ICDS-25

25th International Conference on

Defects in Semiconductors

St Petersburg, Russia, July 20–24, 2009

BOOK OF ABSTRACTS

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Foreword

This book contains 416 abstracts of works included in the programme of the 25th International Conference on Defects in Semiconductors (St Petersburg, Russia, July 20–24, 2009). The abstracts are grouped in three chapters:

Plenary sessions — abstracts of 3 plenary talks.

These sessions include talks which are of general interest for semiconductor physicists. The sessions are held in the Great Hall (**A**) in the morning of Monday, July 20, and Friday, July 24.

Topical sessions — abstracts of 109 invited talks and oral contributions.

The title of a session, which a paper belongs to, is indicated at a page header. The list of topical sessions is given in the first table below.

The topical sessions are held in parallel in two conference halls, **A** and **B**.

Poster sessions — abstracts of 304 poster contributions.

The sessions take place in the afternoon on Monday, July 20, Tuesday, July 21 and Thursday, July 23. The topic, which a contribution belongs to, is indicated at a page header. The list of topics is presented in the table below.

Paper code that appears before each abstract is arranged as follows:

for oral presentation

⟨Day⟩-⟨Hall⟩-⟨Sequential number of a session in the Hall⟩.⟨Sequential number of a presentation at the session⟩⟨Paper type⟩

for poster presentation

⟨Day⟩-⟨Topic number⟩.⟨Paper number in the topic⟩⟨Paper type⟩.

Possible values of *Paper type* are **pl** (plenary), **i** (invited), **o** (oral) and **po** (poster).

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Defects in SiC	Mon-B-2.?i,o	
Defects in oxides I	Tue-A-1.?i,o	Tuesday, July 21
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Defects in nanostructures III	Tue-B-3.?i,o	
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Defects at interfaces	Wed-B-1.?i,o	
Defect engineering	Wed-A-2.?o	
Defects in silicon I	Wed-B-2.?i,o	
Hydrogen in semiconductors I	Thu-A-1.?i,o	Thursday, July 23
Defects in silicon II	Thu-B-1.?i,o	
Hydrogen in semiconductors II	Thu-A-2.?o	
Defects in isotopically controlled silicon	Thu-B-2.?o	
Defects in low dimensional structures	Thu-A-3.?o	
Defects in germanium	Thu-B-3.?i,o	
Defects in organic semiconductors	Thu-A-4.?o	
Transport phenomena in Si, Ge, and Si-Ge alloys	Thu-B-4.?i,o	
Defects in SiGe	Fri-A-2.?i,o	Friday, July 24
Defects in compound semiconductors IV	Fri-B-1.?i	
Magnetic impurities	Fri-B-2.?o	

Poster session topics

Topic	Paper code format	Session date
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2. Defects in compound semiconductors	Mon-2.??po	Monday, July 20
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	Thu-2.??po	Thursday, July 23
3. Magnetic impurities	Thu-3.??po	Thursday, July 23
4. Defects in organic semiconductors	Thu-4.??po	Thursday, July 23
5. Microscopic studies of defects	Thu-5.??po	Thursday, July 23
6. Positrons and muons in defect studies	Thu-6.??po	Thursday, July 23
7. Defects at interfaces	Thu-7.??po	Thursday, July 23
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Transport phenomena in Si, Ge, and Si-Ge alloys

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Magnetic impurities

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Plenary sessions

ICDS-25

Mon-A-1.1pl

Non-equilibrium molecular dynamics for impurities in semiconductors: vibrational lifetimes and thermal conductivities

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Keywords: molecular dynamics, vibrational lifetimes, thermal conductivity

Calculating the vibrational properties of impurities in semiconductors such as Si has kept theorists busy since a couple of decades. The early focus has been on predicting the IR- or Raman-active local vibrational modes. However, the knowledge of the entire dynamical matrix (DM) of a supercell is precious. Not only does it allow the identification of all the localized modes in the system (local, pseudo-local, resonant modes), but the eigenvectors of the DM can be used to 'prepare' a supercell in thermal equilibrium at any (not too high) temperature — a process that normally involves tens of thousands of 'thermalization' time steps. This opens the door to non-equilibrium MD simulations with controlled temperature fluctuations.

One application of this approach deals with the temperature dependence of vibrational lifetimes. Several lifetimes have been measured by transient bleaching IR spectroscopy. The data provide an important test for non-equilibrium MD in 'prepared' supercells. The theoretical approach can be extended to the calculation of thermal conductivities from first principles in periodic supercells using 'temperature-controlled' MD. This allows the study of the impact of specific impurities on thermal conductivities, and a few surprises are emerging.

Mon-A-1.2pl

Semiconductor defect science and technology opening the door to solar energy

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Keywords: photovoltaics, technologies, conversion efficiency, materials

The world needs a fast, fundamental change of its energy production technology, away from CO_2 — emitting power plants based on the burning of our limited fossil fuels towards the dominant use of renewable energy. Among the renewable energies, Solar energy is the only virtually limitless source of energy, and photovoltaic energy conversion is one of the most efficient ways to produce electricity directly from the sunshine.

Photovoltaic (PV) energy conversion is a mature technology of more than 30 years of age, but the most important flaw is still its cost, that makes it too expensive compared to fossil-fuel based energy and even to other kinds of renewable energy. However, the rapid increase in production volume in the last 5 years resulted in the development of production technologies on such a large scale that full price competitiveness comes within reach in the next 10 years.

Our ability to produce PV energy at low cost and on a large scale requires the understanding and control of defects in the semiconductor material. The most widely used material for PV is crystalline silicon that allows conversion efficiencies in the 15–21% range. The development in this field is on the one side towards higher-efficiency cell technologies outside the scope of our conference, but on the other side towards the use of cheaper silicon feedstock material with higher impurity content ('dirty silicon' or 'upgraded metallurgical silicon') that requires thorough understanding and control of lattice defects and impurities in these materials. Solar cells and modules based on thin film technologies such as amorphous or microcrystalline Si and heterostructures with a-SiGe compounds, CuIn(Ga)Se and CdTe today offer the lowest-cost PV energy, but the conversion efficiency is still limited by defects in those structures to values around 10%. Multijunction heterostructures of III/V layers offer theoretical efficiencies exceeding 50%. At our institute we recently achieved a new world record of 41.1% in 450x concentrated light. This success could only be achieved through the careful defect control in relaxed lattice mismatched heterostructures. Finally, organic and dye-sensitized solar cells still promise lowest production costs, but with efficiencies barely exceeding 5% those technologies still require breakthroughs in our understanding of carrier transport in these complex structures before they might become important for large-scale energy production.

In this presentation I will discuss those semiconductor defect science challenges that are the key to further improve the efficiencies and lower the cost of photovoltaic energy production, and whose solution will accelerate the introduction of this desirable technology on a global scale.

Fri-A-1.1pl

First-principles material design and perspective on semiconductor spintronics materials

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Semiconductor spintronics, in which one tries to use the spin degree of freedom of electrons in semiconductor technology, is one of the candidates for next generation electronics. So far dilute magnetic semiconductors (DMS) systems have been investigated intensively as a spintronics material. The purpose of this lecture is to show perspective on spintronics materials by proposing some ideas to answer the most important question in material science for semiconductor spintronics, namely, how we can realize high-T_C DMS.

To understand materials design of high-T_C DMS proposed in this lecture, firstly, I discuss electronic structure of transition metal (TM) impurities in semiconductors [1]. As fundamental mechanisms of magnetic interactions in DMS, double exchange, p-d exchange and super exchange mechanism are introduced, and it is pointed out that relative importance of these mechanisms depends on the occupancy of d-states of TM impurities and calculated chemical trend of the magnetism in III-V and II-VI DMS is discussed [2].

Next, I discuss magnetic properties of DMS at finite temperature. To calculate T_C, I will explain how to map the first-principles total energy results on classical Heisenberg model to estimate magnetic properties [3]. Accuracy in estimating T_C depends strongly on the approximations used. It will be shown that the mean field approximation is not justified particularly in the double exchange systems for low concentrations. Here, I emphasize that the magnetic percolation is the biggest problem that prevents us from realizing high-T_C [4].

Then, I propose two scenarios for realizing high-T_C DMS. The first one uses spinodal decomposition [5]. Thermodynamics consideration based on calculated total energies of DMS tells us that strong inhomogeneity is in general induced in DMS and clusters with high concentration of TM (thus high-T_C), whose structure is coherent to host matrix, are formed. If the cluster size is large enough, due to the super-paramagnetic blocking phenomena the system shows hysteresis even at high temperature. The other way is a co-doping method. When we dope TM impurities in semiconductors, by introducing compensating donor impurity at the same time the solubility of TM impurities increases owing to the reduction of mixing energy. If we use interstitial donors for the co-dopants, we can remove the co-dopants by low-temperature annealing after the crystal growth to recover the ferromagnetism [6]. To realize the above two proposals, I will emphasize that the understanding on the defect properties in DMS is very important.

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Topical sessions

ICDS-25

Mon-A-2.1i

Dealing with defects in indium nitride

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Keywords: indium nitride, surface effects, Hall effect measurements

The electron affinity of indium nitride is nearly 6 eV and is the largest of all III–V semiconductors. This leads to a strong thermodynamic driving force for the formation of native donor defects both in the bulk and at the surface. These, in turn, dominate the semiconducting properties of InN. For example, undoped InN thin films are always n-type and all as-grown InN surfaces, regardless of polarity, crystal orientation, or doping, have an electron-rich surface layer that reflects pinning of the Fermi level about 0.9 eV above the conduction band. Because the surface electron layer interferes with standard electrical characterization methods, it has been difficult to measure accurately the electrical properties of InN films. For example, it is not possible to make a metal Schottky contact and single field Hall effect measurements of Mg-doped films invariably see only the surface layer and cannot assess possible p-type conductivity in the bulk. Recently, new experimental approaches have been developed that mitigate the effects of the surface layer and have led to a more complete understanding of transport and conductivity control in InN. For example, by using a liquid electrolyte as an insulating layer, it is possible to deplete the surface accumulation/inversion layer and measure space charge due to donors/acceptors in the near-surface reason. For Mg-doped InN, this shows clearly the formation of a net concentration of acceptors. While direct electrical characterization of hole transport had been impeded by the electron inversion layer, thermopower measurements find a positive, and in some cases, large Seebeck coefficient showing that holes are the majority charge carrier. Detailed analysis of Hall and thermopower data is used to reveal the dominant electron scattering mechanisms and to establish the effective mass for electrons. Currently grown InN films have dislocation densities in the 10^9-10^{10} cm^{-2} range. Their electrical conductivity and their possible role in creating electric fields inside InN films will be discussed in the light of recent thermopower and electrolyte gated Hall effect measurements.

Mon-A-2.2o

Unintentional conductivity of InN

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Keywords: conductivity, indium nitride, native defects, hydrogen, electron accumulation

InN has enormous potential application in a wide range of electronic and photonic devices. However, every undoped InN sample grown to date exhibits a high unintentional n-type conductivity, which it is important to understand and control if its device potential is to be realised. To date, the origins of this conductivity have proved somewhat controversial [1–3]. Here, we present evidence that the carrier density is rather inhomogeneous throughout the film [1, 4], containing contributions from a background bulk density, a surface electron accumulation, and an increase in carrier density approaching the InN/buffer layer interface due to donors localised at dislocations. This inhomogeneous electron distribution leads to a pronounced film-thickness dependence of the electron concentration and mobility determined by single-field Hall effect measurements. A parallel conduction treatment is used to model both the electron concentration and mobility variation, incorporating dislocation and ionised impurity scattering, and the differing mobilities of bulk and surface electrons.

Microscopic origins of the n-type conductivity are considered. From a combination of experimental and theoretical work, both native defects, such as N-vacancies, and impurities, such as hydrogen, all acting as donors, are attributed as the cause of the residual background conductivity. Such defect centres decorating dislocations are plausible candidates for the increase in electron density approaching the InN/buffer layer interface. In-adlayers are a possible candidate for the donor-type surface states giving rise to the surface electron accumulation, however, this seems to be a "sufficient but not necessary" criterion for electron accumulation to exist. In all cases, an overriding bulk band structure origin is identified as making n-type conductivity very favourable: the large size and electronegativity mismatch of the In and N atoms result in a very low conduction band minimum at the Gamma-point, which therefore lies below the charge neutrality level [5]. Consequently, the formation energy for donor-type defect and impurity centres lies below that of acceptor-type ones for typical Fermi level positions, and unoccupied donor-type states are favourable at the surface.

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Mon-A-2.3o

Electrical and electrothermal transport in InN: roles of point and extended defects

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Keywords: InN, thermopower, transport, dislocation, mobility

The exceptionally large electron affinity of InN (> 5.5 eV) lowers the formation energy of donor-type defects, leading to unique electronic properties such as surface electron accumulation and an extreme propensity for n-type conduction. This, combined with a small energy gap and strongly energy-dependent effective mass, makes an accurate analysis of charge transport and the determination of band structure parameters experimentally and theoretically challenging. In this work we show that a combination of electrothermal (Seebeck coefficient) and traditional electrical transport (Hall effect) measurements can reveal the specific roles of point and extended defects in determining the charge transport properties of n- and p-type InN.

In high quality n-type films, the LO phonon scattering mobility limit is on the order of 10^4 cm^2/Vs. Despite steady improvement in recent years, currently grown films with mobilities on the order of 10^3 cm^2/Vs are still limited by ionized center scattering. Thermopower and Hall mobility measurements are performed over a range of temperatures and analyzed employing Rode's iterative Boltzmann equation method for transport modeling. Comparison of thermopower and Hall mobility data with self-consistent calculations helps to distinguish the role of charged line defects (donor-type charged dislocations) as scattering centers from the role of charged point defects.

In p-type films, detection of hole conduction by traditional techniques such as single-field Hall effect measurement is prevented by the surface electron accumulation (inversion) layer. Positive Seebeck coefficients are observed for some Mg-doped InN samples, demonstrating the presence of mobile holes and providing direct, quantitative evidence of hole transport in InN. An optimum Mg doping concentration for p-type conductivity is observed; the lower limit depends on the background electron concentration donated by impurities, native point defects, and possibly dislocations, which must be overcome with Mg acceptors, while the upper limit is determined by the formation of compensating defects at high Mg concentrations.

Mon-B-1.1o

3d transition metal impurities in diamond: electronic properties and chemical trends

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Keywords: transition metal impurities, synthetic diamond, magnetic impurities

Diamond is a material which stands alone in nature, carrying a unique combination of electronic, mechanical, thermal, and optical properties. High pressure-high temperature (HPHT) methods have been widely used to grow macroscopic diamond out of graphite, in which 3d transition metal alloys are used as solvent-catalysts. These transition metals can end up being incorporated as impurity complexes in the resulting material, forming electrically and optically active centers. Nickel has been unambiguously identified in HPHT diamond [1], while more recently cobalt-related centers have also been identified [2]. Other 3d transition metals, such as titanium, chromium, and iron, have also being identified in diamond by several experimental methods [3]. The major challenge has been to build consistent microscopic models that could explain that zoo of transition metal-related active centers in diamond [4, 5].

We present a theoretical investigation, based on the spin-polarized full-potential linearized augmented plane wave method [6], on the atomic structures, energetics, hyperfine parameters, and chemical trends of transition metal impurities (from Ti to Co) in diamond. We focused on the configurations formed by isolated (substitutional and interstitial) impurities and complexes (transition metal plus vacancies). Our results are discussed in the context of available experimental data [3].

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Mon-B-1.2o

Oxygen distribution and speciation in bulk of monocrystalline diamonds and its correlations with other impurities

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Keywords: diamond, oxygen, point defects, extended defects

Oxygen in diamond lattice remains elusive impurity. Mass-spectrometry and nuclear probes show presence of oxygen in all diamonds in concentrations ranging from < 100 to 1000 at.ppm. Some oxygen is present as adsorbed species on diamond surfaces, whereas a second fraction is resent in sub-microscopic inclusions. Detailed studies [1] have shown that in virtually every diamond there exists "inclusion-independent" oxygen which is believed to be present as a structural impurity. Recent studies of natural diamonds showing strong absorption by CO_2 in IR spectra [2] suggest that these monocrystalline diamonds contain oxygen as a lattice impurity. Calculations [3, 4] show that O-related defects may exist in diamond lattice. However, up until now evidence for incorporation of O during diamond growth is scarce and little is known about related defects.

The aim of the current study is to show conclusively whether or not O can exist as a structural impurity in diamond. Several types of monocrystalline diamonds with and without CO_2 IR absorption were analysed by techniques sensitive to chemical composition (SIMS) and to structure (Small-Angle X-ray Scattering (SAXS) and X-ray topography).

For the SIMS investigation high ion current of 100 nA Cs^+ ions in conjunction with an 8 μm field-of-view were employed. Due to prolonged storage of the sample mount in high vacuum conditions the O background signal was very low. Both spot analyses and mapping of O lateral and depth distributions were performed. In some CO_2-rich diamonds oxygen is distributed heterogeneously at the micron-scale, suggesting its presence in submicron inclusions, which, in turn, are irregularly distributed throughout the sample. Such inclusions could correspond to heterogeneities with sizes of 100–200 nm revealed by SAXS. However, in some of these diamonds O is distributed homogeneously, suggesting that it might be present as a lattice impurity. The last statement could be disputed, but the most important proof of structural position of oxygen impurity comes from simultaneous measurements of N and O concentrations. Plots of N vs O concentrations show clear correlations, obeyed as for several analyses spots on individual diamonds as well as for sets of diamonds. Notably, the slopes of the N–O correlations differ between diamonds showing CO_2 absorption in IR and for "normal" diamonds. As expected, O contents are higher in the former group, suggesting that in CO_2-rich diamonds oxygen is present both the lattice and in microscopic inclusions. This study is the first work showing correlation of structural nitrogen impurity with oxygen content of diamonds, thus providing strong analytical support for earlier hypothesis [3] that O may be present as a lattice impurity in natural diamonds.

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Mon-B-1.3o

Theoretical study of surface step defects on monohydrogenated (100) diamond surfaces

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Keywords: hydrogenated diamond surfaces, TBMD, hydrogen migration

Mono-hydrogenated diamond surfaces are very stable, reconstruct as C(100)(2x1):H with well-defined dimer rows, usually achieved by plasma etching, and present remarkable electronic properties such as p-type conductivity [1]. Subsurface hydrogen impurities [2] have been for a long time proposed as the origin for such behavior, even if recently also the role of oxygen has been discussed [3]. On the other hand, it has also been proposed [4] that the head of the dimer row (on a step boundary) is the starting point for etching by H-plasma.

We here present a study of the local changes on C(100)(2x1):H surface morphology, focusing on different step regions, by means of finite temperature simulations using a Tight Binding Molecular Dynamics (TBMD) scheme [5].

We find that the presence of dangling bonds, characteristic of carbon atoms at the head of an interrupted dimer row, introduces localized electronic states inside the gap and directly affects the local surface stability, leading to dynamical local disorder effects, and to hydrogen subsurface insertion.

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Mon-B-1.4po

Boron-Hydrogen complexes in diamond: energy levels and metastable states

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Keywords: diamond, n-type doping, hydrogen, defects, boron-hydrogen complexes

Diamond is a unique wide band gap semiconductor suitable for high temperature, high frequency and high power applications.

Boron doped diamond is a well known p-type semiconductor, while deuteration of B doped diamond results in the passivation of boron acceptors. Further introduction of an excess of deuterium results in the reversible formation of shallow n-type conductivity in such B doped layers. However the nature of this shallow donor has been the subject of continued debate.

In particular, most *ab initio* models predict B-H_2 to possess deep levels in the diamond band gap, inconsistent with the shallow n-type conductivity observed in B doped diamond samples with an excess of deuterium.

We therefore carefully calculate donor and acceptor levels of Boron-Hydrogen related complexes, taking into consideration possible metastable states, using accurate *ab initio* plane wave Density Functional Theory (DFT) methods.

Mon-A-3.1i

Microscopic observation of vacancy, self-interstitial and the formation of Frenkel pairs by Mössbauer spectroscopy

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Keywords: III–V semiconductors, vacancies, interstitials, Frenkel pairs, Mössbauer spectroscopy

Mössbauer spectroscopy (MS) can provide information on defects in semiconductors at the atomic scale. We use MS to create and study single Frenkel pairs in the III–V semiconductor InSb by making the Mössbauer probe ^{119}Sb the primary knock-on atom (PKA) receiving 12 eV recoil energy by a preceding neutrino emission in the decay of ^{119}Te. This simplest possible defect creation enables the identification of vacancy and self-interstitial and the mechanism of the defect formation itself.

We have chosen InSb due to its low defect production threshold of about 8 eV [1] and the compatibility with the atomic species of the Mössbauer probe: we use the radioactive ^{119}Sb decaying to ^{119}Sn and add to this standard scheme the precursor ^{119}Te decaying to ^{119}Sb: ^{119}Te>^{119}Sb>^{119}Sn. ^{119}Te induces a recoil of 12 eV to the ^{119}Sb by a high energy neutrino emission. Thus ^{119}Sb becomes the PKA and can end up as an interstitial or associated with one vacancy (and nothing else). All configurations are probed by the Mössbauer active ^{119}Sn which lives only for 10^{-8} s and thus reveals the structure of the ^{119}Sb-related defects.

In former experiments [2] the feasibility of this recoil technique was shown. The present ones were performed with much higher statistical accuracy to identify the defects, study the details of the defect formation and the charge dependence of the processes.

The resulting Mössbauer spectra (n-type: undoped and Te-doped) measured at 10K show a main line with isomer shift IS=1.95 mm/s corresponding to substitutional ^{119}Sb/Sn on Sb sites known from earlier experiments [3] and from theory [4]. In addition, two well resolved spectral components show that Frenkel pairs were created: (1) a singlet with very large isomer shift, IS=3.7 mm/s, and (2) a quadrupole split line with IS=2.28 mm/s and splitting $\Delta = 1.18$ mm/s. A small third component (3) has IS similar to (2), 2.1 mm/s, and a large splitting Δ of 2.2 mm/s. Line (1) and (3) anneal in the range 90 to 120K whereas line (2) anneals at 390(10)K.

From the very large IS (high electron density) of defect line (1) the probe atom ^{119}Sb/Sn can be very clearly and uniquely assigned to an interstitial site as already suggested in (2). The large IS reflects the loss of bonding of the ^{119}Sb/Sn atom. The annealing around 100K agrees with [1], likely by close pair recombination. Configuration (2) and (3) with large splittings and IS close to that of the substitutional site are probe-vacancy configurations, the probe either on a normal lattice site or antisite.

The p-doped sample (Cd) does not show defect creation at all displaying strong Fermi level dependence of the Frenkel pair production directly at the threshold. With normalization of the spectra it can be inferred that 55(5)% of the ^{119}Sb recoils produce Frenkel pairs (n-type).

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Mon-A-3.2o

Formation of In vacancies in Si-doped InN

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Keywords: InN, vacancies, positron, mobility, Si doping

Recently, strong efforts are undertaken to increase the understanding of the physics behind InN, a material of highest interest and industrial relevance, which still remains to be the least investigated of the III-nitride family. Its remarkable properties, such as the very high electron mobility and saturation velocity, as well as the narrow band gap of 0.7 eV [1] make it a very attractive material for optical communication applications as well as a promising candidate for the realization of high-speed electronic devices and high-efficiency solar cells. Despite a remarkable progress in crystal growth over the past years, as-grown InN remains to exhibit considerably high defect concentrations, as well as a strong n-type tendency [2]. Recent theoretical calculations predict that In vacancies are the most relevant native defects in n-type InN [3] and are also expected to form complexes with other defects [4]. In this contribution we present results obtained from studies of MBE-grown Si-doped InN with electron concentrations from 1×10^{18} cm^{-3} to 6.6×10^{20} cm^{-3}, using Positron Annihilation Spectroscopy. Temperature dependent Doppler Broadening measurements showed In vacancies in concentrations from 2×10^{16} cm^{-3} to 7×10^{17} cm^{-3} with increasing electron concentration. These values are remarkably higher than what can be estimated based on the theoretically predicted formation energies of In vacancies in InN and the experimentally determined Fermi levels in the investigated samples [5]. Additionally, a strong inhomogeneity of the defect distribution with an increasing vacancy concentration towards the layer/substrate-interface can be observed. This suggests a locally reduced formation energy of In vacancies in the vicinity of extended defects, which are especially abundant in the interface area, possibly through the formation of defect complexes. In spite of their still relatively low concentration the observed threshold for the In vacancy formation suggests, together with earlier results in He-irradiated InN [6], that In vacancies play an important role in reducing the electron mobility.

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Mon-A-3.3o

Stable In-defect complexes in GaN and AlN

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Keywords: GaN, AlN, PAC, nitrides, radiative centres

Perturbed angular correlation measurements in Indium implanted GaN and AlN have shown that after annealing up to 50% of the In probes occupy relatively undisturbed substitutional group III sites at 293 K while the remaining fraction traps a nearest neighbor point defect. Above 293 K this fraction decreases strongly until, at 1100 K, all In probes are found in undisturbed substitutional sites. The effect is completely reversible. A model involving an Indium-nitrogen vacancy complex is suggested to explain this behavior. Possibly this complex can act as radiative recombination centre or as seed for phase segregation during growth.

Mon-A-3.4o

Irradiation-induced In and N vacancies: dominant donors in InN?

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Keywords: InN, vacancy defects, irradiation, RTA

Indium nitride, with its small band gap of $\sim$ 0.7 eV, is a promising material for long-wavelength optoelectronic devices, extending the wavelength of III–N materials into the infrared region. Also, its high electron-mobility and peak-drift velocity, and radiation hardness make it a desirable material for high-speed electronic applications and multi-junction solar cells. Recently, high-energy particle irradiation of InN films followed by thermal annealing has been shown to create InN films with high electron concentrations and mobilities [1]. We apply positron annihilation Doppler

broadening spectroscopy to investigate the role of point defects in the electronic transport properties of InN irradiated with 2-MeV ^{4}He$^+$-ions to fluences in the range 5×10^{14}–2×10^{16} cm^{-2}, and subsequently subjected to rapid thermal annealing (RTA) below 500°C.

Our results show that negative In vacancies are introduced in the He irradiation at a low rate of 100 cm^{-1}, with their concentration saturating in the mid-10^{17} cm^{-3} at an irradiation fluence of 2×10^{15} cm^{-2} [2]. This is completely opposite to the behaviour observed in GaN, where the Ga vacancies act as important compensating centers in similarly irradiated material, introduced at a rate of 3600 cm^{-1} and showing no saturation. The RTA treatment is found to result in efficient clustering of the In vacancies introduced in the irradiation, indicating that a high concentration of both In and N vacancies need to present prior to the thermal annealing, as the thermal formation of vacancy defects is not efficient at the applied temperatures [3]. It should be noted that typically vacancy concentrations above 10^{20} cm^{-3} are required for migration-catalyzed vacancy clustering to be observed. The vacancy clustering seen in the positron data is in good agreement with results on void formation obtained by transmission electron microscopy (TEM).

The estimated concentration of the N vacancies is in excellent agreement with the donor concentration introduced by the irradiation. Hence our results support the identification of these donors as N vacancies. Further, the above results indicate that the majority of the irradiation-induced In vacancies is invisible to positrons, supporting the suggestion [1, 2] that the isolated $\mathrm{V_{In}}$ could undergo an acceptor-to-donor transition: $\mathrm{V_{In}} \leftrightarrow (V_{\mathrm{N}} + N_{\mathrm{In}})$. Results of growth and doping studies show that the In vacancy formation is strongly affected by the structural quality of the InN lattice [3, 4]. Therefore it seems plausible that the acceptor-like In vacancies that are observed right after irradiation have been created in the vicinity of extended defects inhibiting the acceptor-to-donor transition.

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Mon-A-3.5o

Electrical properties and deep traps spectra in AlGaN films with nitrogen and gallium polarities prepared by molecular beam epitaxy

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Keywords: AlGaN films

Polarity of wurtzite (0001) AlGaN films and AlGaN/GaN heterojunctions plays a big role in controlling their physical properties. In standard growth conditions the films usually grow with Ga polarity, but it is desirable to also be able to grow films with N polarity. So far experiments were mostly carried out for MOCVD structures where it was found that nitridation of sapphire substrates promotes N-polar growth while growth on miscut substrates facilitates good surface morphology of N-polar films which is very hard to achieve for on-axis sapphire. In this work we show that, in molecular beam epitaxy, AlGaN films with composition ranging from 0% to 60% can be grown with good morphology for on-axis (0001) sapphire substrates with novel AlN/AlGaN superlattice buffer. The films show nitrogen polarity when the AlN nucleation layer is prepared in the N-rich conditions and gallium polarity for Ga-rich nucleation conditions. Electrical properties, deep traps spectra, luminescence spectra were studied for such undoped N-polar and Ga-polar films. Current-voltage I-V measurements and capacitance-voltage C-V measurements on Au Schottky diodes show that the layers are n-type for N-face growth and p-type for Ga-face deposition for all studied layers, whatever the Al composition. The residual donors in n-type AlGaN films show the ionization energy dependence on Al mole fraction that is similar to that of Si donors, as evidenced by Hall measurements, current versus temperature I-T measurements and admittance spectroscopy measurements. The donors become deep, close to 0.2 eV, for the Al composition of 60%. The residual acceptors in Ga-polar AlGaN films show the composition dependence of ionization energy similar to that reported for typical acceptors, Mg and C. Technological considerations suggest that the acceptors in question should be due to carbon. It is argued that N-polar growth promotes incorporation of shallow donors, but, in contrast to previous reports for MOCVD grown N-polar GaN, these donors are related to Si rather than to oxygen. For Ga-polar films the donor contamination is strongly reduced and the Fermi level is pinned by the residual acceptors, most likely carbon. The concentration of these residual acceptors is actually low and, because acceptors in AlGaN are relatively deep, the films are highly resistive. Deep traps spectra studies on N-polar films show the predominance of electron traps with activation energies 0.25 eV, 0.6 eV, 0.9 eV and hole traps with activation energy 0.2–0.3 eV in GaN. The traps become deeper in

AlGaN N-polar films. For Ga-polar layers the dominant deep traps are the ones that pin the Fermi level. Possible identities of the observed deep centers will be briefly discussed.

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Mon-A-3.6o

Vacancy defects in Fe doped GaN studied with positron annihilation spectroscopy

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Keywords: vacancy defects, GaN, semi-insulating, positron annihilation

GaN is a promising material for the use in high power, high frequency semiconductor devices due to its wide band gap, good thermal stability and high breakdown voltage. Semi-insulating (SI) GaN is the most desirable material for the use as insulating layer between active areas and as a substrate. One way to achieve SI GaN is to dope it with iron to compensate the residual Si and O donors and to pin the Fermi level to mid gap.

Positron annihilation is an effective method for studying neutral and negative vacancy defects in semiconductors. Positrons can get trapped to negative and neutral vacancies, which results in observable changes in the positron lifetime and momentum distribution of the annihilating positron-electron pair. The resulting annihilation data can be used to determine the Ga vacancy concentration in GaN. Additional information about the defect concentration can be obtained by studying the diffusion length of positrons that decreases due to the trapping at vacancies and additionally negative ions.

We have studied 7 MOCVD grown GaN:Fe thin film layers using positron annihilation spectroscopy. The Fe doping concentration varied from 5.7×10^{14} cm^{-3} to 8.7×10^{18} cm^{-3}. The Ga vacancy concentrations estimated from annihilation parameters decrease, although only slightly, varying from 9.0×10^{17} cm^{-3} to 6.0×10^{17} cm^{-3} with increasing Fe content. This behaviour can be expected from the formation energy of Ga vacancies that increases when the Fermi level moves down to mid gap. The positron diffusion length shows a much stronger trend, i.e., it increases by a factor of 3 with increasing Fe concentration, indicating that the concentration of defects capable of trapping positrons decreases by more than an order of magnitude. This suggests that also negative ions trap positrons also at room temperature at least in the low Fe-doped samples. Further experiments, such as measuring the positron parameters as a function of temperature, are required in order to better understand the interplay of charged defects in Fe-doped GaN.

Tue-A-3.1i

Hydrogen in ZnO

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Keywords: ZnO, hydrogen, donor, molecule

Hydrogen is a common impurity in ZnO that strongly influences its electrical and optical properties. First principles investigations suggest that hydrogen acts as a shallow donor in ZnO and might be responsible for the natural n-type conductivity of this material [1].

A combined study of Raman scattering, IR absorption, photoluminescence, and photoconductivity on ZnO is reported. Two shallow donors-hydrogen at the bond-centered lattice site, H_{BC}, and hydrogen bound in an oxygen vacancy, H_O,-were identified. Donor H_{BC} has an ionization energy of 53 meV. The recombination of an exciton bound to H_{BC} gives rise to the 3360.1 ± 0.2 meV photoluminescence line. A 1s-to-2p donor transition at 330 cm^{-1} is detected in the Raman scattering and photoconductivity spectra. The stretch mode of the associated O-H bond is detected in IR absorption at 3611 cm^{-1} with an effective charge of 0.28 ± 0.03 e. The concentration of H_{BC} was determined from the frequency shift of the E_1(LO) phonon-plasmon mode at 591 cm^{-1}. The H_O donor in ZnO [2] has an ionization energy of 47 meV. The excitonic recombination at H_O leads to the previously labeled I_4 line at 3362.8 meV [3]. Photoconductivity spectra reveal the 1s-to-2p donor transition at 265 cm^{-1}.

It is shown that H_{BC} migrating through the ZnO lattice forms electrically inactive interstitial H_2. Vibrational modes of H_2, HD, and D_2 were identified at 4145, 3628, and 2985 cm^{-1}, respectively. These results suggest that interstitial H_2 is responsible for the hidden hydrogen in ZnO [4].

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Tue-A-3.2o

Defects in In_2O_3

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Keywords: In_2O_3, bandgap, surface, Muonium, charge neutrality level

In_2O_3, doped with tin, is the ubiquitous so-called transparent conducting oxide (TCO) material. However, there has been recent interest in considering In_2O_3 as a semiconductor in its own right. Despite this, even its basic optoelectronic properties have proved controversial, and little is known about the behaviour of defects in this material. We have shown that its band gap has negligible indirect nature [1, 2], in contrast to previous reports, but rather optical transitions between the valence band maximum and conduction band minimum (CBM) are dipole forbidden. Considering this, its fundamental band gap value can be determined as ~ 2.9 eV [2], almost 1 eV lower than commonly reported. In light of this, we have reinvestigated the surface electronic properties of this material. While it has previously been reported to exhibit electron depletion, we have shown that In_2O_3 can sustain a large build up of electron charge at its surface [3]. This surface electron accumulation layer is present in high-quality material independent of growth method, surface orientation, or even bulk polymorph [2]. By extrinsic n-type doping with Sn, the electron accumulation is quenched, allowing the so-called charge neutrality level (CNL) to be experimentally located ~ 0.6 eV above the CBM [2, 3], in contrast to the majority of materials where it lies within the band gap.

This has important implications for the electrical behaviour of defects in In_2O_3: native defects will tend to be donors, giving one explanation for its high unintentional conductivity. Furthermore, the formation energy for compensating acceptors to form when n-type doping In_2O_3 will remain comparatively high until the Fermi level moves above the CNL, explaining the very high carrier concentrations attainable by extrinsic doping, for example with Sn, and hence its use as a TCO. Finally, the CNL can be equated with the donor/acceptor transition energy for Hydrogen [4], suggesting H should form a shallow donor here. To test this prediction, we have performed muon spin rotation spectroscopy, and have found that Muonium does indeed form a shallow donor state in In_2O_3 [5]. Therefore, by analogy, H may also be a cause of unintentional conductivity in In_2O_3, and indeed, similar oxide semiconductors.

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Tue-A-3.3o

Formation of Indium-acceptor complexes in ZnO

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Keywords: ZnO, p-type ZnO, cluster-doping, co-doping

One of the main obstacles to the optoelectronic application of ZnO represents the difficulty to achieve reliable and sufficient p-type doping. Possible explanations are the tendency of the acceptors of pairing with native defects or other impurities present in the material and, thereby, forming electrically inactive complexes. Concepts to overcome this problem and to enhance the solubility of acceptors are the so-called cluster-doping [1] or co-doping [2], both being proposed on theoretical grounds. In this concept, the formation of donor-acceptor complexes enhances the solubility of the acceptor atoms. Experimentally, this idea has been confirmed for the case of In–N co-doping of ZnO films: Here, an increase of hole concentration by a factor of 1000 compared to exclusive N doping has been observed using Hall effect measurements, which was accompanied by an enhancement of the incorporation of N as observed by SIMS [3].

On an atomic scale, a pairing of defects would give rise to unique electrical field gradients (EFG) which would be detectable at the site of a defect involved in the pairing process. In this way, the behavior of the donor In in ZnO was investigated using the perturbed $\gamma\gamma$ angular correlation technique (PAC) with the radioactive probe atom ^{111}In/^{111}Cd [4]. After having applied different procedures for In–N and In–P co-doping (diffusion and/or implantation), indeed, in both cases the formation of In-acceptor complexes has been observed.

Each complex is characterized by two slightly different EFG as it is expected for the wurtzite structure of ZnO having different nearest neighbor distances along the c axis and in the basal plane, respectively. The magnitude of the EFG is similar to that of the EFG known for Indium-acceptor complexes in the II-VI semiconductors CdTe, ZnTe, and ZnSe [5]. The efficiency of the different co-doping procedures and their dependency on the diffusion and/or annealing conditions will be discussed.

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Tue-A-3.4o

Dynamical nuclear polarization by means of shallow donors in ZnO quantum dots

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Keywords: EPR, ENDOR, quantum dot, nuclear polarization

Dynamic nuclear polarization (DNP) effects have been observed in ZnO quantum dots (QD's) with using high-frequency (95 GHz) pulse electron paramagnetic resonance (EPR) and electron nuclear double resonance (ENDOR) at the temperatures of 1.3–2 K. Free standing ZnO nanocrystals with diameters of 2.2, 2.8, 3.4, 4.0 and 4.2 nm were prepared via a wet chemical method and the QD's consist of a ZnO/Zn(OH)$_2$ core-shell structure. The polarization of the nuclear spins is achieved by saturating the EPR transition of the shallow donor present in the ZnO nanoparticles and this polarization manifests itself via the creation of a hole and an antihole in the EPR absorption line of the shallow donor. The polarized nuclear spins create an internal magnetic field and as a result the resonance line of the electron spins, subjected to the microwave irradiation, shifts to a lower external field value resulting a shift of the hole (antihole) in the inhomogeneously broadened EPR line.

DNP effect, is shown, to arise not only from an almost complete polarization of the ^{67}Zn nuclear spins in the ZnO QD's but also of the ^{1}H nuclear spins in the Zn(OH)$_2$ capping layer. To check whether a polarization of the ^{1}H nuclear spins affects the resonance line of the electron spin ENDOR experiments on the protons have been carried out. The strong ENDOR signals around the Zeeman frequency of the ^{1}H nuclear spins indicated that the wave function of the shallow donor (shallow donor Bohr radius of $\sim$ 1.5 nm) extends into the capping layer. The observation of the resonance frequency of the ^{1}H nuclear spins shifts caused by DNP was explained by the polarization of the ^{1}H nuclear spins, which produce an internal field and thus shift their resonance frequency.

The shift of holes (antiholes) in magnetic field due to DNP increases considerably when performing the experiments on QD's with smaller diameters. The arguments to explain the increase of this shift by DNP of the ^{67}Zn nuclear spins and of the ^{1}H nuclear spins in the $Zn(OH)_2$ capping layer, in combination with the effect of confinement of the electronic wave function of the shallow donor are presented.

The DNP is produced by a spontaneous-emission type, one phonon, cross-relaxation that is mediated by the zero-point fluctuations of the phonon system in the ensemble of QD's. To explain the relatively fast spin-lattice relaxation of the shallow donor in the ZnO QD's we propose that in the dry powder, used in the experiments, the QD's are in physical contact with each other and that the phonons are not confined to one particle.

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Tue-A-3.5o

Atomic scale correlation between stacking fault density and AlGaN blocking layer in m-plane GaN by transmission electron microscopy

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Keywords: TEM, m-GaN, stacking faults, blocking layer

GaN-based nitride semiconductors have attracted considerable attention in high-brightness light-emitting-diodes (LEDs) and laser diodes (LDs) covering from green to ultraviolet spectral range. LED and LD heterostructures are usually grown on (0001)-Al_2O_3. The large lattice mismatch between Al_2O_3 substrates and the GaN layers leads to a high density of defects (dislocation and stacking faults). Moreover, Ga and N atoms are arranged along the polar [0001] crystallographic direction, which leads to spontaneous polarization. In addition, in the InGaN/GaN MQWs heterostructures, stress applied along the same axis can also give rise to piezoelectric polarization. The total polarization, which is the sum of spontaneous and piezoelectric polarizations, is aligned along the [0001] direction of the wurtzite heterostructures. The change in the total polarization across the heterolayers results in high interface charge densities and spatial separation of the electron and hole wave functions, redshifting the photoluminescence peak and decreasing the peak intensity [1]. The effect of polarization charges in the GaN-based heterostructures can be eliminated by growing along the non-polar [ ] (a-axis) or [ ] (m-axis) orientation instead of the commonly used polar [0001] (c-axis).

For non-polar GaN growth on non-polar substrates, the GaN films have high density of planar defects (basal stacking fault; BSFs, prismatic stacking fault; PSFs), because the SFs are formed on the basal plane (c-plane) due to their low formation energy. A significant reduction in defect density was recently achieved by applying blocking layer such as SiN, AlN, and AlGaN in non-polar GaN [2].

In this work, we investigated the process for reducing the number of defects (SFs and dislocations) by inserting AlGaN blocking layer during the m-GaN growth. In cross-sectional configurations the m-GaN inserting the AlGaN blocking layer has been investigated by transmission electron microscopy. Based on the microstructural observation, the defects in m-GaN film are expected to disappear owing to AlGaN blocking layer, which prevents the propagation of SFs and dislocations into the surface due to the matching of the lattice spacing between the AlGaN blocking layer and GaN.

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Wed-A-1.1i

Mg acceptors in GaN

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Keywords: Mg-doping, GaN, photoluminescence, annealing, instability

In the recent development of III-nitride based light emitting devices efficient p-doping is a bottleneck for obtaining high radiative output. Mg is so far the only acceptor useful for p-doping in GaN. While the electrical properties of Mg-doped p-GaN can be reasonably understood using a model with a single acceptor level, the optical signatures for Mg acceptors are far from understood. Early studies of photoluminescence (PL) of p-GaN showed that the characteristic donor–acceptor pair (DAP) or free-to bound (FB) emission peaking at 3.27 eV was unstable with annealing above 500°C, while the Mg acceptor responsible for the electrical hole activation was known to be activated and stable in this temperature range, by release of H from Mg–H complexes. Several studies of the 3.27 eV PL concluded that the instability was caused by instable shallow donors, believed to be related to H or to N vacancies. In this work we present strong evidence that the instability instead is connected with the acceptor involved in the 3.27 eV PL, while the shallow donors involved at low temperatures are stable. So it is found that Mg introduces two acceptors in GaN, one of them is unstable in p-GaN.

This work includes studies of donor and acceptor bound excitons (DBEs and ABEs) in Mg-doped GaN. To avoid strain induced broadening and energy shifts of BE transitions we have employed about 1 μm-thick Mg-doped layers grown by MOCVD on strain free thick (200–300 μm) bulk GaN templates. Samples were grown both at Meijo University and Bremen University. The ABE spectra show a dramatic sensitivity to the annealing in p-GaN. The ABE1 peak at 3.466 eV is observed for the unannealed condition, and the ABE2 peak at about 3.454 eV is dominant in the annealed condition, both are severely broadened at high Mg concentrations ($> 10^{19}$ cm^{-3}). Thus the acceptor A1 is unstable against annealing, and A2 shows properties expected for the regular stable Mg acceptor. The stability of the optical spectra can also be observed via studies of PL versus UV laser excitation time. A transformation of the BE spectra is observed for virgin samples: ABE1 decreases continuously with excitation time. Thus A1 is unstable against electron injection, typical for H-related complexes. If the sample is warmed up to 300 K and re-measured again at 2 K, the original spectrum is restored. For the same sample measured after annealing ABE2 is dominant, but is stable against UV excitation. Similar observations are made for the lower energy DAP spectra. This low temperature metastability of the A1 acceptor is explained as a motion of an H atom into a metastable excited state of the Mg–H complex, from where it can be thermally restored at elevated temperatures.

The above PL data allow the following conclusions. (i) The dominant shallow donors in Mg-doped p-GaN are stable O and Si donors. (ii) There is clear evidence for two separate acceptors in Mg-doped GaN, A1 and A2. (iii) A2 has the annealing properties expected for the substitutional Mg acceptor, while A1 is unstable versus annealing as well as vs UV (or electron) excitation in p-GaN. (iv) The instability occurring only in p-GaN is strong evidence that H is involved in the transformation processes, since H^+ is highly mobile in p-GaN. (v) The two acceptors have very similar binding energies for the hole. (vi) The strong phonon coupling for the A2 3.15 eV DAP spectrum is similar to other substitutional deeper acceptors on Ga site.

Wed-A-1.2o

Structural distortions in nitrogen doped GaP and GaAs

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Keywords: A_3B_5, nitrogen, distortions, energies

A_3B_5 semiconductors, where the group V element is partially replaced by nitrogen, have been a subject of extensive investigation in recent years due to their unusual properties. In this work we try to take into account microstructure of the crystal around the impurity atom and evaluate the contribution of structural distortions in properties of the materials.

At the first the atomic relaxation in $3a \times 3a \times 3a$ (a — zinc blend lattice constant) cluster is derived by valence force field approximation. Then semi empirical tight-binding approach is used taking into account the second nearest-neighbors interaction and atomic potential change with electronic density change nearby the atoms. The condition of electroneutrality of cluster makes it possible to derive the selfconsistent solution.

Several configurations of nitrogen atoms are investigated: isolated nitrogen atoms, Ga+$N_kP(As)_{4-k}$ ($k = 1 \ldots 4$) tetrahedrons, nitrogen atoms pairs NN_i (where i indicates the separation between nitrogen atoms in atomic shells, $i = 1, 2, 3$). The cluster energy levels strongly depend on the number of N-Ga bonds. Cluster states are unchanged in energy for GaP and for GaAs, due to the band offset in GaAs some of the states fall into the conduction band and in GaP they are in band gap near the conduction band minima. Cluster states are strongly localized near the nitrogen atoms and almost do not depend on nitrogen concentration.

Nitrogen atoms cause strong crystal lattice deformations and significant shift of energy levels. Ability to remove the strain by change of atomic positions determines the final position of cluster states. Isolated nitrogen atoms cause graphitic distortions. Surrounding Ga atoms freely relax in all directions within 5–6 atomic shells. In the case of NN_1-pair forces acting on the Ga atom lie in one plane and cause small vertical displacement of Ga atom. In the case of NN_2 pair a twist distortion takes place. It aspirates to place all chemical bonds of the tetrahedron into one plane. Strain in NN_3 pair is partially compensated by inclination of one valence angle relative another. In the case of NN_4 pair the shear distortions lead to displacement of As atom in [001] direction and to dehybridization of sp^3 orbitals.

Deformations of Ga-centered tetrahedrons containing N strongly depend on behavior of central Ga atom. The Ga+NP_3 case corresponds to isolated nitrogen atom, while Ga+N_2P_2 case corresponds to NN_1 pair. In Ga+N_3P the central Ga atom moves toward three nitrogen atoms, increasing the length of Ga-As bond. In Ga+N_4 case the central Ga atom have no possibilities to relax, the configuration is highly strained and has the lowest energy.

Our calculations demonstrate that deformation energy of NN_1 pair is the highest, than comes NN_4, NN_3 and NN_2 pairs. Consequently NN_1 energy level is the lowest and NN_2 level is the highest one. This mutual disposition differs from generally accepted.

Wed-A-1.3i

Simulation of defects and defect microstructure evolution in GaN-based alloys

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Keywords: defects, electronic structure, migration, GaN

GaN-based materials are promising wide band-gap semiconductor for micro- and optoelectronic applications. Many of their properties and unusual features are ascribed to specific defect microstructure of these materials. To be able to predict the physical properties of GaN-based samples after non-equilibrium processing (annealing, mechanical loading, etc.) one needs to realize both the energetics of various defect types and the features of defect kinetic behavior (migration and clustering). Here we discuss the results of electronic structure calculations of various defects in GaN and its triple alloys with In and Al, as well as multiscale modelling of microstructure evolution during high-temperature annealing of GaN and GaInN. In particular, nitrogen vacancies, shown recently to be the dominant defect type in GaN, will be considered in detail. We show a sufficiently high mobility of nitrogen vacancies in n-type GaN at annealing temperature that together with noticeable binding energies between nitrogen vacancies and other point defects (Ga vacancies and impurities) creates favourable conditions for vacancy clustering.

Fri-B-1.1i

EPR identification of intrinsic and transition metal-related defects in $ZnGeP_2$ and other II–IV–V_2 compounds

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Keywords: compound semiconductors, native defects, transition metals, magnetic resonance

The $A^{II}B^{IV}C_2^{V}$ compounds (A=Zn, Cd, B=Ge, Si, C=P, As) are ternary compounds that crystallize in the tetragonal chalcopyrite structure and were studied in the last two decades mainly for their potential as nonlinear optical (NLO) material for frequency-conversion applications in the mid-infrared region [1, 2]. Point defects play an important role in the efficiency of these materials for these applications.

The importance of the ternary pnictides became even more eminent with the discovery of room-temperature ferromagnetism in highly Mn-doped semiconducting $CdGeP_2$ [3], $ZnGeP_2$ [4] and other pnictides, because semiconductors that exhibit room-temperature ferromagnetism (RT FM) are central to the development of semiconductor spintronics. The existence of RT FM is also predicted for other transition metals. At variance with other semiconductors the pnictides open in addition the possibility to combine the observed RT FM with their excellent nonlinear optical properties, resulting in a new class of material for nonlinear optics and spintronics applications. However, like for other diluted magnetic semiconductors, the origin of the RT FM is still not settled and different models are discussed. A unique explanation of the microscopic origin of the detected FM in the various compounds doped with different TMs can only be accomplished by an efficient combination of various experimental techniques and current state-of-the art theoretical methods. To decide between the different theoretical predictions in particular detailed knowledge concerning the incorporation of TM in the different charge states at the different lattice sites and the TM-induced local change of the free parameter x_f of the chalcopyrite structure are necessary. Such data can be obtained in a unique way by magnetic resonance methods, especially by electron paramagnetic resonance (EPR) and by photo-EPR measurements. These methods particularly address the site selection of the doping atoms and their interactions which each other, with other defects both intrinsic and induced by strong TM-doping and with free carriers. Photo-EPR delivers data energy level positions of the various charge states of the different native defects and TMs. For the ternary compounds such investigations are more complex than for binary III-V and II-VI compounds because there are two metallic sites A and B that can be substituted by a TM ion. A site preference of TM ions is crucial for a potential realization of FM since it depends on the valence state of the TM whether holes or electrons are released [5, 6].The EPR studies of isolated TMs on the two different cation lattice sites, on exchanged coupled pairs as well as the interaction of TMs with native defects will be critically reviewed and the obtained experimental results are compared with theoretical predictions.

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Mon-B-2.1i

Point and extended defects in SiC and their impacts on modern technological processes

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Keywords: silicon carbide, deep level, carrier lifetime, stacking fault

Silicon carbide (SiC) has received increasing attention as an attractive wide bandgap semiconductor for developing high-power, high-frequency, and high-temperature devices. Through rapid progress in SiC growth technology, production of almost micropipe-free 4 inch wafers as well as growth of high-quality homoepitaxial layers have been realized. However, various kinds of point and extended defects are still existing in the SiC epilayers employed for device development. In this paper, recent progress in characterization and reduction of these defects, and application to prototype devices are presented.

4H-type SiC (4H-SiC) epilayers were prepared by hot-wall chemical vapor deposition at 1550–1650°C with a high growth rate of 25–50 μm/h [1]. The typical thickness and doping concentration were 50 μm and 1×10^{15} cm^{-3} (intentionally doped n-type or p-type), respectively. DLTS measurements were performed in the wide temperature range from 90 K to 750 K to monitor both shallow and midgap levels in SiC. Photoluminescence (PL) measurements, molten KOH etching, and TEM analyses were performed to study extended defects.

Among various deep levels present in SiC, the $Z_{1/2}$ ($E_C - E_T = 0.63$ eV) [2] center has been identified as an efficient lifetime killer in n-type 4H-SiC crystals [3, 4]. The authors have found that the major deep levels can be significantly reduced by means of thermal oxidation. By thermal oxidation of epilayers at 1150 $\sim$ 1300°C, the $Z_{1/2}$ concentration has been reduced from $0.3 \sim 2 \times 10^{13}$ cm^{-3} (as-grown) to below the detection limit (1×10^{11} cm^{-3}). The depth-profile analysis of the $Z_{1/2}$ center has revealed that the $Z_{1/2}$ center is eliminated to a depth of about 50 μm from the surface after thermal oxidation at 1300°C for 5 h. The reduction mechanism of the $Z_{1/2}$ and other defects centers will be discussed in detail. The carrier lifetime in an n-type 4H-SiC epilayer measured by differential microwave photoconductance decay has been significantly improved from 0.73 μs (as-grown) to 1.62 μs (after oxidation). The impacts of lifetime enhancement on the device performance are also presented.

After nearly complete elimination of micropipe defects in SiC wafers, the stacking faults (SFs) are the major device-killing defects in 4H-SiC epilayers [5]. The authors have characterized a number of samples by micro-PL spectroscopy and PL intensity mapping [6], and four types of major SFs have been classified. Each SF exhibits a peculiar PL peak (420, 455, 480, and 500 nm at room temperature) associated with electronic states of its quantum-well structure. By cross-sectional TEM observation, the exact stacking structures of the four types of SFs have been identified. The shapes and distributions of SFs have been profiled by micro-PL intensity mapping. The formation mechanisms of each SF are also discussed.

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Mon-B-2.2o

Microstructural and magnetic study of Fe-implanted silicon carbide

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Keywords: diluted magnetic semiconductors, ion implantation, defects, X-ray diffraction, Rutherford backscattering spectroscopy

Silicon carbide is a wide band gap semiconductor with excellent transport properties and has reached a mature state of industrial development. It could thus be a good candidate for diluted magnetic semiconductors (DMS) with a critical temperature up to 270 K as previously observed [1]. Moreover, it was found that particularly large values of the Curie temperature are expected for materials built up from light elements [2] and *ab initio* calculations [3] have shown that Fe at low concentration on the Si site of hexagonal 6H-SiC leads to a ferromagnetic ordering. Moreover, XRD is a powerful tool for studying ion implantation-induced strain in monocrystalline samples [4]. Thus, we started a detailed XRD study of Fe-implanted SiC samples a few years ago.

Commercial (CREE) single crystalline 6H-SiC near (0001)-oriented samples were multi-implanted with $^{56}\mathrm{Fe}^{+}$ and $^{57}\mathrm{Fe}^{+}$ ions at different energies and fluences leading to an iron concentration reaching a plateau of $\sim 2\%$ at a depth between 20 nm and 120 nm from the sample surface. The temperature was kept constant at 550°C during implantation.

First microstructural results from XRD, TEM, GISAXS and CEMS [5] on samples implanted with $C_{Fe} \sim 7\%$ at 380°C and then furnace-annealed (900–1000°C/10-805; 1300°C/4-30) reveal the presence of small (a few nm) iron-rich crystalline clusters into a light matrix strongly damaged but still partly crystallized rather than purely diluted iron atoms.

From these first results, in order to limit iron aggregation, we decided to limit the iron concentration around 2% and to explore other ways of treatments for implantation-induced damage recovery and iron incorporation and activation in the SiC matrix: the effects of furnace annealing on microstructure and magnetic properties of Fe-implanted 6H-SiC is compared to those of Rapid Thermal Annealing (RTA) and laser processing in the solid phase [6].

Increasing the implantation temperature up to 550°C induces a still crystalline implanted region and iron atom dilution (STEM-HAADF) with a strong substitution rate (RBS/C and ALCHEMI). Microstructural state of as-implanted and annealed samples is studied by XRD, RBS/C and TEM. Annealed samples exhibit magnetic response, contrary to as-implanted samples (SQUID, PNR and VSM). Further studies of annealed samples are in progress in order to understand where the magnetic signal comes from.

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Mon-B-2.3o

Charge carrier removal rates in n-type silicon and silicon carbide subjected to electron- and proton irradiation

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Keywords: silicon carbide, irradiation, DLTS, electron

In contrast to irradiated Si, the information on removal rates of charge carriers in irradiated SiC is meager and often contradictory [1]. This is due to serious difficulties in crystal growth which, in turn, may have a profound effect on properties of initial materials. In the present work we compare the influence of electron ($\approx$ 1 MeV) and proton (8 MeV) irradiation on float-zone Si (FZ-Si) and 4H-SiC (CVD). Electrical measurements were carried out with the help of the Van der Pauw technique and capacitance-voltage technique at 1 kHz for FZ-Si and SiC, correspondingly. In addition, the spectrum of radiation-produced defects in SiC was determined with the aid of DLTS. Besides, calculations of introduction rates of primary defects were made for the both materials. The calculations for SiC showed that the introduction rates of primary defects under the electron irradiation are around 2.0 cm^{-1} and 1.3 cm^{-1} on the silicon and carbon sulattices, respectively, whereas the introduction rates under the proton irradiation are much higher, 610 cm^{-1} and 285 cm^{-1} on the same sublattices, respectively. It has been shown that the spectrum of radiation-produced defects in each polytype appears to be almost independent of the growth technique and doping level. This suggests that the defects considered are intrinsic in their nature and they are not contain impurity atoms. Under irradiation of SiC the formation of deep acceptor centers takes place and, as a result, the usual compensation of shallow donor states is observed. As expected, the formation of E-centers (the complex of vacancy–group–V impurity atom) is dominant in irradiated FZ-Si. It has been established that the production rates of radiation-produced acceptors in FZ-Si and 4H-SiC (CVD) are rather close to each other for the both materials, about 0.1 cm^{-1} and 150 cm^{-1} for the fast electron- and proton irradiation, correspondingly. A possible explanation in this case can be offered taking into account that the threshold energies of atomic displacement in Si and 4H-SiC differ insignificantly.

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Mon-B-2.4o

Mechanisms of changes of hole concentration in Al-doped 6H-SiC by electron irradiation and annealing

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Keywords: radiation damage, electron irradiation, SiC, 6H-SiC, p-type SiC

SiC is a promising wide band gap semiconductor for fabricating high-power and high-frequency electronic devices capable of operating under radiation environments, because the minority-carrier-lifetime degradation by irradiation in SiC was reported to be lower than in Si and GaAs [1]. Compared with Si [2], however, the understanding of radiation damage in SiC is far from complete [3].

According to our simulation [4], irradiation with 200 keV electrons can replace only substitutional C atoms in SiC, while irradiation with 100 keV electrons cannot. Moreover, electrons with $\geq$ 400 keV can replace all atoms in SiC.

The temperature dependence of hole concentration $p(T)$ in Al-doped 6H-SiC epilayers was obtained by Hall-effect measurements, from which the densities and energy levels of acceptors were determined. Before irradiation, the density of acceptors (N_{A1}) at $E_{\text{V}} + 0.24$ eV in the epilayer was determined to be 1.6×10^{15} cm^{-3}, and the density of acceptors (N_{A2}) at $E_{\text{V}} + 0.4$ eV was 1.0×10^{15} cm^{-3}.

Irradiation with 200 keV electrons reduced $p(T)$. After irradiation with a 1×10^{16} cm^{-2} fluence, N_{A1} decreased to 6.0×10^{14} cm^{-3}, while N_{A2} increased to 2.2×10^{15} cm^{-3}. After second irradiation with the same fluence, N_{A1} decreased to $< 10^{14}$ cm^{-3}, whereas N_{A2} remained. Third irradiation resulted in incapable measurement due to too high resistivity of the irradiated epilayer. After 500°C annealing for 2 min in Ar, however, N_{A1} increased to 4.0×10^{14} cm^{-3} and N_{A2} decreased to 1.6×10^{15} cm^{-3}, compared with the second irradiation. This is an unexpected phenomenon.

First irradiation with a 1×10^{16} cm^{-2} fluence of 100 keV electrons did not change $p(T)$. However, second irradiation with a 2×10^{16} cm^{-2} fluence increased $p(T)$ at low temperatures, which is also an unexpected phenomenon.

Possible mechanisms of changes of $p(T)$ by electron irradiation and annealing will be discussed.

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Mon-B-2.5o

Defects and polytypic transformation in LPE grown SiC epilayers on (111) 3C-SiC seeds grown by VLS

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Keywords: SiC, LPE, VLS, TEM, LTPL

It is well known that due to one-dimensional polymorphism silicon carbide exists in a large variety of crystal structures which differ only by the stacking sequence of n successive Si-C bilayers. The different polytypes are distinguished by their lattice structure which ranges from zinc-blende for 3C-SiC to wurzite for 2H-SiC. All other variants combine cubic and hexagonal stacking, resulting in either a hexagonal or rhombohedral symmetry. Depending on the degree of hexagonality, the band gap energy E_g varies from 2.39 eV for 3C-SiC to 3.33 eV for 2H-SiC. Unfortunately, the development of SiC based device applications has long been hindered by the difficulties in polytype stabilization and easy formation of structural defects, especially in the cubic form.

The most serious problem, when the growth of 3C-SiC is concerned, is that the growing crystals can undergo polytypic transition and/or spontaneous generation of defects, mainly stacking faults and double-positioned boundaries, especially at high temperature. The growth of bulk 3C-SiC and the investigation of the defects generated during this growth are particularly challenging issues. Understanding the mechanisms of polytypic conversion and defining optimized growth conditions are still open questions that need to be solved in the future development of the 3C-SiC technology.

In the current work TEM (transmission electron microscopy) and LTPL (low-temperature photoluminescence) studies of liquid phase grown epilayers are presented. First, a VLS (vapour liquid solid) grown 3C-SiC buffer layer is deposited on on-axis Si face 6H-SiC (0001) substrate, with a thickness of 3.3 μm. The thickness of this first layer is next increased using a LPE (liquid phase epitaxy) process at 1650°C with pure Si as solvent (see ref [1] for more details). The typical thickness of the overgrown layer is about 45 μm.

The TEM investigation shows that the 6H-SiC seed is completely covered by the 3C-SiC polytype during the VLS process. During the LPE process some polytype instabilities occur, and several rhombohedral polytypes are stabilized one after the other. These are 21R, converted after several microns to 57R and eventually leading after few microns to the final transition of the 3C-SiC polytype back to 6H-SiC. This interplay of the polytypes results in a complex optical signature with specific LTPL features. In conclusion, all these findings show that the conversion of 6H into 3C is a very delicate process in which high quality seeds, free of any polytype inclusion are needed.

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Mon-B-2.6o

Influence of the defect density (twins boundaries) on electrical parameters of 3C-SiC epitaxial films

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Keywords: 3C SiC, twins, mobility, magnetoresistance, X-ray

3C-SiC epitaxial layers were grown by sublimation epitaxy in a vacuum on the (0001)C face of SiC substrates. The low-temperature conductivity and magnetoresistance of the films have been studied as functions of their doping level and structural quality. The epitaxial structures were examined using X-ray topography in the back-reflection configuration. It is known that, as a cubic epitaxial layer starts to grow simultaneously at different regions of a hexagonal substrate, 3C-SiC nuclei are oriented along the growth surface in two ways, with an angle of 60° between the two orientations (twin structure). Commonly, the structural quality of 3C-SiC epitaxial films is characterized by the twin density. However, this is convenient when the twin density is high and separate twins have about the same geometrical dimensions. The best of the samples we obtained contained only several twins and, while present in the same amounts, they strongly differed in shape and size. Because the main structural defects are concentrated at twin boundaries, samples with the same (and small) number of twins with different shapes may contain strongly different amounts of defects. Therefore, it seemed to us to be more convenient to use for evaluation of the structural quality of our films the parameter $L_{Tw} = l_{Tw}/S$, where l_{Tw} is the sum of lengths of all the twin boundaries in a sample, and S is the sample area.

In the structures under study, we examined the electrical conductivity and the Hall effect in the temperature range 300–1.5 K. For all of the samples, the resistance is independent of the magnetic field up to $H = 1$ T when the field is directed along the plane of a 3C-SiC layer. For a field perpendicular to the film plane, the resistance initially decreases with the magnetic field increase. The value of $R(H)/R(H = 0)$ is $\sim 2 \times 10^{-2}$–1×10^{-4}. The further magnetic field increase leads to the positive magnetoresistance, irrespective of the field orientation. The behavior of the type $R \sim H^2$ holds up to the highest magnetic fields available in the experiment ($\sim 15T$).There is no noticeable relation between the doping level of n-3C-SiC films and the NMR magnitude ($\Delta R/R$). The total resistance of the epitaxial structures grows as N_d–N_a in n-3C-SiC decreases, but remains small in absolute value.A comparison of n-3C-SiC samples with different degrees of structural quality demonstrated that the presence and magnitude of NMR as well as the electron mobility depend on the parameter L_{Tw}. A decrease in the degree of structural quality (an increase in L_{Tw}) results in a decrease of the mobility and in a decrease of the NMR (up to its complete suppression in the sample with the minimum density of twins).The decrease in the carrier mobility and NMR magnitude is possibly observed as the twin density becomes lower because twin boundaries play a role of a sink for defects responsible for the carrier scattering in n-3C-SiC films.

Tue-A-1.1i

Oxygen vacancies in oxides

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Keywords: oxides, electronic structure, density functional theory

Wide-band gap oxide semiconductors constitute a large class of materials with a rich variety of crystal structures and physical properties, including transparency to visible light, high electrical conductivities, strong luminescence, high dielectric constants, and piezoelectricity. Although many semiconducting oxides are widely used in various technological applications, their use as semiconductors in electronic and optoelectronic devices is rather limited due to the lack of control over conductivity. Many of these materials exhibit unintentional n-type conductivity, the cause of which has been intensely debated. The traditional explanation is the presence of oxygen vacancies which would act as donors. However, this traditional model has been recently challenged by first-principles calculations [1–4] which show that in ZnO, SnO_2, and In_2O_3, prototypes of transparent conducting oxides, oxygen vacancies are deep donors and cannot contribute to n-type conductivity. In view of the recent developments, the study of the electronic properties of oxygen vacancies in wide-band-gap oxides based on state-of-the art density functional calculations will be critically reviewed, and connections with experimental results will be made whenever possible.

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Tue-A-1.2o

Nitrogen and hydrogen in bulk single-crystal ZnO

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Keywords: zinc oxide, hydrogen, nitrogen, local vibrational modes

Zinc oxide (ZnO) is a wide band gap II–VI semiconductor with optical, electronic, and mechanical applications. The lack of reliable p-type doping has prevented it from competing with other semiconductors such as GaN.

Nitrogen is a promising acceptor dopant. We successfully incorporated nitrogen-hydrogen (N–H) complexes in ZnO during chemical vapor transport (CVT) growth, using ammonia as an ambient. Using commercial ZnO as a seed, we obtained bulk single-crystal growth. The N–H bond-stretching mode gives rise to an infrared (IR) absorption peak at 3150.6 cm^{-1} at liquid helium temperatures. Isotopic substitutions for hydrogen and nitrogen result in the expected frequency shifts, thereby providing an unambiguous identification of these complexes. The N-H complexes are stable up to $\sim$ 700°C. The introduction of neutral N–H complexes could prove useful in achieving reliable p-type conductivity in ZnO [1].

Along with passivating acceptors, hydrogen also acts as a shallow donor. In previous work, we observed an IR peak at 3326 cm^{-1} that corresponded to a hydrogen donor [2]. However, other samples show a hydrogen peak at 3611 cm^{-1} [3, 4]. By comparing the trace impurities in Cermet and Eagle-Picher samples, we proposed that the 3326 cm^{-1} mode may arise from Ca–OH or Mg–OH complexes [5]. First-principles calculations verified that the Ca–OH complex is a likely candidate [6]. However, unambiguous experimental proof is still lacking.

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Tue-A-1.3o

On quantum efficiency of photoluminescence in ZnO layers and nanostructures

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Keywords: quantum efficiency, photoluminescence, ZnO

ZnO has attracted great interest as potential material for short-wavelength light-emitting diodes, laser diodes, UV detectors, and other optoelectronic applications. Among the most important characteristics of wide-bandgap semiconductors to be used in optical devices are radiative efficiency (the ratio between the emitted and consumed power) and concentrations of defects involved in the recombination process. The most common method employed for characterization of wide-bandgap semiconductors is photoluminescence (PL). Surprisingly, no standards of PL quantum efficiency (QE) of wide-bandgap semiconductors exist, and almost nobody evaluates the concentrations of radiative defects in these materials! There have been very few attempts to estimate the absolute value of internal and external QE of PL in wide-bandgap semiconductors. The solution to this problem and the development of radiative efficiency metrology standards would enable one to quantitatively evaluate important characteristics of wide-bandgap semiconductors from a relatively simple analysis of the steady-state and time-resolved PL, namely: QE of different recombination channels, concentrations of radiative defects, their capture cross-sections, charge states, and lifetimes of minority carriers.

In this work we studied PL in ZnO layers and nanostructures, including ZnO layers on sapphire substrate grown by MBE, ZnO–$\mathrm{Zn}_{x-1}\mathrm{Mg}_x\mathrm{O}$ single quantum well (SQW) structures grown on sapphire substrates by MBE, and ZnO nanowires grown on sapphire by MOCVD. The external QE in O-face ZnO layers exceeded that in Zn-face ZnO layers by two orders of magnitude at low temperatures. In addition to a very strong excitonic emission in O-face ZnO layers, broad green and orange bands related to defects were observed and studied in detail. In a sample with SQW the combined external QE from the 4-nm-wide SQW and 100-nm-thick $Zn_{x-1}Mg_xO$ barriers achieved 28% at 15 K. The highest external QE was observed in one of the samples with ZnO nanowires 50% at 15 K and 2% at 300 K. Remarkably, contribution of defect-related PL bands in ZnO nanowires samples was extremely low. In selected samples with high external QE the absolute internal QE of PL has been determined indirectly from analysis of carrier recombination statistics in conditions of varying temperature.

Tue-A-1.4o

Electrically active defect centers in hydrothermally grown ZnO after high temperature treatments

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Keywords: ZnO, defects, DLTS, SIMS

Zinc oxide (ZnO) is a wide band gap semiconductor ($E_g = 3.4$ eV) who has received considerable attention the last few years due to its potential applications as light emitting diode and in photovoltaics being a transparent conducting oxide. However, the technological advances have been hindered by the difficulty in controlling and understanding the electrial behavior of intrinsic and impurity related defects. So far, temperature dependent Hall (TDH) measurements have been an important technique to obtain information about electrically active defect centers in ZnO. However, deep level transient spectroscopy (DLTS) and thermal admittance spectroscopy (TAS) can give quantitative and more direct information about defect concentrations, activation energies, and capture cross sections. Only a few studies using Deep level transient spectroscopy (DLTS) and thermal admittance spectroscopy (TAS) on ZnO have been reported due to the difficulty in producing high quality Schottky barriers. However, recent progress, see e.g. ref. [1], shows promising results for Schottky contacts of sufficient quality to pursue ZnO studies using DLTS.

In the present study, Deep level transient spectroscopy (DLTS) and thermal admittance spectroscopy (TAS) have been employed to study electron traps in hydrothermally grown ZnO after thermal treatments up to 1500°C, resulting in different impurity concentrations, in particular of Lithium. Schottky barrier contacts were formed by e-beam evaporation of Pd on bulk n-type ZnO, followed by DLTS, TAS, and secondary ion mass spectrometry (SIMS) in order to determine both electron traps in the upper part of the band gap and the impurity concentration of the most prominent impurities. The results from DLTS and thermal admittance spectroscopy showed at least five different levels having energy positions of Ec -20 meV, Ec -55 meV, Ec -220 meV, Ec

-320 meV, and Ec -570 meV (Ec denotes the conduction band edge). SIMS results showed that the most pronounced impurities were Li, Al, Si, Mg, and C, with concentrations up to $\sim 5 \times 10^{17}$ cm^{-3}. The hydrogen concentration was below the detection limit, about 5×10^{17} cm^{-3}. TAS show that the Ec - 55 meV level is annealed out in samples subjected to heat treatments above 1300°C, and a level at Ec -20 meV arise. Moreover, the Li concentration is reduced from $\sim 10^{17}$ cm^{-3} for as-grown material to $\sim 10^{15}$ cm^{-3} for samples treated at 1500°C.

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Characterisation of point defects in ZnO thin films by optical deep level transient spectroscopy

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Keywords: ZnO, DLTS, point defects, photo cross-section

We employed a variant of optical DLTS, where optically excited emission from deep levels additionally to thermal emission is being determined by illuminating the sample with monochromatic light having energies lower than the band gap energy. From this data, the photo cross-sections of deep levels can be calculated. These can be distinguished for two optically excited processes: the emission of an electron from the occupied trap into excited states or an energy band; or secondly, from an energy band onto the empty trap. The photo cross-sections represent the probabilities of these processes.

ZnO thin films (n-type) with varying Zn/O-ratio have been characterised by standard DLTS. A total of six deep levels have been found, including the E3 and E4 levels (both in [1–3]), as well as the recently reported T2 [4]. Further deep levels are located at energies of (247 ± 20) meV (in the following labelled T3) and (680 ± 80) meV below the conduction band edge. The latter is energetically comparable to (and will be referred to as) E5 [3]. It might also be related to the deep level reported in [5].

We have determined the relative photo cross-section spectra for emission to the conduction band for E4 and T2 in the photon energy range from 0.7 to 3.0 eV from ODLTS. E3 and E5 appear as optically inactive, having a photo cross-section at least four orders of magnitude smaller than E4.

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Point defects in ZnO: electron paramagnetic resonance study

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Keywords: ZnO, point defects, magnetic resonance

ZnO is wide band semiconductor currently of interest for possible electronic and optical applications. Optical, electrical, and magnetic properties of ZnO strongly depend on the impurities and defects in this material. Depending on the growth method, nominally undoped ZnO single crystals may contain In, Ga, Al, Pb donors, Li acceptors and a row of transition metal impurities (TM = V, Mn, Cu, Co, Fe, Ni) even in the same sample. The most successful experimental technique for identifying and studying the defects in semiconductors is the electron paramagnetic resonance (EPR), detected either directly (EPR and photo-EPR), or optically (ODEPR). In spite of many investigations of paramagnetic centers in ZnO several important problems concerning identification of EPR spectra and properties of point defects in ZnO are open so far.

In this study the results of EPR investigation of different point defects in ZnO single crystals, ceramics and powders are reported. The main attention is given to EPR and photo-EPR studies of such important intrinsic defect as oxygen vacancy (V_O) being in scope of many experimental and theoretical investigations. The properties of EPR spectra related to oxygen vacancies and such impurities as Li and Pb atoms observed under illumination with different quantum energies are reported. The results of EPR and photo-EPR investigations are compared with the optically detected ODEPR spectra. The optimal experimental conditions for detection EPR and ODEPR spectra were analyzed.

Unusual time dependences of the V_O and Pb EPR spectra under photoexcitation were found. Depending on the light quantum energy, the fast increase of intensity of these spectra followed by slow decrease almost to zero value is observed when light is switched on. These dependences were explained taking into account the optical recharge of centers and double donor nature of Pb in ZnO. Based on the experimental results on the photoexcitation and quench of the V_O and Pb EPR spectra the conclusion about the level positions of these centers was done.

Tue-A-2.2o

Vacancy clustering in ion implanted ZnO: Fundamental properties and influence of group-I elements

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Keywords: ZnO, ion implantation, group-I, vacancy

ZnO is a direct band gap semiconductor having exciting properties and understanding of intrinsic defects is essential for making progress in realizing ZnO-based devices. Vacancies and their clusters are fundamental defects in ZnO and a significant effort has been devoted to investigate properties of these defects partly, because excess vacancy concentrations are readily formed during ion implantation. Considering the behavior of Zn vacancies (V_{Zn}) during post implantation anneals, V_{Zn} may in general either annihilate by interacting with Zn interstitials (Zn_i) or agglomerate to higher order clusters. It has recently been shown that vacancy clustering dominates at relatively broad annealing temperatures/time conditions [1]. However, little is known if and how group-I impurities may influence the V_{Zn} concentration in ZnO [2]. For example, Na may efficiently interact with V_{Zn}, and thus changing the defect evolution in ion implanted ZnO.

In this contribution we report on a systematic study of how group-I elements (Na and Li) influence V_{Zn}-related defect reactions in ion implanted ZnO. Importantly and in comparison with a host of previous studies employing other implant ions, Na^+ implants (i) result in significantly lower V_{Zn} concentrations and (ii) practically no V_{Zn} clustering is observed during post-implantation anneals. A major part of the V_{Zn} defect/cluster observations are made by positron annihilation spectroscopy (PAS) and scales accordingly with the Na concentration measured by SIMS, thus confirming that it is evidently Na that is affecting the V_{Zn} evolution. In addition, our preliminary RBS-C measurements indicate more Zn_i surviving post-implantation anneals in samples containing Na compared with control implants. Note that Na implants were made, for comparison, into Li-rich ($\sim 10^{17}$ Li/cm^3) and Li-lean ($< 10^{13}$ Li/cm^3) samples and competing roles of Na and Li were also investigated. Moreover, diffusion mechanisms of Na and Li are discussed, and last but no least, the electrical properties of the samples, investigated using Hall effect measurements and scanning spreading resistance microscopy (SSRM), will be discussed.

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Lattice location of the group V elements As and Sb in ZnO

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Keywords: ZnO, Sb in ZnO, As in ZnO, lattice location, ion implantation

Modifying the properties of ZnO by means of incorporating P, As or Sb impurities is of interest since these group V elements have been reported in the literature among the few successful p-type dopants in this II–VI compound. However, the large size mismatch between O^{2-} (ionic radius 1.38 Åand the potential acceptor ions P^{3-} (2.12 Å), As^{3-} (2.22 Å) or Sb^{3-} (2.45 Å) makes the simple substitution of O^{2-} anions unlikely [1], while the much smaller radius of the triply positive ions P^{3+} (0.44 Å), As^{3+} (0.58 Å) or Sb^{3+} (0.76 Å) should favour the substitution of Zn^{2+} (0.60 Å) cations, resulting in double donor formation. There is therefore an ongoing debate whether the experimentally observed p-type character is due to P, As or Sb simply replacing oxygen or to the formation of more complicated defects: In particular the formation of electrically active acceptor complexes of the type $As_{Zn}/2V_{Zn}$ or $Sb_{Zn}/2V_{Zn}$ has been suggested to be responsible for the p-type behaviour [2].

Experiments that reveal the lattice location of group V impurities in ZnO are therefore crucial in order to understand the mechanism of p-type doping. We have previously determined the lattice sites of ion implanted As in ZnO by means of conversion electron emission channeling from radioactive ^{73}As [3]. In this contribution we present new data on beta emission channeling experiments using the implanted isotope ^{124}Sb ($t_{1/2} = 60.2$ d) and compare the behaviour of the two dopants. Preliminary data on the lattice location of radioactive phosphorus ^{33}P ($t_{1/2} = 25.3d$) in ZnO will be briefly addressed as well.

We find, in contrast to what one might expect from their nature as group V elements, that both As and Sb do not occupy substitutional O sites in ZnO but mostly substitutional Zn sites. Possible fractions of As or Sb on O sites in our experiments, if existing at all, could at maximum have been a few percent. Arsenic and antimony in ZnO are thus interesting examples for impurities where the major impurity lattice site is determined by ionic size rather than their position in the periodic system. While our results cannot settle the interesting issue whether substitutional As or Sb on oxygen sites or $As_{Zn}/2V_{Zn}$ or $Sb_{Zn}/2V_{Zn}$ complexes are responsible for the acceptor action, the fact that implanted As and Sb prefer the substitutional Zn sites is clearly a strong argument in favour of the complex acceptor model, while it discourages the notion that As and Sb act as simple chemical acceptors in ZnO.

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Impurity doping in silicon nanowires and nanocrystals

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Keywords: Si, nanocrystal, nanowire, shallow impurity

Silicon (Si) nanowires and nanocrystals (nano-Si) are believed to be new building blocks for future Si-based electronic and optoelectronic devices. One of the crucial issues to realize nano-Si based devices is a precise control of shallow impurities and to understand the physics of doped nano-Si. In this work, we first discuss the mechanism of shallow impurity doping in Si nanowires grown by the vapor-liquid-solid (VLS) process. We show that mapping of Raman spectra in a single Si nanowire and the analysis of the Fano-type spectral shape provides information on distribution of active B concentration in Si nanowires. From the B distribution of modulation-doped Si nanowires, we discuss the mechanism of in-situ impurity doping during the VLS growth. The second topic is shallow impurities in Si nanocrystals. Because of a so-called self-purification effect, Si nanocrystals always tend to push impurities out of them during thermal treatments. To avoid this effect, we grow doped Si nanocrystals in heavily impurity (P and/or B) doped SiO_2 glasses. We show that shallow impurity doping modifies the photoluminescence (PL) properties significantly. From PL, infrared absorption, and electron spin resonance (ESR) studies, we discuss the energy band structure of doped Si nanocrystals. We also demonstrate that nonlinear optical responses of Si nanocrystals are strongly enhanced by shallow impurity doping.

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Phosphorus doping of Si nanocrystals: doping efficiency and electronic confinement

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Keywords: Si nanocrystals, doping, phosphorus, magnetic impurities

Owing to their interesting physical properties and the potential of cost-effective processing, silicon nanocrystals (Si–NCs) are a promising candidate for a variety of applications e.g. in solar cells or thermoelectric power devices. For most of these applications, it is inevitable to tailor the electronic properties via controlled doping with impurity atoms. However, doping of NCs is in general quite distinct from their bulk counterparts [1]. In this work, we use electron paramagnetic resonance (EPR), secondary ion mass spectroscopy (SIMS) and electrically detected magnetic resonance (EDMR) to investigate the P doping of freestanding Si–NCs with mean diameters between 4 nm and 45 nm.

The NCs were produced by microwave-induced decomposition of silane in a low-pressure microwave plasma reactor and can be doped with substitutional P via addition of phosphine during growth [2, 3]. SIMS results do not indicate a size dependence of the P incorporation efficiency. However, it is found that 90–95% of the P segregates to the Si–NC surface region, which is oxidized after exposure to air. The concentration of electrically active, paramagnetic P detected by EPR further falls below this SIMS concentration by about one order of magnitude for Si–NCs with diameters larger than 15 nm. Charge compensation by Si dangling bonds, which are investigated using room temperature EPR and which can be passivated by H, is shown to be the reason for this deviation and can quantitatively be described by a statistical model.

For efficient doping at room temperature, also the donor ionization energy is crucial. The ionization energy correlates with the donor localization which we probe via the Fermi contact hyperfine coupling of isolated donor electron spins with the nuclear spins of their impurity sites. Applying EDMR to Si-NC networks, we find that the localization effect sets in for Si-NCs as large as 20 nm. For Si–NCs with a diameter of 6 nm the hyperfine coupling is increased by 100% with respect to the bulk value. A quantitative comparison with different theoretical models shows that the observed localization can only be explained taking into account a size-dependent change of the dielectric screening inside the Si–NCs, rather than by a pure quantum confinement model [4].

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Energy transfer processes between Si nanocrystals and Er^{3+} ions in SiO_2

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Keywords: silicon nanocrystals, erbium ions, silicon dioxide, photoluminescence, energy transfer mechanisms

The material composed of Si nanocrystals (NCs) dispersed in SiO_2 doped by Er is a subject of big interest for creation of amplifiers or lasers on the basis of silicon technology [1–3]. There are a lot of experimental results concerning this material, and particularly the nanocrystals properties and the mechanism of the Er^{3+} ions excitation [4, and references therein]. Here we present the results of theoretical study of the energy transfer processes between Si nanocrystals and Er^{3+} ions.

Energy transfer between electrons and holes in NCs and f-electrons of Er^{3+} ions is considered as an Auger process (i.e. via the Coulomb interaction). The energy can be transferred to an erbium ion either when a confined electron-hole pair recombines, or when an intra-band transition of a *hot* confined carrier occurs. Both processes can be assisted by multiphonon transitions to fulfill the energy conservation law, as the energy spectra of both electron systems are discrete. We have calculated the probability of these processes as a function of Er^{3+} distance from the Si NC. The details of calculations can be found in [5]. It is shown that the Er^{3+} ion excitation accompanied by the confined exciton recombination is an effective process only if Er^{3+} ion is situated inside a NC or at the boundary of a NC. In this way, the Er^{3+} ion is transferred to one of the higher excited states and undergoes then a multiphonon relaxation on a microsecond time scale to the first excited state giving rise to technologically important 1.55 μm emission. On the other hand, up to 50% of all the Er^{3+} content is in the effective range of fast excitation by intraband relaxation of *hot* carriers transferring Er^{3+} ions directly into the first excited state.

We have studied also the possibility of erbium excitation directly in the light absorption process and demonstrated that the process is of particular importance for Si NCs where light absorption is phonon-assisted due to the indirect band-gap energy structure. When the energy of photon is large enough for simultaneous excitation of Er^{3+}ion and confined exciton generation, the Er-assisted light absorption can take place and no additional particle is required to fulfill the momentum conservation law. Finally, we have considered the reverse de-excitation processes. A clear understanding of the experimentally observed nanosecond dynamics of the Er-related 1.55 μm photoluminescence in SiO_2 sensitized with Si NCs [6] is achieved.

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Tue-B-1.4o

Doping and segregation of impurity atoms in silicon nanowires

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Keywords: silicon nanowire, boron, phosphorus, Raman scattering, electron spin resonance

Silicon nanowires (SiNWs) are of great interest in the fields of both fundamental and application research. In order to realize nanoscale silicon devices using SiNWs, it is important to investigate the impurity doping.

SiNWs were synthesized by laser ablation of a Si target with nickel as a metal catalyst and boron (B) and phosphorus (P) as dopants which were placed in a quartz tube heated at 1200°C in a flowing Ar gas. A frequency-doubled NdYAG laser (532 nm, 7 ns pulse width, 10 Hz, 150 mJ/pulse) was used to ablate the targets. Micro-Raman scattering measurements were performed at room temperature with a 532-nm excitation light. Electron spin resonance (ESR) measurements were carried out at 4.2 K using an X-band ESR spectrometer to investigate the state of P donors in SiNWs.

A Raman peak was observed at about 618 cm^{-1} for SiNWs synthesized by using a Si target with B. The peak frequency is in good agreement with that of a local vibrational mode of B in Si crystal. The Fano broadening due to a coupling between the discrete optical phonon and a continuum of interband hole excitations was also observed in the optical phonon peak, which indicates heavily B doping. The observation of B local vibrational peaks and Fano broadening were observed for the first time in our experiments [1, 2]. These results prove that B atoms were doped in substitutional sites of the crystalline Si core of SiNWs [1]. ESR measurements were also performed to investigate defects and P donor/conduction electrons in P-doped SiNWs. The observation of ESR signal due to conduction electrons clearly showed that P atoms were doped in substitutional sites of the crystalline Si core of SiNWs [2, 3]. The codoping of B and P were also investigated and the compensation effect in SiNWs was detected [4]. The segregation behaviors of B and P were investigated by using B local vibrational peaks and Fano broadening for B-doped SiNWs, while an ESR signal of conduction electrons was used for P-doped SiNWs. The results showed that the segregation of B is faster than that of P.

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Tue-B-1.5o

Relation between photocurrent and DLTS signals observed for quantum dot systems

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Keywords: nanostructures, quantum dots InAs/GaAs, Laplace DLTS, photocurrent

Quantum dots in a semiconductor matrix can create binding potentials for electrons in the conducting band and/or holes in the valance band depending on the specific quantum dot material/semiconductor material system. Despite the fact that the dots are formed by hundreds of atoms usually they are able to bind only one or two carriers, thus from a point of view of their electrical characteristics they are like point defects. Thus quantum dots can be of a donor or acceptor type depending on a position of the Fermi level. In this study we attempt to characterise the binding potentials for electrons and holes for the quantum dot system where we manipulate with the dot occupancy using a monochromatic (continuous or pulsing) light illumination resonant with the excitonic transition for the dots. The carrier binding potentials are characterised with a use of the conventional or Laplace DLTS methods, while the spectral characteristics of the dot system electrical activity is investigated with a use of photocurrent measurements in a wide range of temperatures and using broad- (high-throughput monochromator) or narrowband (the OPO laser) light sources. We combine the observed electron and hole related DLTS signals with resonant light dot excitation energy to link the given carrier binding energy with the energy of an exciton created in the dot. We clearly demonstrate that the quantum dots can contribute to the observed photocurrent at temperatures where the carrier binding energies are not too strong to prevent the dot autoionisation process. At these temperatures we observe the dot-related thermal ionisation process as DLTS signals avoiding a confusion with other defects related signals. The photocurrent measurements also showed that with increasing temperatures the dot-related photocurrent peak shifts to lower energies with a rate similar to the GaAs bandgap shrinkage. Finally, the dot parameters are broadened as a result of their spontaneous creation procedure and we attempt to evaluate these broadenings for different sets of quantum dots grown at different conditions. In this study we investigate different densities and sizes the InAs quantum dots in the GaAs matrix grown by the MBE technique with some preliminary results for the CdTe/ZnTe dot system.

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Surface segregation of dopants in nano-crystalline silicon: density-functional studies

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Keywords: nanostructures, doping, segregation

Semiconductor nanocrystals may find future applications in a wide variety of technologies, such as light emitting devices and solar cells. Doping nano-sized structures presents a remarkable task, where effects such as self-purification and enhancement of ionization energy of dopants have been suggested to pose significant difficulties. Nonetheless, recent experimental studies have proven the feasibility of incorporating foreign elements into different types of semiconductor nanocrystals. Here we present a study of the energetics and electronic structure of phosphorus and boron dopants in silicon nanocrystals, the material of choice for the production of semiconductor inks for printing of semiconductor thin films. To this goal we model large atomic clusters with more than 1000 Si atoms. It is found that a size driven self-purification mechanism has a low impact on hindering P and B doping when compared to surface segregation. This is suggested as a dominant sink for dopants, especially in the case of phosphorous.

Tue-B-2.2o

Epitaxial growth of Ge/Si nanostructures under low-energy ion irradiation

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Keywords: epitaxy, nanocluster, strain, ion irradiation, simulations

The effect of pulsed irradiation by a low-energy (50–250 eV) ion beam with a pulse duration of 0.5 s on the nucleation and growth of three-dimensional germanium islands during molecular-beam heteroepitaxy of Ge/Si(100) structures is investigated experimentally. It is revealed that at specific values of the integrated ion flux (less than 10^{12} cm^{-2}) pulsed ion irradiation leads to an increase in the density of islands and a decrease in their mean size and size dispersion as compared to those obtained in the case of heteroepitaxy without ion irradiation [1]. The observed phenomena are explained in the framework of the model based on the concept of the change in the diffusion mobility of adatoms due to the instantaneous generation of interstitial atoms and vacancies under pulsed ion irradiation [2]. It is shown that there are areas of local tensile strain above interstitial atom and vacancy clusters which are responsible for the change in the binding energy of the adatoms. Thus, the places where the ions impact the surface become centers of preferential nucleation of three-dimensional islands. The model takes accounts of annihilation of vacancies and interstitial atoms on the surface of the growing layer. The results obtained from the Monte Carlo simulations based on the proposed model are in good agreement with the experimental data.

Influence of ion beam flux on the mechanical strain of epitaxial layer of Ge was investigated using the high-energy electron diffraction (RHEED) method. To obtain additional information about nature of nucleation centers, substrates doped by boron impurities, which serve as traps for interstitial atoms, were used for growth experiments. Surface morphology was investigated by scanning tunneling microscopy (STM). Point defects introduced by ion irradiation was detected by electron paramagnetic resonance (EPR).

The knowledge of the mechanism of ion-assisted nucleation during heteroepitaxy will provide an additional tool for controlling the growth of nanostructures.

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Tue-B-2.3o

ODMR and EDEPR of impurity centres embedded in silicon microcavities

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Keywords: silicon microcavity, quantum well, EPR, bound exciton, trigonal centers

We present the findings of the excitonic normal-mode coupling (NMC) with the single silicon quantum well (SQW) embedded in the silicon microcavity that exhibits the high efficient photoluminescence of bound excitons at the iron-boron pairs and the erbium-related centers inserted in SQW.

The n- type Si (100) wafers preliminary doped with iron and erbium were oxidized at 1150°C in dry oxygen containing CCl4 vapors. Short-time boron doping was done from the gas phase under fine surface injection of both self-interstitials and vacancies into the window, which was cut in the oxide overlayer after preparing a mask and performing the subsequent photolithography. The four-point probe under layer-by-layer etching and SIMS measurements allowed the depth of the $p+-$ boron diffusion profile, 8 nm. The CR angular dependencies have shown that the profile prepared contains the low density p-type SQW confined by the delta barriers heavily doped with boron. The boron centers inside the delta barriers are found to be the impurity dipoles, $B(+) - B(-)$, which cause the GHz generation under applied voltage or optical pumping. Spectroscopic studies confirmed this pattern and furthermore the STM images have demonstrated that the SQW is incorporated into the microcavity system of the fractal type formed by the microdefects of the self-interstitials type. This silicon microcavity is revealed by the angle-resolved transmission spectra that exhibit the NMC regime with a single SQW in the spectral range of the Rabi splitting at $T = 300$ K. Moreover, the bound excitons at a single point defect appeared to cause giant exchange splitting in the absence of the external magnetic field that is created by strong coupling between d or f-electron states of the center and the s-p electronic states of the host SQW. This strong sp-d or sp-f mixing is revealed by the angle-resolved photoluminescence and absorption that seem to be the ODMR spectra in zero magnetic fields under the NMC conditions, because the EPR frequency is able to be selected from the GHz range generated by the delta barriers confining the SQW being in self-agreement the exchange splitting value. The values of the EPR frequency , 87 GHz and 200 GHz, which allow the transmission spectra under the ODMR saturation, appeared to correlate respectively with the line splitting value of the bound exciton at the trigonal iron-boron pair and trigonal erbium-related center. The EPR frequencies appeared to be selected from the GHz range by preparing additional microwave cavity. Finally, the possibilities of this GHz selection have been verified by measuring of the electrically-detected EPR (EDEPR) of the same centers embedded in the silicon microcavity that was carried out, for the first time, without external resonator.

Tue-B-3.1i

Defect engineering in single-walled carbon nanotubes

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Keywords: carbon nanotubes, low-energy irradiation damage, metal-semiconductor transition

Single-walled carbon nanotubes (SWNTs) are damaged by irradiation of low-energy particles, such as electrons and photons [1]. The threshold energy of the low-energy irradiation damage was evaluated to be about 6 eV [2], several orders of magnitude smaller than the threshold energy of the knock-on damage. The irradiation-induced defects have some unique properties. The formation and healing of the defects are reversible, meaning that the number of carbon atoms is preserved [3]. The damage strongly depends on the SWNT diameter; that is, a thicker nanotube is less damaged [3]. Because of a small activation energy of the defect healing ($\sim$ 1 eV), the defects are gradually healed at room temperature [4].

Moreover, the irradiation converts the room temperature electric properties of a metallic SWNT to semiconducting [5, 6]. The conversion can be explained by defect-induced energy barrier formation and gate-induced band bending of a metallic SWNT [7]. When the defects act as tunneling barriers, Coulomb oscillation is also observed at room temperature [5].

The low-energy irradiation damage could lead to reversible, diameter-selective, and highly spatially selective defect engineering of SWNTs.

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Tue-B-3.2o

Imaging charge transport in GaN nanowires using near field optical microscopy

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Keywords: nanowire, GaN, transport, diffusion, imaging

A unique system has been developed for the imaging of carrier transport within semiconductor nanostructures by operating a near field scanning optical microscopy (NSOM) within a scanning electron microscope. Luminescence associated with carrier recombination is collected with high spatial resolution to monitor the motion and recombination of charge generated by the use of the electron beam as an independent point source. Light is collected in the near field from a scanning fiber using tuning fork feedback in an open architecture combined AFM/NSOM system (Nanonics MultiView 2000) allowing for independent motion of sample and tip. The technique builds upon, but is different from conventional CL in that spatial information on the carrier recombination is maintained [1]. Fiber apertures ranging from 150 to 300 nm are used to collect the light. From a single image, it is possible to obtain a direct measure of minority carrier diffusion length and determine the effects of doping, surface passivation, wire diameter and defect density on minority carrier transport. The approach will be illustrated with imaging of carrier diffusion in various planar double heterostructures using standard far field imaging techniques [2]. Extension to the near field allows for the resolution required to image transport along a single nanowire or nanorod.

This technique has been used in the near-field collection mode to image the diffusion of charge in n-type GaN and GaN–AlGaN core-shell nanowires, grown via Ni-catalyzed MOCVD [3]. The tapered nanowires range in diameter from 100 to 1000 nm, with lengths up to $\sim$ 30 microns. We measure 1-dimensional carrier diffusion lengths ranging from 200 to 1000 nm, depending on material and wire diameter. In addition, it is possible to map the luminescence that is waveguided to the end of the structure, directly imaging the waveguide modes. Initial results from imaging charge carrier drift under applied bias will also be presented.

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Magnetic resonance spectroscopy of single centers in silicon quantum wells

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Keywords: single centers, hydrogen, EPR, quantum well, silicon microcavity

The high mobility silicon quantum wells (Si–QW) confined by high temperature superconductor delta-barriers are of a great interest to be embedded in silicon microcavities for the studies of single centers by the electrically-detected magnetic resonance (EDEPR).

These single Si–QWs are prepared by the short-time boron diffusion that is carried out from the gas phase into 350 μm thick n-type monocrystalline Si(100)-wafers with resistivities 20Ω cm. The wafers are previously oxidized at 1150°C in dry oxygen containing CCl_4 vapors. Impurity doping is done during five minutes into windows, which are performed in the Hall geometry by cutting in the oxide overlayer after the preparation of a mask and subsequent photolithography. Using the four-point probe, SIMS, Cyclotron Resonance (CR), Infrared Fourier spectroscopy and Scanning Tunneling Microscopy (STM) techniques, the ultra-narrow, 2 nm, a single p-type Si–QW confined by the delta-barriers heavily doped with boron has been identified. Besides, the ESR studies show that the delta barriers appear to consist of the trigonal dipole centers, $B(+) - B(-)$, which are caused by the negative-U reconstruction of the shallow boron acceptors, $2B(0) \Rightarrow B(+) + B(-)$. The temperature and magnetic field dependencies of the resistance, thermo-emf, specific heat and magnetic susceptibility demonstrate the high temperature superconductor properties for the delta barriers that seem to result from the transfer of the small hole bipolarons through these negative-U dipole centers of boron, which cause the GHz generation under applied voltage or optical pumping with the enhancement by varying the dimensions of doping area. Spectroscopic studies confirmed this pattern and furthermore the STM images have demonstrated that the SQW is incorporated into the microcavity system of the fractal type formed by the microdefects of the self-interstitials type. This silicon microcavity is revealed by the angle-resolved transmission spectra that exhibit the excitonic normal-mode coupling (NMC) regime with a single Si–QW in the spectral range of the Rabi splitting at $T = 300$ K. The silicon microcavity of the fractal type is able to exhibit a tuning of the absorption and emission line positions in the ranges $1.2-5.5$ μm, $8.1-17$ μm, $18-27$ μm, which seem to be revealed by the transmission and electroluminescence spectra. Therefore, this series of microcavities in the NMC regime has been used to develop new methods of the analysis of the properties for the residual centers related to hydrogen, oxygen and carbon, which are in wide use to prepare semiconductor nanostructures. The first test was to observe the angle-resolved transmission spectra of the Si–QW microcavity structure in the range $7.5-10$ μm that seem to reveal bound excitons related to the hydrogen molecule-oxygen center, which is created by the localization of the hydrogen molecule at natural atomic oxygen under thermal treatment. Besides, the high efficient bound exciton absorption and photoluminescence in the range of the Rabi splitting allow the identification of other single centers embedded in the Si–QW such as the C–H center and the carbon interstitial-related center. Finally, the GHz generation induced by the voltage applied to the delta barriers is used to observe the EPR spectra of these single centers by magnetic field scanning in the absence of external resonator.

Tue-B-3.4i

Optical properties of Si/Si:Er multi-nanolayer structure grown by SMBE method

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Keywords: Si:Er, nanolayers, SMBE, optical gain, photonics

Among Er-doped crystalline Si materials, Si/Si:Er multi-nanolayer structures grown by sublimation molecular beam epitaxy (SMBE) technique [1] present extraordinary optical properties. After appropriate annealing procedures, characteristic spectrum comprising only a few intense lines is formed with very narrow linewidth of DE < 8 meV at 4 K, the smallest value ever measured in RE-doped semiconductors. Based on this spectrum, the splitting of the ground state of Er^{3+} ions and the presence of only a single type of Er-related optical center, labeled Er-1, have been conclusively established [2, 3].

In this contribution, we will review the unique optical properties of Si/Si:Er multi-nanolayer structures. In particular, we will present:

Preferential formation of the Er-1 center and its microscopic structure [2, 3].
Level of optical activity of Er [4].
Direct evidence of an Er-related donor level and its effects on optical properties [5].
Microscopic evidence for the role of oxygen in Er-related emission [6].
Terahertz transitions within the ground state multiplet of Er^{3+} [7].

Finally, we will also report on the most recent results on optical gain in Si/Si:Er multinanolayers. By comparison of photoluminescence intensities from the variable stripe length (VSL) and the shifted excitation spot (SES) experiments, we will show that induced absorption cross-section of free carriers is about 4.3×10^{-18} cm^2, which precludes observation of the net optical gain.

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Wed-B-1.1i

Massive point defect redistribution near semiconductor surfaces and interfaces and its impact on Schottky barrier formation

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Keywords: defect, interface, ZnO, Schottky barrier, segregation

Until now, native point defects in semiconductors were not considered a significant factor in Schottky barrier formation due to their relatively low bulk densities. Instead, many theories have postulated localized states, including adsorption-induced defects, at the semiconductor surface with high enough densities to “pin” the Fermi level. It is now possible to measure the energies and densities of point defects below the semiconductor free surface and its metal interface with nanoscale precision. Using depth-resolved cathodoluminescence spectroscopy (DRCLS) of deep level emissions calibrated with deep level transient spectroscopy (DLTS) as well as capacitance-voltage ($C-V$) measurements of free carrier densities — all at the same interface, we can now demonstrate that native point defects can (i) increase by orders-of-magnitude in densities within tens of nanometers of the semiconductor surface, (ii) alter free carrier concentrations and band profiles within the surface space charge region, and (iii) dominate the Schottky barrier formation for metal contacts to ZnO and many other single crystal compound semiconductors. Previously we used this combination of techniques to show that surface adsorbates, hydrogen donors, and subsurface native point defects each contribute independently to interface charge transport and Schottky barrier formation [1]. Furthermore, metal deposition [2] and subsequent annealing [3] induce additional native point defects extending tens of nanometers or more below the free ZnO surface that increase tunneling, recombination and hopping transport. These effects are orientation-dependent, with significantly higher defect and free carrier densities below the free (000-1) O face versus (0001) Zn face and their interfaces with many different metals [4].

The spatial redistribution of electrically-active defects within the surface space charge can be understood in terms of temperature-dependent atomic diffusion enabled by low formation energies and driven by strain and electric fields as well as metal-specific chemical reactions near room temperature. Self-consistent electrostatic calculations based on subsurface trap distributions, energies and carrier densities yield a wide range of effective Schottky barriers, in agreement with measured values for different metals on a wide array of ultrahigh vacuum clean ZnO crystals grown by various methods. These results are not unique to ZnO. Indeed these sub-surface and near-interface native point defects dominate the Fermi level movement across the band gaps of most compound semiconductors. We will discuss this dramatic native defect redistribution and its electronic effects using first-principles calculations of interfacial segregation [5] and migration barriers [6].

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Wed-B-1.2o

Role of the surface in the electrical and optical properties of GaN

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Keywords: GaN, surface photovoltage, photoluminescence, photoadsorption

In spite of significant progress in the development of wide-band-gap semiconductors for optoelectronics, the detrimental effect of the surface on the electrical and optical properties of materials and devices based on these semiconductors is often underestimated. In particular, a depletion region caused by upward bend bending near the surface can affect device properties. The height of the near-surface barrier and the width of the depletion region are ambient dependent. We have studied the effect of temperature and different ambients (air, oxygen, nitrogen, and vacuum) on the electrical and optical properties of undoped and Si-doped GaN in an original set-up based on a high-vacuum Kelvin probe system combined with an optical cryostat. The value of band bending at the surface and its change due to illumination (photovoltage) were studied with the Kelvin probe. Complementary information about the depletion region and carrier recombination paths was obtained from the analysis of photoluminescence (PL) measured using the same experimental conditions. We observed the surface photovoltage (SPV) signal at photon energies between 1.2 and 4.0 eV, with the maximum value of 0.7 V at photon energies close to the GaN bandgap, indicating that the initial (dark) upward band bending decreased by at least 0.7 eV under UV light with an intensity of about 0.03 W/cm^2. In the intensity range from 10^{-9} to 10^{-2} W/cm^2 the SPV signal increased as a logarithm of the light power. In air or oxygen gas ambient the SPV signal under near-band-edge illumination increased quickly to a maximum and then gradually decayed while illumination of the sample continued. In contrast, in vacuum or nitrogen gas ambient the SPV signal continuously and slowly increased under UV illumination. To explain these effects we propose that in air the UV light assists adsorption of oxygen species (photo-induced adsorption), whereas in vacuum it causes the desorption of negatively charged species from the surface. These observations are consistent with PL transients under continuous illumination with a UV laser: the PL intensity gradually decreases in air (depletion region width increases due to photoadsorption of oxygen), whereas it increases in vacuum (depletion region width decreases due to photodesorption of oxygen).

Wed-B-1.3i

Energy state distributions at oxide-semiconductor interfaces investigated by Laplace DLTS

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Keywords: SiO2/Si interface, Pb centres, dangling bond, Laplace DLTS

The dangling bond represents one specific case among the various point defects observed in bulk silicon and these defects have well-defined electronic levels in the band gap. At disordered interfaces the lattice mismatching results in dangling bonds (here referred to as P_b centers) forming a rather broad distribution of energy states. Electron-Spin Resonance measurements revealed the existence of two types of centers, termed P_{b0} and P_{b1}, only slightly differing in the structure. The P_{b0} state has been identified as related to a $\langle 111 \rangle$ oriented dangling bond of the interfacial silicon atom bonded to three other silicon atoms, while in the case of P_{b1} the dangling bond orientation is $\langle 211 \rangle$ as a result of the oxygen atom(-s) bridging the second nearest bond(s) to the silicon dangling bond. Only P_{b0} states were observed at the (111) and (110) oriented Si/SiO$_2$ interfaces while both types of P_b's were observed at (100) Si/SiO$_2$.

In this study the energy distribution of the P_b centers at the Si/SiO$_2$ interface has been determined using isothermal current Laplace DLTS [1] for the (100), (111) and (110) orientations. The (111) and (110) distributions are similar and centered at 0.38eV below the silicon conduction band. This is consistent with only P_{b0} states being present. For the (100) orientation two types of the interface states are observed; one similar to the (111) and (110) orientations while the other has a negative-U character in which the emission rate versus surface potential dependence is qualitatively different from that observed for $P_{b0}$and is presumed to be P_{b1}. The negative-U character of P_{b1} could explain the controversy as to whether the P_{b1} center has an energy level in the Si band gap.

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Wed-A-2.1o

Formation of vacancy and oxygen containing complexes in Cz-Si by rapid thermal annealing

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Keywords: silicon, quenching, vacancies, oxygen, FTIR

Introduction of vacancies (V) and oxygen (O) containing complexes (V_nO_m), previously known only from radiation experiments, is reported in the presented work as a result of rapid thermal annealing (RTA) of Si wafers without applying any irradiation. The creation of such complexes due to interaction of thermally induced V with O during fast cooling (quenching) was expected many years before, from both the physical consideration of the quenching processes on the atomic scale and from the very reliable technological effect of the enhancement of thermally induced O precipitation in Si after treatment with RTA. Such enhancement of precipitation implied that V-containing point defects should be created after RTA acting as the nucleation centers for O precipitation. Nevertheless, the existence of V_nO_m after RTA remained still not established experimentally. Probably, the insufficient sensitivity of the vibrational absorption infrared spectroscopy, mainly used as a selective method for monitoring of V_nO_m in radiation experiments, was the key reason for the lack of the experimental confirmation of interaction of thermally induced V with O atoms in Si.

In the present study, a modernized method of Fourier Transform Infrared (FTIR) spectroscopy was applied, with a sensitivity exceeding in approximately two orders the conventional FTIR [1]. Industrial grade Si wafers and industrial grade RTA equipment were used to perform RTA in clean room conditions. The usage of half wafers during RTA processing and the usage of the second untreated part of the same wafer as a reference during precise differential FTIR measurements allowed us to reveal, quite reproducibly, the small RTA-induced changes in the absorbance on the level of ca. 1E-5 in absorbance units. Special attention was paid in order to separate the real contribution from the bulk from the possible surface related contribution in recorded differential absorbance spectra. The surface-to-bulk absorbance ratio was changed for this aim by changing optical path length, angle of incidence, and polarization.

As the result, the quantitatively reproducible absorption bands of known V_nO_m were revealed in each of the examined wafers after RTA. The concentration of the observed complexes was ca. 1E13 cm-3 as estimated from the bandwidth rescaled calibration factor for interstitial oxygen (O_i). Additionally, changes in other O states

(O_i, O_{2i}, O_{3i}) after RTA were monitored. The obtained results agree quantitatively with some previous theoretical considerations of “frozen-in” V_nO_m.

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Wed-A-2.2o

Microscopic mechanisms behind efficient self-healing of ZnO

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Keywords: vacancy clusters, self-healing, implantation, positron annihilatio spectroscopy

The wide band-gap of ZnO ($\sim$ 3.4 eV at 10 K) makes it suitable for the construction of opto-electronic devices working in the blue-ultraviolet wavelength range. Its physical and chemical properties and the progress in crystal growth processes have renewed the interest on this material. The material shows a remarkable radiation hardness and the amount of damage created in these room-temperature irradiations is two orders of magnitude lower than in GaN [1, 2].

Vacancy defects are introduced in typical material processing steps, either during growth or post-growth treatments such as ion implantation and subsequent thermal annealing. Electron irradiation experiments have shown that irradiation damage in high-purity ZnO can be removed in thermal treatments already at around 300°C [3], while temperatures up to 700°C [4] are required when significant amounts (above 10^{17} cm^{-3}) of Li are present in the material. Irradiation-induced single vacancy defects have been shown to cluster very efficiently when the induced vacancy concentration increases above 10^{19} cm^{-3}, again indicating fast and easy movement of the lattice damage already at room temperature [5]. Interestingly, Li ion implantation-induced heavy damage can be removed by slow thermal treatments at temperatures around 800°C, while millisecond-range flash annealing in temperatures 900–1200°C result in efficient clustering of vacancies [6].

Positron annihilation spectroscopy is a powerful technique for studying vacancies and vacancy clusters. We will present experimental results on the thermal evolution of the lattice damage created in N and Li implantation of ZnO already containing Li, an important impurity in commercially available hydrothermal ZnO substrates. The results show that the catalytic properties of Li in vacancy cluster formation inhibit the efficient self-healing of ZnO. The interaction of Li with the V_{Zn}, or its lack, could help determining the microscopic mechanisms leading to the apparent radiation hardness of ZnO.

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Wed-A-2.3o

Amorphous diamond synthesized from graphite by shock compression

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Keywords: diamond, graphite, defect, irradiation, shock compression

We report the discovery of a novel pathway for the transformation from highly oriented pyrolitic graphite foils into amorphous diamond platelets [1]. The transformation from graphite to diamond is a long time issue. Recently, polycrystalline diamond of 10–20 nm across, which exhibits an excellent hardness, was synthesized by direct conversion of graphite under static high pressure and temperature [2]. By utilizing shock compression, the ultimate smallest crystalline size of diamond was synthesized from C_{60} fullerene and labelled as “amorphous diamond” [3]. However, graphite has not been found to transform into amorphous diamond but to crystalline diamond by martensitic mechanism [4]. Here, we show a transformation from graphite to transparent amorphous diamond tiles for the first time. The platelets are transparent and show photoluminescence but no diamond Raman peak. This pathway consists of three stages of neutron irradiation, shock compression, and rapid quenching. Pre-irradiation of graphite with high energy neutron is the key to success. Wigner defects produced by irradiation are considered to work as the nucleation sites for diamond [5]. The combined method of irradiation and shock compression should be a promising way to synthesize new carbon materials such as the amorphous diamond.

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Wed-A-2.4o

Depth profile of donor-acceptor pair transition revealing its effect on the efficiency of LEDs

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Keywords: GaN, light emitting diode, quantum well, donor-acceptor pair, cathodoluminescence

Group-III nitrides are probably the most promising compound semiconductors to produce full spectrum light emitting diodes (LEDs) and laser diodes (LDs). Recent research has focused on the challenge to bridge the “green gap”, the relative efficiency underperformance of the system in the green spectral region. The challenge in growth technology to accommodate very dissimilar materials properties for GaN and GaInN alloys of barriers and quantum wells, respectively, leaves ample opportunity for the generation of line and point defects which are likely to act as non-radiative recombination centers.

Our efforts to develop light emitters for the 500–580 nm spectral region first concentrates on reducing high densities of dislocations (threading, misfit dislocations and stacking faults). This proved critical also to avoid alloy in homogeneities and premeditated phase separation. Substantial strides have been achieved by homoepitaxial growth on thick HVPE-grown polar c-axis GaN templates that with process optimization reproduces the low threading dislocation density of the bulk (5×10^6 cm^{-2}) into the epitaxial layers. By the availability of such thick templates, we now have even been able to claim the same perfection for non-polar m-axis and a-axis growth. Such achievements indeed result in substantial LED efficiency gains, yet detrimental shunt processes seem to dominate recombination nevertheless. This brings into consideration point defects such as dopant impurities.

In low temperature luminescence pronounced donor acceptor pair (DAP) recombination is frequently observed. In order to evaluate their role, we evaluated their correlation with LED device performance and depth resolved cathodoluminescence. By the implementation of a ternary GaInN alloy layer with variable bandgap energy inside the LED active region, we find conditions under which DAP recombination can be suppressed and LED performance simultaneously enhanced. This provides evidence for possible charge transfer mechanisms between the different recombination schemes and could possibly point at the role of defect recombination as well at approaches to ameliorate such loss processes.

We draw on the collective experience of epitaxial growth, defect and device characterization efforts to identify new opportunities to overcome the remaining hurdles for full scale deployment of group-III nitride based solid-state lighting for energy efficiency.

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Wed-A-2.5o

Rich formation of defects in ZnO via an attractive interaction between O vacancies and Zn interstitials

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Keywords: ZnO, n-type doping, O vacancy, Zn interstitial, theory

It is well-known that O-deficient ZnO can easily become n-type even without the introduction of any intentional dopants. The mechanisms leading to the n-type behavior are, however, still controversial. Even though native defects resulting from this deficiency have been excluded as the main source of the high free electron density, the n-type conductivity of ZnO is seen to be closely related to its O deficiency which manifests itself through the formation of O-vacancy and/or Zn-interstitial defects. In this work, we propose that as the concentration of intrinsic defects in ZnO becomes sufficiently high, interactions between defects leads to a significant reduction in their formation energies. In particular, we show that the formation of both O-vacancy and Zn-interstitial in O-deficient ZnO becomes significantly enhanced by a strong attractive interaction between them, making these defects an important source of n-type conductivity of ZnO [1].

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Wed-A-2.6o

Raman lasers due to scattering on donor electronic resonances in silicon

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Keywords: silicon, Raman, laser, terahertz

New principals to generate stimulated emission in terahertz frequency range from silicon doped by shallow donor centers have been demonstrated. Lasing in the frequency bands covering the range of 5.0–6.7 THz, has been achieved from silicon crystals doped by all group-V donors under optical pumping by radiation of frequency-tunable mid-infrared free electron laser at cryogenic temperatures. Analysis of the data shows that the emission corresponds to Stokes-shifted Raman-type lasing. The Stokes shift is determined by the 1s(E)-1s(A_1) donor electronic resonance.

Wed-A-2.7o

Strength and dislocation mobility in wide bandgap semiconductors

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Keywords: wide bandgap, dislocations, strength, GaN, ZnO

Dislocations lead to spatial variations in the electrical and optical functions of a semiconductor crystal and can be the cause of degradation of devices. Dislocations are induced into a crystal under stress by means of generation followed by multiplication during crystal growth and device fabrication processes. Thus, a great deal of effort has been made to understand details of the dynamic behavior of dislocations as well as the relation of their electrical and optical properties in semiconductors. In contrast to diamond and sphalerite structure semiconductors such as Si, GaAs, and so forth, knowledge of the dynamic behavior of dislocations is far more limited in recent wide band-gap semiconductors with a hcp-based wurtzite structure which are recently increasing significance in a wide range of applications for optoelectronic devices with a blue to ultraviolet wavelength range operating around room temperature and for high power devices.

We herein summarize our recent results on mechanical strength of various wide bandgap single crystals (GaN, ZnO, ZnSe) obtained by a conventional compressive deformation method at elevated temperatures. The dislocation mobility in wide bandgap crystals together with that in some elemental semiconductors and IV–IV, III–V, and II–VI compound semiconductors is evaluated and discussed.

II–VI compounds ZnSe and ZnO can be deformed under a stress around 10–20 MPa at low temperatures 150–400 and 650–850°C, much lower than that of GaN and SiC, commensurate with the mechanical instability of these materials. Dislocations are highly mobile in ZnSe and ZnO since the activation energies for dislocation motion in the crystals are evaluated to 0.5–0.7 and 0.7–1.2 eV and those for dislocations 2–5 eV in GaN and SiC. It is found that the activation energies for the motion of dislocations within various groups of semiconductors maintain a linear dependence on the band-gap energy with clear distinctions among the elemental and IV–IV, III–V, and II–VI compound semiconductors, irrespective of the crystal structure, being diamond, sphalerite, or wurtzite.

Wed-B-2.1i

Strange lifetimes of the vibrations of interstitial oxygen in SiGe alloys

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Keywords: SiGe, oxygen, vibrations, lifetime

To our knowledge, there are no data available on the decay of vibrations of impurity atoms in semiconductor alloys. Given the considerable amount of data available for the vibrations of interstitial oxygen in crystalline silicon, a suitable candidate for investigation appears to be oxygen in dilute SiGe alloys ([Ge] less than 7%).

We show that pump-probe measurements in SiGe alloys give lifetimes at low temperature of $\sim$120 ps for the 1136 cm^{-1} band in SiGe alloys, even when the Ge content is only 1%. This figure contrasts with the 10 s of pico-seconds observed for oxygen in crystalline silicon [1]. Surprisingly, the lifetime is the same for all excitation wavelengths within the alloy-broadened 1136 cm^{-1} band. The lifetime is close to that reported in crystalline Ge, of 115 ps [2], which we show is quantitatively compatible with a simple three-phonon de-excitation process.

Quantitative analysis of the vibrational bandshapes for oxygen in SiGe alloys shows that the coupling of the ν_3 (1136 cm^{-1}) and the low energy ν_2 modes is severely quenched in the alloys, as first found by Yamada-Kaneta [3]. This effect can result in strange effects at $T > 0$ K, such as the bandshape in the alloy being sharper than in the crystalline material. However, we have not yet identified any mechanism local to the oxygen that can lengthen the lifetime.

It appears that the long lifetime in SiGe alloys is a result of the lifetime of the 1136 cm^{-1} mode being critically dependent on the maximum lattice frequencies, and even at a small alloy composition, a three phonon process is required rather than the faster two-phonon process that may occur in crystalline silicon.

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Wed-B-2.2o

Trivacancy and trivacancy-oxygen complexes in silicon

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Keywords: silicon, trivacancy, energy levels, DLTS, modeling

High-resolution Laplace DLTS and ab-initio modeling have been used to determine the energy levels and structure of the trivacancy (V_3) and trivacancy-oxygen (V_3O) defects in Si.

Phosphorus doped Si samples with different concentrations of oxygen and carbon were irradiated with 6 MeV electrons at 25°C and subjected to isochronal and isothermal anneals in the tempearature range 50–400 °C. Two electron traps, E4 and E5, with activation energies for electron emission, E_n, 0.36 and 0.46 eV and present in equal concentrations were observed in the DLTS spectra of all the irradiated samples. Disappearance of the traps upon annealing of the samples in the temperature range 50–100°C occurred simultaneously with the appearance of another electron trap with $E_n = 0.075$ eV (E_{75}). An application of forward bias injection with $I = 10-15$ A/cm^2 at 300 K to the irradiated and annealed p$^+$–n diodes resulted in the complete regeneration of the E4 and E5 peaks and the disappearance of the E_{75} trap. Multiple annealing/injection induced transformations between the state giving rise to the E4/E5 pair and that responsible for the E_{75} trap occurred without any loss in magnitudes of the corresponding DLTS signals. It was found from Laplace DLTS measurements under uniaxial stress that the center responsible for the E_{75} trap has trigonal symmetry. Heat-treatments of the irradiated oxygen-rich Si samples in the temperature range 200–275°C resulted in the disappearance of the E_{75} trap (or the E4/E5 pair) and appearance of another pair of electrons traps, E4* and E5*, with E_n values of 0.34 and 0.455 eV. It is argued that the E4/E5 pair and E_{75} trap are related to acceptor levels of V_3 defect in two configurations, and the E4*/E5* pair to the V_3O complex.

*A*b-initio density functional studies have been carried out and a detailed picture of the electronic structure of the V_3 and V_3O complexes is presented. The calculations confirm that V_3 is a bistable complex. While planar $V_3[C_{2v}]$ stands as the ground state structure for positive and negative charge states, the extended trigonal $V_3[D_3]$ atomistic structure has lower energy in the neutral charge state. The presence of Si dangling bonds in $V_3[C_{2v}]$ induce deep acceptor and donor levels which are predicted to lie at $E(-/0) = E_c - 0.38$ eV, $E(-/0) = E_c - 0.50$ eV and $E(0/+) = E_v + 0.24$ eV. On the other hand, the four-fold coordination nature of $V_3[D_3]$ structure leads to a single shallower electron trap at $E(-/0) = E_c - 0.23$ eV. These results support the assignment of E4, E5 and E_{75} to $V_3[C_{2v}](=/-)$, $V_3[C_{2v}](-/0)$ and $V_3[D_3](-/0)$, respectively. Interstitial oxygen is predicted to act as an efficient trap for V_3 complexes. The binding energy is estimated as 1.8 eV and the electronic structure of V_3O is rather similar to that of V_2O. Energy levels of V_3O are calculated to be at $E(=/-) = E_c - 0.27$ eV, $E(-/0) = E_c - 0.42$ eV and $E(0/+) = E_v + 0.22$ eV.

Wed-B-2.3o

Trivacancy-oxygen complex in silicon: local vibrational mode characterization

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Keywords: silicon, infra-red, radiation damage, oxygen

Infrared (IR) absorption spectroscopy has been known to be a very powerful tool in studies of oxygen-related defects in Si (e.g. see [1] and references therein). However, regarding the multivacancy-oxygen-related defects (V_nO, $n \geq 2$) previous IR absorption studies have not led to a clear and self-consistent picture. One of the main reasons is that all members of the V_nO family contain a Si–O–Si bonding structure like the one in VO. The vibrational bands of V_nO centers appear in a close vicinity of the main VO band and they are hardly distinguishable in the absorption spectra.

In the present work a careful FTIR study of the evolution of multivacancy-oxygen-related defects in the temperature range 100–350°C in Czochralski-grown Si samples irradiated with different particles (2 and 10 MeV electrons, 5 MeV neutrons) has been carried out. The spectra were measured at 20 K and at room temperature. A clear correlation between disappearance (upon annealing) of the divacancy (V_2) related absorption band at 2767 cm^{-1} and appearance of two absorption bands positioned at 833.4 and 842.4 cm^{-1} at 20 K (at 825.7 and 839.1 cm^{-1} at room temperature) has been found. Both these two emerging bands have previously been assigned to a divacancy-oxygen defect formed via interaction of mobile V_2 with interstitial oxygen (O_i) atoms [2, 3]. The present study shows, however, that the two bands arise from different defects since the ratio of their intensities depends on the type of irradiation. The 842.4 cm^{-1} band is much more pronounced in neutron irradiated samples and we argue that it is related to a trivacancy-oxygen defect (V_3O) formed via interaction of mobile V_3 with O_i atoms.

Both defects, V_2O and V_3O are electrically active centres and possess deep states in the gap [4–6]. FTIR studies of the effects of illumination at low temperature allowed us to assign two weaker bands at 837.0 and 848.7 cm^{-1} to optically excited states of the V_2O and V_3O defects, respectively.

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Wed-B-2.4o

Electron paramagnetic resonance of boron in silicon revisited

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Keywords: magnetic resonance, silicon, isotopes, shallow acceptors

Electron paramagnetic resonance (EPR) has contributed extensively to the current understanding of shallow donor states and of defects in silicon already in the early days of semiconductors. In contrast, EPR studies of shallow acceptors have been impeded by the fourfold degeneracy of the acceptor ground state which is easily lifted by any symmetry breaking perturbation, e.g. by randomly distributed, defect-induced local strains. This leads to strong inhomogeneous broadenings of acceptor related EPR lines. It was only in 1978, when Si became available with sufficient crystalline quality, that EPR of B acceptors in externally unstrained Si was reported for the first time [1]. Since then, a number of fundamental questions concerning the line shape, the magnitude of the residual broadening, and the substructure of the six EPR resonances that were assigned to transitions between the four Zeeman levels of the spin 3/2 acceptor state, have remained unsolved.

We show that local fluctuations of the valence band edge due to different isotopic configurations in the vicinity of the B acceptors can quantitatively account for all inhomogeneous broadening effects of B-related EPR lines in high purity Si with a natural isotope composition. For this, we adapt a theoretical model which has successfully been applied to understand the residual acceptor ground state splitting in the absence of a magnetic field as an effect due to the presence of different Si isotopes [2]. The crucial parameters for the excellent agreement between our model and the experimental data are the valence band offsets between pure ^{28}Si, ^{29}Si, and ^{30}Si which were extracted from calculations of the temperature dependence of electronic band states [2, 3]. Using our model to recalculate the residual acceptor ground state splitting in the absence of a magnetic field, we show that the 30% discrepancy between theory and the experimental value determined by phonon absorption spectroscopy, obtained originally in [2], is not due to an uncertainty in the values assumed for the valence band offsets but rather to an inaccuracy of the used acceptor wave function.

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Wed-B-2.5o

Switching the localized hole states by acoustic solitons

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Keywords: acoustic soliton, deformation, quantum well, acceptor

The strain induced effects are known to be an efficient tool to study fundamental properties of bulk semiconductors and nanostructures yielding information of their point-group symmetry, band structure, spin-orbit coupling, etc. During the last decade, there emerged the possibility to study strain induced effects at extremely short time scale of picosecond range. This could be done employing solitary acoustic waves (solitons) [1, 2].

Here we propose a new, mechanical, way for switching between degenerate states of carriers in semiconductors. We show that an acoustic soliton effectively interacts with localized hole and the soliton propagation through the area of hole localization leads to switching between states of the holes with different projections of angular momentum. The effect is analyzed here on the example of heavy holes localized at shallow acceptors in silicon-based quantum wells where the ground state of the heavy hole is twofold degenerate (excluding spin).

Microscopically, the effect of conversion is caused by splitting of the hole states by elastic deformation of the soliton. Such a splitting introduces a phase shift between the split states. Therefore, after the interaction with the soliton, the final state of the hole differs from the initial one. In particular, the soliton of certain amplitude interconverts the localized holes with opposite projections of angular momentum.

The detailed microscopic calculations show that the amplitude of the strain soliton pulse required for the efficient switching is of order of 10^{-4}, which is typical for the acoustic solitons studied experimentally. Such an effect of switching, particularly between two easily distinguished states, can be of interest from fundamental point of view and may also be potentially utilized for information processing and storage.

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Wed-B-2.6o

Effects of group-V impurities on the elastic properties of silicon

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Keywords: silicon, strain, PAC, elastic properties

Besides reduction in device size the application of strained silicon in transistor design plays a crucial role in improving device speed and power consumption. Microscopic investigations are fundamental to understand the mechanical behaviour of strained Si layers, especially in combination with impurity atoms.

Thus, the influence of group-V impurities on the elastic properties of silicon was studied by means of the perturbed angular correlation (PAC) method using the acceptor ^{111}In as probe. This nuclear technique is well suited for studying strain on an atomic scale. After ion implantation of the group-V atoms and subsequent annealing in a rapid thermal annealing apparatus the Si samples were bent along the $\langle 110 \rangle$ crystal axis resulting in a uniaxial tensile strain.

The distortion of the cubic charge symmetry of silicon due to applied stress leads to an electric field gradient (EFG) at the probes site. From the corresponding quadrupole interaction (QI) frequency the resulting strain can be determined.

For nitrogen-implanted silicon the response of the crystal lattice to mechanical stress shows no difference to undoped samples, e.g. a linear stress dependence was found for the QI frequency. However, after implantation of the donors P, As and Sb a significant strain relaxation is observed. The experimental results are compared to ab initio calculations based on density functional theory (DFT) using the SIESTA code.

Thu-B-1.1i

On the threshold energy of atomic displacement in Si

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Keywords: point defects, threshold displacement energy, density-functional theory, molecular dynamics

The threshold displacement energy of a material E_d is the single most fundamental quantity in determining the primary state of radiation damage in any material. Knowing E_d in silicon is essential not only for the well-known use of the material in the manufacturing of semiconductor devices, but also because of contexts such as particle accelerators, where silicon elements in detectors are exposed to extensive hadron damage. In spite of this vast technological interest in the quantity, and its extensive study during the last few decades, the E_d averaged over all lattice directions remains poorly known in the material. Experimental methods show a widely varying scale of results for the average E_d in the range of 10–30 eV, and simulations carried out previously using classical potentials show a similarly wide range of results.

We have used Density Functional Theory (DFT) molecular dynamics (MD) simulations to study E_d in bulk Si. We calculated E_d with the DFT code SIESTA over all lattice directions. We found a global minimum of 12.5 eV for the minimum E_d, in excellent agreement with experiment, and a value of 36 eV for the average E_d [1].

We also showed that a large fraction ($\sim 65\%$) of the produced Frenkel pairs have a tetrahedral interstitial, even though the dumbbell is the ground state configuration for the isolated interstitial. This is because the formation energy of a close Frenkel pair is lower when the interstitial is tetrahedral rather than a dumbbell. Moreover, we found that the other dominating end state is the bond defect complex. If the bond defect is counted in as a stable defect, one obtains a lower threshold displacement energy than without counting it. The average threshold energy for producing either a bond defect or a Frenkel pair was found to be 24 eV, i.e. much lower than when only Frenkel pairs are considered.

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Thu-B-1.2o

Atomic and electronic structures of the deca-vacancy V_{10} in crystalline silicon

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Keywords: silicon, defects, electronic structures, spin polarization

Silicon has premier status in semiconductor technology and extensive research on its defects has been already reported. In particular, it has been established that the mono- and di-vacancies induce deep electron levels in the energy gap accompanied with Jahn-Teller (JT) type symmetry lowering distortion of surrounding atoms. As to the multivacancy V_n, however, clarification of its properties has been less pursued although its existence is indirectly evidenced through several experiments such as EPR or positron annihilation measurements. We here report first-principles calculations which clarify atomic and electronic structures of the deca-vacancy V_{10} which has been speculated to be abundant from a simple dangling-bond counting model [1] and later from more sophisticated calculations [2]. We have found that V_{10} is spin-polarized in its stable form with various charge states, virtually keeping tetrahedral (T_d) symmetry even after relaxation of surrounding atoms, in sharp contrast to the small vacancies.

Calculations have been performed with the local-spin-density approximation (LSDA) in the density-functional theory. We employ super-cell models with 216 or 512 atomic sites to simulate the V_{10} in an otherwise perfect crystal. Norm-conserving pseudo-potentials are used to describe nuclei and core electrons. Calculational parameters including the cut-off energy in the plane-wave basis set are carefully examined to assure the numerical accuracy. In the ideal (non-relaxed) V_{10}, 16 dangling bonds are generated. Structural optimization leads to 6 rebonds consisting of 12 dangling bonds in the ideal structure, but the remaining 4 dangling bonds are separated from each other by about 7Å, keeping overall T_d symmetry. These isolated dangling bonds induce deep levels near the valence band top and spin polarized in the stable structure. Addition of electrons or holes, i.e., negatively or positively charged V_{10}, induces further breathing-type distortion by which exchange-correlation splitting is substantially modified. We have found that the interplay of spin vs lattice renders the V_{10} a negative-U system, in contrast with the V_1 where the JT distortion is essential for its negative-U behavior.

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Thu-B-1.3o

Metastable interstitial complexes in silicon

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Keywords: silicon, interstitial defects, simulation

The kinetic pathways of self-interstitial clustering into bigger size complexes can involve metastable, rather than ground state configurations of interstitial clusters (as is the case e.g. with the rod-like defects in Si). In order to identify metastable clusters with energies only slightly higher than the ground state energy, one can, inparticular, apply long term molecular dynamics (MD) for tracing the kinetic behaviour of interstitial clusters, and pick up low-energy intermediate configurations from the simulation output for further rectification by ab initio techniques [1]. In this way one can identify both the ground state and the most frequent metastable cluster configurations, but its evident shortcoming is the sensitivity to the employed model of interatomic interaction. Unfortunately, long term calculations of interstitial kinetics with ab initio are too ambitios, so one has to rely upon description of atomic interactions in terms of tight-binding approximation [1], or semi-empirical potentials (e.g. [2]). This bears a risk of simply overlooking the relevant configurations, if these are not favoured by the particular interatomic interaction description used.

Here we apply the above-mentioned strategy to the investigation of di- to tetra-interstitials in silicon. The MD counterpart involves calculations with three most widely used semiempirical potentials, namely EDIP, Tersoff and Stillinger-Weber. we show that both the predicted lowest-energy cluster configurations and their kinetic behaviour are completely different for these potentials. The best correlation of MD predictions with the outcome of ab-inito based post-processing is obtained for EDIP potential. We compare our results to the earlier proposals for the ground states of di-, tri- and tetra-interstitials and discuss, whether small interstitial clusters can be considered as multi-configurational defects (i.e. with several metastable configurations of nearly the same energy as the ground state), like it has been recently reported for vacancy-type defects in silicon [3].

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Thu-B-1.4i

Quantum coherence and manipulation of phosphorus electron and nuclear spin states in silicon

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Keywords: phosphorus, silicon, quantum information processing, quantum coherence

Pulse EPR and ENDOR spectroscopy of phosphorus doped isotopically controlled silicon is reported.

We obtain extremely long coherence time $\sim$ 300 ms at 6 K of an electron spin bound to phosphorus and $\sim$ 3 s at 6 K of a ^{31}P nuclear spin in a high quality isotopically enriched ^{28}Si single crystal that has been depleted of ^{29}Si nuclear spins. Those coherence times in natural Si, which is composed of 4.7% of ^{29}Si nuclear spins, are much shorter suggesting that the background ^{29}Si nuclear spins are the dominant decoherence sources of phosphorus electron and nuclear spins. Theory predicts that the coherence time of nuclear spins should reach two times relaxation time of electrons. Indeed, such relation is confirmed with our isotopically controlled silicon with the least amount of phosphorus doping ($\sim 1 \times 10^{13}$ cm^{-3}). However, such relation breaks for higher phosphorus concentrations as shown in our systematic study varying the concentration between 1×10^{13} and 4×10^{15} cm^{-3}. Hopping conduction between phosphorus that increase with the concentration may be playing a major role in the electron relaxation.

Other surprising observation is the shift of ^{31}P nuclear transition energies (ENDOR peak positions) as we change the background silicon isotopic composition. Our analysis shows that the four nearest neighbor silicon isotopes of phosphorus affect strongly the nuclear transition energy of ^{31}P. Experimental results will be discussed in terms of isotopic mass and nuclear spin difference.

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Thu-A-1.1i

Donor level of interstitial hydrogen in semiconductors: deep level transient spectroscopy

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Keywords: experiment, group IV and compounds, defects, hydrogen, irradiation

The behavior of hydrogen in crystalline semiconductors has attracted considerable interest during several decades. Due to its high diffusion rate and ability to react with a wide variety of lattice imperfections such as intrinsic point defects, impurities, interfaces, and surfaces hydrogen is an impurity of fundamental importance in semiconductor materials. It has been already evidenced in previous investigations that the most fundamental hydrogen-related defects in-group IV semiconductors are interstitial hydrogen atoms occupying the bond center site (BC) or the interstitial tetrahedral site (T). Using first-principles calculations Van De Walle predicted similar properties of isolated hydrogen in other II-VI and III-V semiconductors. Another interesting prediction shown in that work was the existence of a universal alignment for the hydrogen electronic $(+/-)$ level. Until now there is no direct experimental information regarding the individual isolated hydrogen states and most reported properties have been inferred indirectly. In the present work *in-situ* conventional deep level transient spectroscopy (DLTS) and high-resolution Laplace DLTS techniques were used to analyze the resulting hydrogen-related levels after low-temperature proton implantation in different II-VI and III-V semiconductors including such as GaAs and CdTe. We demonstrate that using phenomenological observations the donor level of isolated hydrogen is found to keep almost a constant value in the absolute energy scale taking into account different band-offsets calculated for the whole group of semiconductors.

Thu-A-1.2o

Raman scattering on H_2 in platelets in silicon

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Keywords: silicon, platelet, hydrogen, molecule

Single-crystal silicon wafers exposed to a radio frequency hydrogen plasma are studied by Raman scattering. This treatment is known to result in formation of ordered planar defects called platelets [1]. In the present study, the {111} platelets filled with molecular hydrogen, H_2, are considered [2, 3].

The rotational transitions $S_0(J)$ for $J = 0, 1, 2$, and 3 are identified at 353, 587, 815, and 1034 cm^{-1}, respectively. Here, J is the rotational quantum number. At low temperatures, ortho-to-para conversion of H_2 trapped within platelets is observed and suggested to be caused by interaction of nearby H2 molecules. At 77 K, the ortho-to-para conversion was found to occur with the rate of 0.09 ± 0.04 h^{-1}. This is about a factor of 10 faster than in the case of interstitial H_2 in Si [4]. The contributions of the ortho and para hydrogen species to the broad band at 4150 cm^{-1}, which originates from vibrational transitions of H_2 in the platelets, are identified.

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Thu-A-1.3o

Defect-level pinning and shallow states of the muonium isotope of hydrogen

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Keywords: defect levels, hydrogen, muonium

Muonium (Mu) is well established as an experimental analog for the defect states formed by isolated hydrogen impurities in semiconductor materials. We recently reported [1] on the deep donor and acceptor levels obtained for Mu in six materials (Si, Ge, GaAs, GaP, ZnSe, and 4H-SiC) in which we have measured the ionization energies for the two separate neutral Mu centers observed in each. These Mu^0 states represent the neutral charge-states of hydrogen donors and acceptors, with the bond-centered (BC) site functioning as the donor and a tetrahedral interstitial (T) site as the acceptor location. Thus, the obtained ionization energies locate the Mu(+/0) and Mu(0/-) levels relative to the band edges. Using the band alignments of Van de Walle and Neugebauer [2], we find that the experimental defect-level energies for Mu in these materials are pinned at a constant energy, but approximately 0.4 eV above the predicted energy for the H(+/-) charge-state transition level after minor corrections are made for the differences in the H and Mu zero-point vibrational energies. This difference between the theoretical and experimental location of the (+/-) transition level implies that more materials may be subject to n-type doping by H, and fewer to p-type doping, than initially predicted. The fact that muon spin research (MuSR) methods probe the states formed during muon implantation and thermalization, well away from the equilibrium site and charge-state populations, allows access to numerous states not easily observable directly for hydrogen. We present our current understanding of deep vs shallow state formation for Mu in both the donor and acceptor sites, with emphasis on materials (Ge, InSb, GaSb, and InAs, for example) for which the theoretical results for H and experimental results for Mu are not presently in full qualitative agreement. Several aspects of the short MuSR experimental time scale are discussed along with questions raised for interpretation. The origin of small real differences that are expected for defect-level energies of H and Mu are discussed in evaluating how well the muonium energy levels should transfer to hydrogen in cases where no direct comparison is available.

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Thu-A-1.4i

Hydrogen in multi-crystalline silicon solar cells

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Keywords: hydrogen, Si, photovoltaics, infrared spectroscopy

The silicon photovoltaics industry has been growing at the rate of 40% per year. The Si materials that are often used to reduce cost give rise to defect issues that must be addressed. Hydrogen is commonly introduced into silicon solar cells to reduce the deleterious effects of defects and to increase cell efficiency [1]. A process that is widely used by industry to introduce hydrogen is by the post-deposition annealing of a hydrogen-rich SiN_x layer that is used as an antireflection coating [2]. A number of simple questions about this hydrogen introduction process and hydrogen's subsequent interactions with defects proved difficult to address because of the low concentration of hydrogen that is introduced into the Si bulk. We have used the fundamental knowledge of hydrogenated defects that has been revealed by recent investigations of impurity-H complexes to develop strategies by which hydrogen in silicon can be detected by IR spectroscopy with high sensitivity. The introduction of hydrogen into Si by the post-deposition annealing of a SiN_x coating has been investigated to answer simple but important questions about hydrogen's properties [3, 4] and its reactions with defects in multi-crystalline silicon solar cells. The work performed at Lehigh University has been supported by the Silicon Solar Research Center SiSoC Members through NCSU Subaward No. 2008-0519-02 and NSF Grant No. DMR 0802278.

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Thu-A-2.1o

Ab initio g-tensor calculation for paramagnetic surface states in μc–Si:H-based solar cells

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Keywords: magnetic resonance, solar cells, surfaces, DFT, g-tensor

Hydrogenated microcrystalline silicon (μc-Si:H) provides an interesting material for efficient and low-cost solar cells [1], which does not suffer from the notorious light induced degradation, known as the Staebler-Wronski effect. Best cell performance is achieved for material grown close to the transition to amorphous growth [2]. Consequently, it contains considerable amorphous fractions leading up to 10% degradation of the cell efficiency. For a further improvement of cell performance a detailed microscopic understanding of the efficieny limiting processes is crucial. Here, we focus on the reduction of the cell efficiency in highly crystalline μc-Si:H. The porosity of this material allows in-diffusion of atmospheric gases [3]. The main effects to consider are adsorption and oxidation on surfaces. Oxidation would provide a non-reversible process with the occurence of the ingerprint of the well-known Pb-centers (Si–O/Si interface dangling bond states [4, 5]), which are not observed in the electron paramagnetic resonance (EPR) measurements. On the other hand, adsorption of oxygen or water would be consistent with the observed reversible in?uence on conductivity and spin densities. However, if the observed increase of the EPR-resonance at $g = 2.0052$ [3] is directly related to the adsorped molecules or not is still in discussion. Adsorption of electron acceptor molecules will create a depletion layer at the surface which will result in a lower overall conductivity, equivalent to a lower-lying Fermi level A charge transition into a paramagnetic intrinsic surface state could then explain the observed increase of the ESR-signal. However, based on the present knowledge the alternative explanation via a direct relation to states of the adsorped species cannot be excluded. In order to elucidate this situation, we calculate the elements of the electronic g-tensor for plausible surface states from first principles, using a recently developed gauge-including projector augmented plane wave (GI-PAW) approach [6, 7] in the framework of density functional theory. Taking the spin-orbit coupling at the surface states explicitely into account our approach is shown to be able to distinguis between different surface states. Besides intrinsic dangling bond-like states on the [111] and [001] silicon surfaces also adsorped oxygen and hydrogen atoms are compared with the experimental ?ngerprints in order to clarify the microscopic origin of the intense $g = 2.0052$ EPR-signal providing a basic key for improved solar cell efficiencies.

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Thu-A-2.2o

Strong enhancement of defect photoluminescence in hydrogenated amorphous silicon upon intense optical pumping

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Keywords: defect generation, photoluminescence

A strong enhancement was discovered of the intensity of defect photoluminescence (PL) at room temperature of films from amorphous hydrogenated silicon containing oxygen (a- Si:H<O>) under powerful interband pumping. In this case, heating of the sample occurs at the laser spot increasing the local temperature to 500–600 K. The intensity of defect PL grew with the temperature exponentially with energy of activation about 0.9 eV. The threshold intensity of pumping after which the sharp increase in the intensity of defect PL was observed grew with decrease in the initial sample temperature. These and further experimental findings obtained from spectroscopic and kinetic investigations both of the intrinsic and defect PL showed that the growth of the intensity of defect PL was caused by the thermally induced creation of intrinsic defects (of the dangling bonds type) in a neutral charge state D^0.

Based on the universally accepted model of "hydrogen glass" [1, 2, 3] describing the thermodynamically equilibrium state of the a-Si:H matrix comprising the glass-like network Si-H and the rigid Si-Si network, we were able to understand the total scope of experimental findings. It was demonstrated that the study of defect PL at strong interband pulse excitation makes it possible to investigate the creation of thermally induced defects in the real time mode in the millisecond time range.

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Thu-A-2.3o

Hydrogen diffusion on graphene surface and related nanostructures

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Keywords: hydrogen, diffusion, nanostructure, graphene, doping

Graphene is an emerging material with many potential applications. To make the graphene an electronic material, hydrogen passivation is often required, for example, to eliminate edge dangling bonds. Although an infinite graphene sheet is a zerogap material, both fully hydrogenated graphene (also termed graphane) and edge-passivated graphene nanosegments are semiconductors. The need for hydrogen passivation raises an interesting question on how the hydrogen species actually transport through the graphene surfaces, which is a necessary step during any hydrogen treatment. So far, however, relatively little is known about the diffusion of hydrogen on graphene and related nanostructures.

We have studied hydrogen diffusion on graphene at the impurity limit, namely, the diffusion of a single hydrogen atom, by first-principles density functional theory calculations. It was found that the diffusion process depends strongly on the charge state of the hydrogen. Both the negatively charged hydrogen ion and the charge neutral hydrogen atom have similar diffusion barriers, being slightly higher than 1 eV. In contrast, the barrier for the positively charged hydrogen ion is only 0.6 eV. In other words, should hydrogen persist in the charge neutral state, there will be no substantial diffusion until at elevated temperatures, but even at room temperature positively charged H ions diffuse. Interestingly, at room temperature, there is a significant fraction of positively charged hydrogen ions on the graphene surface. This is not only because of the zero gap of the material but also because the singly occupied dangling bond state (locally associated with a neutral hydrogen atom) is high enough in energy to be thermally excited. Our calculation thus predicts a thermally activated diffusion process for hydrogen on graphene surfaces to be experimentally verified. On the other hand, on graphene nanostructures, due to the band gap of the materials, such an auto-ionization usually cannot take place. Nevertheless, positively charged hydrogen ion still possesses substantially smaller diffusion barrier over their charge neutral counterpart (and as a matter of fact the effect can be more pronounced in terms of percentage reduction). This opens the opportunity to control the hydrogen profile in graphene nanostructures via selective p-doping.

Thu-A-2.4o

Donor nature of native defects, surface states and hydrogen and in n-type CdO

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Keywords: oxides, hydrogen, particle irradiation, interfaces, experiment

The group-II oxide materials represent a rapidly emerging class of semiconductor compounds, with recent advances in growth producing high quality single-crystalline material that presents opportunities for a wide range of device applications. Research in these materials has largely focused on ZnO, which has enormous promise for devices such as light-emitting diodes. However, the smaller band gap compound CdO ($E_g \sim 2.2$ eV at the Brillouin-zone centre) has received far less attention, despite its potential in transparent electronics and its importance when alloyed with ZnO to extend the operation of ZnO-based devices into the visible spectral range.

By irradiating single-crystal CdO thin films with high energy He^+ ions to introduce native defects, an increase and then stabilization of the Fermi level at the charge neutrality level (CNL) is observed with increasing irradiation displacement damage dose. Consequently, we show that the CNL is located above the conduction band minimum in CdO [1]. Changes in the Fermi level as a function of annealing nominally undoped CdO samples in ultra high vacuum, and in atomic oxygen and hydrogen atmospheres are also investigated to provide information on the charge character of defects and dopants within this material [2]. In particular, hydrogen is observed to be a donor in CdO, as in ZnO, consistent with the CNL lying well above the particularly low Gamma-point conduction band minimum. Finally, we also observe that the surface Fermi level is above the bulk Fermi level, indicative of a surface electron accumulation layer. The properties of donor-type native defects, surface electron accumulation and hydrogen as a donor in n-type material are emerging as common properties of significantly cation-anion mismatched semiconductors, such as ZnO [3], InN [4], In_2O_3 [5] and SnO_2 [6]. While theoretical calculations of some or all of these phenomena have been performed for most of these semiconductors, theoretical investigations of defects in CdO have yet to be undertaken, but may be motivated by this experimental study.

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Thu-B-2.1o

Isotopic fingerprints of gold-containing luminescence centers in 28Si

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Keywords: isotopes, luminescence, deep defects, silicon

We have recently shown that the dramatic reduction in linewidth of many deep luminescence centers in highly enriched 28Si can lead to the observation of isotopic fingerprints, revealing not only that a specific element is involved in the defect complex, but also the number of atoms of that element [1–3]. This has lead to a number of surprises regarding the actual constituents of supposedly well known luminescence centers, as well as the discovery of an entire family of four-atom centers containing Cu, Ag and Au. More recently, we have also found that Li can be a constituent in these centers. There is as yet no detailed understanding of the stability of this family of defects, but progress has been made in understanding the prototypical Cu_4 center [4].

The isotopic fingerprint of Au is problematic, since only 197Au is stable, but we have now used the relatively long-lived 195Au to reveal the number of Au atoms in several of these centers. Our earlier suggestion [1] that the Cu_3Au center contains a single Au is found to be correct, and we find a further series of four-atom centers containing one Au plus Cu and Li. Surprisingly, the Au isotopic fingerprint also reveals a series of five-atom centers containing a single Au plus Cu and Li. Further evidence for the ubiquity of these four- and five-atom defects is provided by two previously observed [5] Pt-containing centers, with luminescence at 884 meV and 777 meV, which are found to contain three and four Cu atoms, respectively.

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Thu-B-2.2o

Electrical detection of phosphorus donor spin states in isotopically controlled silicon

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Keywords: phosphorus in silicon, electrically detected electron spin resonance, Bell state, isotope effect, low magnetic field

We demonstrate electrical detection of the Bell states formed by phosphorus electron and nuclear spins embedded in silicon (Si) bulk single crystals and of isotope effect using isotopically controlled ^{28}Si under low magnetic field (< 200 G). The Hamiltonian of the phosphorus in silicon is composed as the sum of the 1) electronic Zeeman, 2) nuclear Zeeman, and 3) hyperfine interaction terms. Extensive studies on Si:P have been performed recently using the conventional electron spin resonance (ESR) [1, 2] and electrically detected magnetic resonance (EDMR) [3, 4] with moderately high magnetic fields that realize four well defined states $|\uparrow\uparrow>$, $|\uparrow\downarrow>$, $|\downarrow\uparrow>$, and $|\downarrow\downarrow>$ where left and right symbols in each ket correspond to the states of the electron spin and nuclear spin, respectively. Because the Hamiltonian is dominated by the hyperfine term rather than the Zeeman terms at such low field, superposition states $\alpha|\uparrow\downarrow> +\beta|\downarrow\uparrow>$ and $-\beta|\uparrow\downarrow> +\alpha|\downarrow\uparrow>$ are formed automatically between phosphorus electron and nuclear spins and transitions between those superposition states and $|\uparrow\uparrow>$ or $|\downarrow\downarrow>$ states are observed clearly and magnetic field control of α and β is possible [5]. The degree of superposition can be controlled by the choice of B and becomes well known Bell states $1/\sqrt{}2(|\uparrow\downarrow> +|\downarrow\uparrow>)$ in the limit of $B = 0$. Moreover, we demonstrate isotope effect of electrically detected magnetic resonance (EDMR) of P doped isotopically controlled Si. A ^{nat}Si has non-nuclear spin free ^{29}Si with I = 1/2(4.7%). The ^{29}Si broadens a linewidth of electron spin resonance [1, 2]. In this study, we can successfully observe same ^{29}Si effect on electrical detected magnetic resonance spectroscopy. The sharpest linewidth is 0.24 G using an isotopically controlled ^{28}Si ($\sim$ 99.999%) sample.

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Thu-B-2.3o

Isotope effects on the resonant states of shallow acceptor in Si

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Keywords: spin-orbit splitting, acceptor, Si

The actual interest to accurate determination of Si band parameters is connected with access to monoisotopic high quality crystals. Within the past years the isotope effects on electronic band gaps and localized states of shallow donors and acceptors have been investigated for isotopically enriched Si and Ge [1-3]. The isotope shifts in the transition energies and ground state binding energies with changing of isotopic mass from ^{30}Si to ^{28}Si have been determined from absorption spectra for the shallow impurities [1].

We present the first high-resolution photoconductive investigation of the isotope effect for transitions of shallow acceptor B from ground to the excited resonant states related to the spin-orbit split-off valence band. We determine the ionization energy of the boron acceptor to the spin-orbit split-off valence band as 88.372 meV for ^{28}Si and 88.58 meV for ^{30}Si. Contrary to previous works [3] we obtain the dependence of spin-orbit splitting on host isotope mass. The spin-orbit splitting increases with increasing mass, as a result of electron-phonon interaction.

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Thu-B-2.4o

Electron paramagnetic resonance and dynamic nuclear polarization of ^{29}Si nuclei in lithium-doped silicon

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Keywords: silicon, lithium donors, electron paramagnetic resonance, dynamic nuclear polarization

Lithium atoms form shallow donor levels in silicon gap. Two electron paramagnetic resonance (EPR) spectra related to lithium atoms in silicon have been reported [1, 2]. First spectrum of trigonal symmetry with g-factors $g_{\|} = g_{[111]} = 1.9978$ and $g_{+} = 1.9992$ has been attributed to Lithium Oxygen (Li-O) complex in Czochralski grown silicon [1]. The second spectrum of tetragonal symmetry $g_{\|} = g_{[100]} = 1.9997$ and $g_{+} = 1.9987$ was observed in Floating-Zone (FZ) silicon crystals under uniaxial stress [2].

We report the results of EPR and dynamic nuclear polarization (DNP) experiments carried out with FZ silicon wafers doped with lithium by diffusion at 420°C in vacuum for 15 min, and in the same samples post annealed at 450°C during 2 hr in vacuum. It was found that the tetragonal Li EPR spectrum dominates in the samples after Li diffusion and well detected without external stress. After 450°C annealing the EPR spectrum of trigonal symmetry arises. In contrast to the phosphorus both Li related EPR spectra detected in the absorption mode are well observable at low temperatures 3.2–10 K. This shows that the Li electron spin-lattice relaxation time is shorter than that for phosphorus in silicon and DNP of the ^{29}Si nuclei due to the saturation of the Li EPR lines is expected to be more effective.

DNP due to solid-effect was observed in all investigated Li doped samples. The DNP enhancement (the ratio of DNP to equilibrium Boltzman nuclear polarization) was obtained about 618 at 10 K and 198 at 3.2 K corresponding to the ^{29}Si DNP degree of 0.41%. The nuclear polarization time was found about 3 hr. At such low temperature the DNP was not observed in silicon doped with phosphorus.

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Thu-A-3.1o

Subsurface satellite dislocation defects formed near InAs quantum dots buried in GaAs

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Keywords: quantum dot, dislocation, microscopy

Quantum dots (QDs) are now important elements of many semiconductor structures and devices. QDs are usually self-organized on the surface and then buried into the bulk by subsequent overgrowth. Since coherent QDs are desirable for most applications, formation of various defects associated with them has been extensively studied. This study, however, has been focused on the processes in and around strained QDs when they are formed on the surface.

In this paper we show that coherent strained state of a surface QD can be destroyed by subsequent overgrowth.

Theoretical analysis shows that the elastic energy of a stressed QD increases when the QD is buried. Under certain condition stress relaxation becomes energetically favorable, which may occur by formation of subsurface satellite subsurface defects near the QD. For a given mismatch between the QD and matrix, the relaxation onset depends on the QD size.

Our experimental research has been done with MBE InAs QDs self-organized on the GaAs (001) surface by Stranski-Krastanow mechanism. The growth conditions and nominal thickness of the InAs layers were varied in order to obtain the QD of various sizes. Then the QDs were overgrown by 300? thick GaAs layer. The buried QDs were examined by transmission electron microscopy (TEM). The TEM revealed three cases. (a) Coherent InAs QDs in GaAs. No stress relaxation occurs in this case.

(b) QDs with dislocations located at the QD/matrix interface and expanded to the free surface. It is likely that these dislocations were generated before the overgrowth procedure. (c) QDs with subsurface satellite dislocation defects. These defects seem to be generated in the bulk.

We analyze the origin of the observed defects and their relevance to the stress relaxation on the surface and in the bulk. The results of the experiment prove the theoretical prediction that stress relaxation by dislocation mechanism may occur not only during the QD formation on the growth surface, but also in the bulk during the overgrowth procedure. Eligible for the latter case are the QDs, which are subcritically stressed on the surface. They, however, become overcritically stressed in the bulk due to the theoretically predicted change in the critical conditions.

Thu-A-3.2o

Effects of dislocations on optical properties of wide bandgap GaN and ZnO

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Keywords: wide bandgap, dislocations, optical properties, GaN, ZnO

Dislocations cause spatial variations in electrical and optical properties and also their degradation of semiconductor devices. Thus, a great deal of efforts is being made in elucidating optical properties of dislocations and their modification through interactions with other defects in order to achieve high yield and efficiency of devices. In wide bandgap semiconductors there has been some experimental works mainly on the properties of grown-in dislocations, i.e., threading dislocations parallel to the growth direction c-axis generated as a consequence of deposition on a foreign substrate. Thus, it is interesting to clarify intrinsic optical properties of dislocations. This paper reports optical properties of GaN and ZnO in which dislocations are freshly induced by the plastic deformation at elevated temperatures.

Optical absorption spectra of plastically deformed GaN have been well understood for red-shift of the absorption edge in a model of the Franz-Keldysh effect by the electric fields associated with charged dislocations. Also, the near-band-edge (3.48 eV) photoluminescence intensity decreased remarkably, which was attributed to the introduction of high-density non-radiative recombination centers and the resulting reduction of free-carrier concentration. The yellow-band luminescence (2.22 eV) decreased due to plastic deformation, while several luminescence bands centered at 1.79, 1.92, and 2.4 eV developed. The dependence of photoluminescence features on deformation and subsequent annealing suggests that yellow luminescence is not related to the native structure of dislocations in GaN.

On the other hand, in ZnO plastic deformation did not influence the PL intensities related to the emissions from near-band-edge (3.354–3.39 eV) due to free excitons and to neutral-donor and acceptor bound excitons and also from mid-gap centers at 1.9–2.4 eV. Alternatively, new excitonic light emissions with photon energies of 3.100 and 3.345 eV developed with increasing dislocation density by the plastic deformation. Those emissions were attributed to the localized energy levels with the depths of 0.3 ± 0.1 or 0.05 ± 0.01 eV, respectively. The origin of the energy levels may be point defect complexes involving dislocations.

Thus, it is known that GaN and ZnO show quite different features of their optical susceptibility on dislocations and related defects.

Thu-A-3.3o

The electron and molecular processes on the surface of wide-bandgap oxides induced by photoexcitation of point defects

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Keywords: wide-bandgap oxides, point defects, spectral sensitization

The step-by-step experimental investigations of the mechanisms of interrelated processes in electronic and atomic subsystems of wide-bandgap oxides (Al_2O_3, MgO, ZnO, TiO_2) surface, illuminated in the UV–vis sub-bandgap range are presented. Point defects in wide-bandgap oxides absorbing in the region $1 < h\nu < 6$ eV are numerous and of varied nature. However the defects of F- type (an oxygen vacancy which captured one or two electrons) and those of V-type (a metal vacancy which captured one or two holes) are of special interest because of their capability to transform light energy into the chemical one.

Various complementary experimental methods such as: mass-spectrometry, thermodesorption spectroscopy, optical (diffusion reflectance), photoluminescence and electron spin resonance spectroscopies, as well as UV (8.43 eV) photoelectron spectroscopy, have been adapted to carry out in situ investigations in three phases: gas, adsorbate and solid state. Single crystals and dispersed powders of nominally pure oxides were irradiated by monochromatic light with the power of 10^{-3} to 10^{-1} W/cm^2 in the UHV $\sim 10^{-9}$ Torr or in a flow of pure gases (H_2, O_2, CO, N_xO_y) under a controllable pressure of $\sim 10^{-8}$–10^{-2} Torr.

The primary steps of electron subsystem excitation are the spectral-selective and site-sensitive excitations of the point defects accompanied with a charge transfer between excited states and the valence or the conduction bands, and terminated by chemical bonds breaking or/and bonds rearrangements on the surface.

The spectral and kinetic parameters of photoexcited centers and the structures of adsorbate complexes are determined for a number of studied oxides (Al_2O_3, MgO, ZnO, TiO_2). The role of photoactivated adsorption, desorption and chemical reactions acting as relaxation channels which compete with radiative and non-radiative decay is treated. Highly active oxygen species are created at photoactivated oxide surface, allowing oxygen vacancies to form or to heal and also to oxidize a number of adsorbed molecules.

We have demonstrated that point defects of F, F^+ and V-type can be used for self-sensitization of photocatalysts to a sub-bandgap spectral range on an example of NO_x/Al_2O_3 and $(NO + CO)/TiO_2$ systems.

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Thu-A-3.4o

Identifying sites for oxygen chemisorption on Si(100)(2×1):H surfaces with STM spectroscopy: an *ab initio* approach

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Keywords: hydrogenated silicon surfaces, oxidation, STM, density functional theory

It is known that hydrogenation of Si surfaces can postpone but cannot avoid oxidation. The main point to be settled concerns the preferred chemisorption site for O atoms in these H:Si surfaces [1–5]. Scanning Tunneling Microscopy (STM) can be a powerful tool for such investigations, and in particular is one of the most adapted techniques to perform complementary experimental-theoretical investigations of surface defects [6].

Here we show theoretical results for different O-impurity configurations on Si(100)(2x1):H that can serve as reference for such experiments. We use for that first-principles Density Functional Theory calculations within the Local Density approximation, and simulate Constant Height Scanning Tunneling Microscopy (STM) images [6–8]. We analyzed 5 different sites for insertion of the isolated Oxygen impurity. Our results indeed show that STM could be used to clearly distinguish between dimer and back bond O-insertion, and also from the silanol (Si–OH) configurations.

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Thu-A-3.5o

Structural study of low temperature grown superlattices of GaAs with delta-layers of Sb an P

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Keywords: LT-GaAs, superlattices, high resolution X-ray diffractometry

High resolution X-ray diffractometry was utilized to study gallium arsenide structures grown at low temperature (LT-GaAs) by molecular-beam epitaxy. A feature of the investigated structures is presence of thin (about 1 monolayer) delta-layers of antimony and phosphorus isovalent impurities, which were formed during low temperature epitaxy. Such delta-layers, being periodically placed in the bulk of the epitaxial film, give rise to the X-ray diffraction picture with a large number of interference peaks. Quantitative analysis of this picture allowed us to reveal information on the thickness, chemical composition and abruptness of the interfaces. Such analysis was done before and after annealing of the samples, which causes formation of the system of nanoinclusions (NI) of As in the bulk of the epitaxial film. Microstructure of As NI were studied by transmission electrom microscopy. We reveal the parameters of the rocking curves, which characterize the process of As NI formation. Formation of the NI As system in LT-GaAs(δ-Sb) was found to result in an enhanced decay of superlattice-related satellite peaks, which is probably due to increased roughness and intermixing of the Sb delta-layers. Such phenomenon was not observed in LT-GaAs(δ-P), which is likely due to absence of heterogeneous precipitation of As at phosphorus delta-layers and lower effective intermixing coefficient for As–P compared to As–Sb. For the samples with a combined system of Sb and P delta-layers the x-ray rocking curves quantitatively verify fabrication of superlattices, containing the As NI system, with mismatch of their averaged lattice parameter to that of GaAs substrate being less than 0.0001%.

Thu-A-3.6o

Hanle effect and spin-dependent recombination at deep centers in GaAsN

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Keywords: spin-dependent recombination, optical orientation

The paper is devoted to the study of a giant electron spin polarization achieved in nonmagnetic semiconductors at room temperature due to spin-dependent recombination through deep paramagnetic centers. Recently, we have found the extremely high optical spin polarization (about 90%) and spin memory ($\sim$ 1 ns) of free electrons in GaAsN alloys at room temperature [1–5]. We have explained these results by formation of nonlinear coupled system of free and localized spins and its dynamic polarization. The system arises due to spin dependent capture of free electrons on deep paramagnetic centres, which are formed under N incorporation into GaAs [2]. The proposed theoretical model [2, 4] qualitatively correctly describes the coupled spin-system. However, a careful fitting of the model parameters is needed to describe the system quantitatively.

In this paper, we measured spin lifetimes of free electrons and electrons bound on paramagnetic centers in GaAsN alloy with nitrogen content $x = 0.021$ using the Hanle effect (the depolarization of free electrons by a magnetic field B directed perpendicularly to the continuous-wave pump beam). Free-electron polarization was created under an interband absorption of circularly polarized light. We measured the steady-state degree ρ of circular polarization of the edge photoluminescence, which is proportional to free-electron polarization.

The measured Hanle curve $\rho\,(B)$ consists of narrow and wide parts which have the widths on the half-height $\approx$ 100 Gauss and $\approx$ 110000 Gauss. The difference between the widths by three orders of magnitude results from the strong difference in spin-life times of bound and free electrons, T_c and T. Using g-factor values of bound and free electrons +2 [2, 6] and +1 [5], respectively, we have found that $T_\mathrm{c} \approx 1000$ ps and $T \approx 2$ ps. The measured values of T_c and T allowed us to describe theoretically the experimental Hanle curve as well as its dependence on pump intensity.

The recent low-temperature measurements of the ODMR [6] revealed that paramagnetic self-interstitial defects Ga^{2+} are the origin of the efficient spin-dependent recombination and giant electron polarization in GaAsN alloys.

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Thu-B-3.1i

Progress towards understanding self-interstitial defects in Ge

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Keywords: self-interstitials, germanium, irradiation, Frenkel pairs

Self-interstitials and vacancies are the primary intrinsic defects in semiconductors. They are highly mobile and reactive, taking part in many defect reactions, mediating the diffusion of impurities and forming complexes stable up to very high temperatures. In Germanium, extensive experimental investigation on 1–3 MeV irradiated material have been carried out in an effort to clarify the properties of these basic defects, revealing a range of tantalising effects which remain difficult to understand [1, 2].

In this talk we will look into the findings of density-functional calculations, trying to understand how they can clarify the effects of radiation in Ge. Further, we suggest some of the reasons why radiation damage in Si and Ge seem to be strikingly different by contrasting the properties of the fundamental intrinsic defects in both materials.

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Thu-B-3.2o

Interstitial-related defect reactions in electron-irradiated Ge crystals: a DLTS study

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Keywords: germanim, self-interstitials, energy levels, DLTS

The electronic properties and structure of self-interstitials in Ge crystals are not well understood. In this work capacitance transient techniques have been used for identification of electrically active interstitial related defects in oxygen-rich and oxygen-lean n-type Ge crystals. The defects were induced in the samples by irradiation with MeV electrons at 80 K and at room temperature. Transformations of the defects upon post-irradiation isochronal and isothermal anneals were also investigated.

It is argued that in oxygen-rich Ge crystals the radiation-induced electron traps with energy levels at 62 meV and 80 meV below the conduction band edge are related to complexes of Ge self-interstitials with oxygen dimers ($\mathrm{I{-}O_2}$). The complexes were formed upon annealing of electron-irradiated Ge:O samples at $T > 50°\mathrm{C}$ and annealed out at temperatures higher than 140°C. The disappearance of the complexes resulted in a substantial decrease in concentrations of vacancy-related defects. It is found from the high-resolution Laplace DLTS measurements under uniaxial stress that the symmetry of the center, which gives rise to the $E_c - 0.06$ eV level, is orthorhombic (C_{2v}).

In the DLTS spectra of oxygen-lean Ge samples doped with different group-V impurities (Sb, P, As) and electron irradiated at 80 K two electron traps with energy levels at $E_c - 0.14$ eV and $E_c - 0.19$ eV were observed after anneals at temperatures higher than 300 K. Concentrations of these traps were comparable with those of the dominant vacancy-related defects, vacancy-group-V-impurity pairs. It is argued that the traps are related to a center incorporating a Ge-self-interstitial. Formation and annihilation kinetics of the traps were studied. Possible interstitial-related defect reactions in Ge crystals with different contents of impurities are discussed.

Thu-B-3.3o

Ab initio studies of Cu-H complexes in germanium

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Keywords: Mn in Ge, ab initio

We perform density functional-pseudopotential calculations upon substitutional Cu–H in large hydrogen-terminated germanium clusters, avoiding the underestimation of the band gap produced by the supercell method. Various configurations, in several charged states (2e to -3e), of H were investigated, namely the bond center between Cu and Ge, and the two anti-bondings positions of the Cu–Ge bond. But, the most stable configurations, for the negative charged clusters, were found for hydrogen on the C site (middle of the first nearest neighbours of substitutional Cu), in C_{2v}symmetry. For the neutral and positive charges the hydrogen is nearby the C site, in C_1 symmetry.

Thu-B-3.4o

Experimental and theoretical study of the solubility and diffusivity of the vacancy in Ge

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Keywords: germanium, vacancy, quenching, ab initio calculation, spectroscopy

Due to its high carrier mobility, there is a renewed interest to use Ge as active semiconducting layer in advanced electronic devices on Si substrates [1]. Successful growth and processing of Ge requires a good understanding of its intrinsic point defect properties which is not available. The present paper reports on the progress of a joint effort to determine the solubility, diffusivity and clustering of the vacancy in Ge.

Experimental data on the thermal solubility of vacancies in Ge are scarce and most are more than 40 years old. The largest amount of experimental data were obtained from quenching experiments assuming that the quenched-in vacancies are acceptors so that their concentration can be determined from resistivity changes (a compilation of the published results was given in [2]).

The formation energy of the vacancy in its different charge states has been calculated before using the VASP (with LDA+U approximation) and CASTEP codes [3, 4].

These results showed a remarkably good agreement between the calculated formation energy of the (double) negatively charged vacancy and the measured activation energy of the quenched-in defects.

In the present work quenching experiments are performed using state of the art n- and p-type Czochralski-grown Ge samples. The vacancy formation energy and thermal equilibrium concentration are determined using van der Pauw and Hall measurements. The results are compared with previously published ones and with recent predictions from ab initio calculations of the formation and migration energy of the vacancy. The quenched-in defects are characterized with DLTS, revealing also that the metal contamination level during quenching can be kept at least one order of magnitude below that of vacancy related quenched-in defects. FTIR analyses are performed in order to obtain more information on the nature of the quenched-in defects.

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Thu-B-3.5o

Quantitative evaluation of germanium displacement induced by arsenic implantation using germanium isotope superlattices

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Keywords: germanium, arsenic, ion-implantation, isotope, superlattice

Arsenic (As) implantation is used for the formation of shallow junctions in germanium (Ge) technology which is expected to realize new transistors because of higher carrier mobility in Ge than that in silicon (Si) and induces radiation damages that can significantly affect the redistribution of dopants during post-implantation annealing. The ion-channeling and cross-sectional transmission electron microscopy (XTEM) can only estimate the fraction of the Ge atoms displaced from the substitutional sites in the single-crystalline region. Such evaluation becomes almost hopeless in the amorphous region induced by the implantation.

This work reports the evaluation of the average distance of the Ge displacements as a function of the depth from the implanted surface both in the amorphous and single-crystalline regions using Ge isotope superlattices composed of alternating layers of natural Ge (natGe) and 70Ge stable isotopes. It enables precise determination of the degree of mixing of Ge host atoms induced by the implantation.

75As+ ions are implanted at 90keV with the doses of $1 \times 10^{13} - 1 \times 10^{15}$ cm^{-2} into 70Ge(5.00nm)/natGe(5.0nm) isotope superlattices grown by solid-source molecular beam epitaxy. When the implanted dose is 1×10^{13} cm^{-2} the alternating depth profiles are unperturbed even after the implantation. Note that the alternation of 70Ge and natGe with the periodicity 10 nm is an excellent depth standard for the depth profile of As and therefore so-called SIMS artifact (nock-on mixing etc.) can be removed completely. Higher dose implantation than 5×10^{13} cm^{-2} leads to mixing of the alternating layers. We have successfully developed a model based on convolution integral to simulate the SIMS profiles of mixed 70Ge and natGe to obtain quantitatively the characteristic length of Ge displacements as a function of the depth. Furthermore comparison with XTEM to measure the thickness of the surface amorphous layer created by implantation allows us to determine how amorphization correlates to the length of the Ge displacement.

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Thu-A-4.1o

Photocurrent studies of sexythiophene -based OFETs

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Keywords: organic FET, deep level spectroscopy

Photocurrent (PC) spectroscopy is proposed as a reliable tool in the investigation of the transport properties of organic thin film transistors (OFETs).

We have applied PC analyses to the study of the electronic density of states distribution (DOS) of the OFETs with crystalline mixed films of two derivatives of a conjugated molecule [a-sexithiophene (6T), and its alkylated analogue a,w-dihexylsexithiophene (DH6T)] as the active semiconductor. Our results on 6T and DH6T OFETs fabricated on different substrates (SiO_2 and Mylar) evidenced a close correlation between the distribution of the electronic density of states and the charge carrier population in the channel. The charge carrier mobility in organic semiconducting materials depends on the effective charge carrier density, which can be modulated, e.g., by gate voltage induced charge in a transistor geometry. We investigated the modifications in the DOS distribution associated to variations in the carrier density in the OFET channel and we detected the formation of deep electrically active states in the below-band-gap region, associated to polaron states induced by a prolonged exposure of the device to atmosphere. The observed deterioration of the macroscopic transport parameters of the OFET devices (reduction of the mobility and shift of the threshold voltage), was correlated to significant modifications in the distribution of the electronic density of states and in the activation of deep trapping states.

Thu-A-4.2o

Dependence of mobility on localized gap states in single-crystal organic field-effect-transistors

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Keywords: mobility, transistor, organic, defect

Recently, organic semiconductors have attracted great interest due to their potential for cost-effective, high-performance devices such as field-effect transistors (FETs), light-emitting diodes (LEDs), and solar cells. In order to optimize the performance of such devices it is important to study the fundamental charge transport mechanisms in the environment of crystalline material [1, 2]. For this purpose, the field-effect mobility, μ_{eff}, is a key parameter to relate electrical performance to a material parameter. We report measurements of the density of localized states in organic semiconducting crystals by a simple spectroscopic method, and relate these states to the field-effect mobility, μ_{eff}, of organic FETs. We find that μ_{eff} is parameterized by two factors, the free-carrier mobility, μ_0, and the ratio of the free carrier density to the total carrier density induced by gate bias. Crystalline FETs fabricated from rubrene, pentacene, and tetracene have a high free-carrier mobility, $\mu_0 \sim 50$ cm^2/Vs, at 300 K with lower device μ_{eff} dominated by localized gap states. This relationship suggests that further improvements in device performance could be possible with enhanced material quality.

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Thu-A-4.3o

Defect studies in nanoscale organic semiconductor films using monoenergetic positron beam

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Keywords: positron annihilation, organic semiconductor, nanoscale material, positron beam

In recent years, there has been a growing interest in studying the properties of organic semiconductors (OSC). This is due to potential applications such as active component of solar devices, gas detectors, laser diode light, photovoltaic devices, light emitting diodes, field effect transistors and memory devices. OSC offers advantage over conventional silicon technology in terms of fabrication methods, materials variety and mechanical flexibility. The electronic and optical properties of OSC thin films strongly depend on their structure and morphology due to large anisotropy in shape and electron orbital of the molecules. Consequently, tailoring these properties requires the ability to control the growth modes of organic materials. Phthalocyanines (Pcs) are a class of planar aromatic organic compounds that exhibit semiconducting properties. Their thermal and chemical stability makes them very suitable for thin films. It has been observed that due to substrate-molecule and molecule-molecule interactions, the films grow in various morphologies which is a function of deposition rate, substrate type and its temperature as well as thickness of the film.

The sensitivity of positrons to defects and free-volume is well documented. In this work slow positron beam that offers depth profiling ability has been used to understand the growth mechanism in OSCs by indexing the free-volume (defect) in metal-Phthalocanine films. Studies have been carried out on amorphous as well as crystalline films of varying thickness(50–150 nm) and grown on different substrates. Variation in microstructure as a function of thickness of the films, substrate type and its temperature is reflected in Doppler broadening S-parameter and diffusion length of positron. Films (FePc) grown at substrate temperature of 30°C and 300°C shows amorphous and crystalline nature, respectively. S-parameter for the amorphous film shows almost flat profile with increasing depth showing the presence of large open space or defects as compared to crystalline film which is having lower S-parameter indicating ordered arrangement of molecules. Variation in S-parameter with the thickness of the films has been studied in FePc films (50–100 nm) and is attributed to the fact that molecular arrangement changes from columnar to granular kind as the film thickness increases. Growth morphology of films as a function of substrate nature is studied in Cobalt-phthalocyanine films grown on glass and single crystal sapphire. S-parameter shows amorphous and crystalline nature for the films grown on glass and sapphire, respectively as reflected from the S-parameter vs depth profile. These films have been characterized using atomic force microscopy as well as grazing incidence x-ray diffraction techniques and the results are seen to be consistent with positron data. Our studies demonstrates the potential of slow positron beam technique in elucidating defect microstructure in nanoscale organic semiconductors.

Thu-A-4.4o

Three-dimensional anisotropic density of states distribution and carrier mobility of solution grown organic single crystals measured by Space-Charge Limited Current

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Keywords: single crystals, carrier mobility, density of states

Organic semiconducting molecules are receiving a large attention because of their potential applications, spanning from OLEDs to plastic photovoltaics to bio-chemical sensors. However, the electronic transport properties of these materials are still not fully understood, and organic single crystals (OSCs) may represent model materials for assessing the charge transport mechanisms, thanks to their high purity and molecular order. The intrinsic structural asymmetry of organic single crystals allows to investigate the correlation between their molecular stacking order and the carrier mobility anisotropy, providing an insight on the effects of crystal packing on the macroscopic electronic device performance. Here we show for the first time that solution-grown, millimiter-sized organic single crystals of 4-hydroxycyanobenzene (4HCB) possess a clear and reproducible three-dimensional anisotropy in their main transport parameters: i) charge carrier mobility, ii) distribution of the electronic density of states and iii) deep traps energy and concentration, and we report intrinsic-like three-dimensional mobility values for these crystals [1]. We have carried out Space Charge-Limited Current (SCLC) and photocurrent spectroscopy analyses on over 30 crystals and we have obtained a remarkable agreement with the mobility values we had previously obtained with air-gap FET measurements [2], emphasizing the intrinsic-like nature of the measured values. These findings demonstrate that the electronic spatial anisotropy of OSCs extends well beyond the carrier mobility, and open the way to the development of novel electronic device architectures based on the simultaneous exploitation of different electronic responses along the three spatial directions of the crystal.

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Thu-B-4.1i

Scientific and technological issues of atomic transport in silicon-germanium alloys

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Keywords: silicon, germanium, self-diffusion, dopant diffusion, composition dependence

Silicon germanium alloys and in particular the elemental semiconductor germanium have received renewed attention due to their potential application in advanced complementary metal oxides semiconductor (CMOS) technology as alternate materials on silicon. Whereas e.g. doping of Ge with the p-type dopant boron meets the requirements for highly doped source/drain regions in Ge pMOS, the fabrication of Ge nMOS remains a challenge due to the low donor activation level and the difficulty to realize abrupt junctions (see e.g. [1]).

The technological issues of doping Ge are discussed against the background of recent experimental and theoretical studies on self- and dopant diffusion in Ge under conditions close and far from thermal equilibrium. An explanation for the different diffusion behavior and activation levels of p- and n-type dopants in Ge is given. Taking advantage of our improved understanding on atomic transport processes in Ge various strategies are discussed to overcome the diffusion and activation issues that hamper a Ge-based CMOS technology.

Compared to elemental Si and Ge our understanding of atomic transport processes in SiGe is still very limited. Recent experiments on self- and dopant diffusion in isotopically controlled $Si_{1-x}Ge_x$-isotope heterostructures reveal a nonlinear composition dependence of both self- and dopant diffusion [2, 3]. The nonlinear dependence of self-diffusion is in contrast to earlier results. A similar nonlinear behavior is predicted theoretically for the stability of donor-vacancy pairs in SiGe. This interrelation indicates that the nonlinear behavior is mainly a consequence of the SiGe alloy system [4].

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Thu-B-4.2o

Radiation enhanced diffusion in germanium

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Keywords: germanium, irradiation, protons, diffusion

Ge isotope heterostructures were irradiated with 2.5 MeV protons at temperatures between 550°C and 640°C. The applied proton flux was varied up to 3.8 μA per cm^2. Secondary ion mass spectroscopy (SIMS) was utilized to record concentration profiles of the Ge-isotopes after the irradiation treatment. The SIMS profiles show a homogenous broadening of the multilayer structure. Continuum theoretical simulations were performed which are based on diffusion models that consider the formation of Frenkel-defects and their annihilation. Best fits to the experimental profiles are obtained when the boundary conditions for vacancies and self-interstitials are assumed differently. Ge self-interstitials are reflected at the surface, whereas the concentration of Ge vacancies approaches the thermal equilibrium value. To check these boundary conditions, experiments on the diffusion of n-type dopants under irradiation were performed.

Thu-B-4.3i

Transport spectroscopy of single defects in silicon

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Keywords: transport spectroscopy, single impurity, MOSFET

With the increasingly nanoscopic dimensions of devices, a new demand to under-

stand the electronic properties of single defects subject to strong electronic fields has emerged. In this talk our recent results on transport through single defects in silicon will be presented [1–6]. We investigate the resonant peaks superimposed on a direct tunneling current in the low temperature transport of Schottky barrier MOSFETs. These devices differ from standard transistors in that the source and drain contacts consist of a metallic silicide, instead of doped regions. The resonant peaks observed are shown to be due to single defects located in the depletion region near the metal silicide/semiconductor contacts. We investigate these states using excited state spectroscopy, in which the excited states of the defect are observed as the source-drain voltage increases while maintaining the gate voltage near resonance. With this technique and application of magnetic field, different charged states and their g-factors are observed. We have been able to identify P, several charged states of Pt and the neutral and 1st charged state of B. We will also discuss recent measurements in which the *g*-factor is determined as a function of magnetic field direction.

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Fri-A-2.1i

Effects of germanium doping on the behavior of oxygen and carbon impurities and impurity-related complexes in silicon

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Keywords: oxygen, carbon, germanium impurities, silicon

Some important characteristics of Si-based devices, among them their thermal stability and resistance to radiation damage, are sensitive to the presence of isoelectronic impurities in Si. These impurities can affect many quasi-chemical reactions of other practically important impurities like oxygen and carbon in Chochralski grown Si (Cz-Si) with point intrinsic defects, vacancies and self-interstitials. Oxygen and carbon atoms can effectively trap intrinsic defects leading to the production of a large variety of impurity-related complexes. The purpose of the present work is to study how the presence of Ge atoms in Cz-Si over a wide concentration range of 10^{18} to 2×10^{20} cm^{-3} affects most important quasi-chemical reactions of O and C under irradiation and subsequent annealing as well as their precipitation processes upon heating. In this report we outline the obtained results.

(i) The production rates of oxygen-vacancy complexes (VO_n, V_nO_m) as well as carbon-related defects (C_iC_s, C_iO_i, $C_iO_i(Si_I)$) in irradiated Si were found to be markedly affected by the Ge presence. However, the role of Ge changes with increasing Ge content. At low Ge concentrations much less than 10^{20} cm^{-3}, the isolated Ge atoms act as temporary traps for vacancies preventing their annihilation with self-interstitials. At high concentrations, Ge atoms tend to form clusters which attract vacancies and self-interstitials, thus enhancing mutual annihilation.

(ii) Thermal annealing of VO_n defects ($1 \le n \le 4$) is also affected by Ge atoms. The disappearance of VO complexes by trapping of self-interstitials is enhanced in the presence of Ge. As a result, the conversion of VO into VO_2 is reduced, too. In contrast, the transformations of $VO_2 \rightarrow VO_3$ and $VO_3 \rightarrow VO_4$ show a noticeable increase. Interestingly, the annealing temperature of VO defects and the growth temperature of VO_2defects in Ge-doped Si turned out to be significantly lower than those observed in materials without Ge. This effect is attributed to the compressive strains introduced by Ge atoms in the Si lattice. On the other hand, the thermal stability of radiation-produced carbon-related defects was found to be insensitive to the presence of Ge. Evidently, the behavior of vacancy- and interstitial- type complexes is different in Ge-doped Si.

(iii) Oxygen precipitation processes upon annealing slow down in heavily Ge-doped Cz-Si. By contrast, carbon precipitation processes are not affected by the presence of Ge in Cz-Si. This is not true for the both impurities in the same materials subjected to irradiation.

(iv) A new band at 994 cm^{-1} associated with Ge impurity atoms was observed; its origin is discussed.

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Fri-A-2.2o

Vacancy-impurity complexes in P- and Sb-doped $Si_{1-x}Ge_x$

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Keywords: E-centers, silicon germanium, positrons

Silicon germanium ($Si_{1-x}Ge_x$) has attracted major research interest recently due to its promising properties in semiconductor technology. The complete solubility of silicon and germanium makes band gap engineering between pure Si and pure Ge values possible. Additionally, carrier mobilities in Ge are higher than in Si which encourages the use of SiGe-based devices in high frequency applications. Due to Si and Ge having similar lattice constants, compatibility with existing Si-based technology is also good.

Positron annihilation spectroscopy is a nondestructive tool for studying neutral and negative vacancy-type defects in semiconductors. Positrons can get trapped in these vacancies, resulting in observable changes in both positron lifetime and the momentum distribution of the annihilating positron-electron pair. In this work we have focused on the latter and used positron Doppler broadening spectroscopy to study defects in $\mathrm{Si}_{1-x}\mathrm{Ge}_x$.

The defect we have been interested in is the vacancy-group V donor-complex, which is often referred to as the E-center in elemental semiconductors. It is probably the most studied point defect in semiconductors. The E-center in phosphorus-doped $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ has been studied extensively by positron annihilation spectroscopy (PAS) here at TKK [1–3]. It has been shown that the E-center in P-doped $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ becomes mobile at 150°C but a new defect type consisting of a vacancy, a phosphorus dopant and a germanium atom is formed after annealing at 150–175°C [1].

In this work we have studied both P- and Sb-doped $\mathrm{Si}_{1-x}\mathrm{Ge}_x$. P-doped $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ was isochronally annealed at temperatures ranging from 250 to 350°C and diffusion theory was applied to the results in order to find out activation energies related to the $E-$center annealing. Both isothermal and isochronal annealings were performed on Sb-doped $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ and the results were compared with the ones earlier obtained for the P-doped case. Coincidence Doppler broadening measurements were also performed on the Sb-doped samples for better understanding of the chemical surroundings of the $E-$centers.

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Fri-A-2.3o

Vacancy related defects in n-type $\mathrm{Si}_{1-x}\mathrm{Ge}_x$: alloying and strain effects

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Keywords: SiGe, E-center, DLTS, chemical disorder

The decrease of the band gap in fully strained $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ is controlled by both the alloying and strain effect. While the band gap shrinkage in fully relaxed $\mathrm{Si}_{1-x}\mathrm{Ge}_x$

alloys is related only to the alloying effect, the partially relaxed $Si_{1-x}Ge_x$ epilayer on Si open the possibility of tuning the band gap by varying the degree of strain only at given Ge content, In fact, fully strained and partially relaxed $Si_{1-x}Ge_x$ can have the same bad gap but for different Ge content. This gives the possibility to control the band gap in partially $Si_{1-x}Ge_x$ independently of the Ge content. We have used deep-level transient spectroscopy (DLTS) to investigate the electronic properties of defects introduced during high energy alpha particle irradiation of epitaxially grown phosphorous doped fully strained and partially relaxed n-$Si_{1-x}Ge_x$ ($0 \leq x \leq 0.1$). It is observed that alpha particle irradiation introduces two major defects in n-$Si_{1-x}Ge_x$ regardless the strain degree and were attributed to doubly negative charge state of the divacancy ($V_2^{=/-}$) and V–P pair (E-center). It has been found that the activation enthalpy (E_H) of $V_2^{=/-}$ in n-$Si_{1-x}Ge_x$ decreases slightly with respect to Si, while a large decrease of E_H is observed between the partially relaxed and fully relaxed n-$Si_{1-x}Ge_x$ at given Ge content. This large difference is explained by a large inward lattice relaxation and is suggested to be due to a combination of in- and out-of plane strain effect. On the other hand, the Gibbs free energy of E-center in $Si_{1-x}Ge_x$ does not change either with Ge-content or strain relaxation and indicates that the V–P level is pinned below the conduction band. The Gibbs free energy for $V_2^{=/-}$ was determined. The alloying and strain dependence of Gibbs free energy of $V_2^{=/-}$ will be presented and discussed in terms of pinning behavior of such defect with respect to the band edge. Finally the impact of the chemical fluctuation in the vicinity of the V-P and $V_2^{=/-}$ on the variation of the ionization energy level will be discussed.

Fri-A-2.4o

On vacancy diffusion in SiGe

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Keywords: interstitial, interstitial Fe-vacancy, defects, diffusion

Silicon-germanium (SiGe) is a promising alternate candidate for silicon (Si) in device processing due to its electronic properties; in particular, the understanding of the diffusivity of dopants in SiGe has been given much attention recently [1]. In this contribution, ^{57}Fe Mössbauer Spectroscopy has been employed after implantation of radioactive $^{57}\mathrm{Mn}^{+}$ ions ($T_{1/2} = 1.5$ minutes) into $\mathrm{Si}_x\mathrm{Ge}_{1-x}$ ($0.1 \leq x < 0.3$) single crystals at the ISOLDE facility, CERN. Pure beams of intensity $> 10^{8}$$^{57}\mathrm{Mn}^{+}$/s were implanted with 60 keV energy into the samples under study held at 300–800 K in an implantation chamber. Mössbauer spectra for the 14.4 keV transition of the ^{57*}Fe ($T_{1/2} = 100$ ns) daughter atoms were measured with a resonance detector equipped with ^{57}Fe absorber layers mounted on a velocity drive unit outside the implantation chamber.

Upon annealing of the implantation damage during the lifetime of ^{57}Mn at $T > 475$ K, Mn enters predominantly substitutional sites [2]. In the β^{-} decay the daughter ^{57}Fe nuclei is given a recoil of average energy 40 eV. This expels majority of the Fe atoms into interstitial sites (Fe_I). The Mössbauer spectra are characterized by lines from both interstitial and substititional Fe (Fe_S). Between 500 K and 700 K, the interstitial line broadens and a new line is observed, assigned to a metastable interstitial Fe-vacancy (Fe_I–V) configuration. The line broadening of the Fe_I gives direct information on the lifetime of the interstitial Fe in its configuration relative to the lifetime of the Mössbauer state. The effective lifetime is shortened, either due to diffusion or/and due to formation of the Fe_I–V pair. By monitoring the linewidth of Fe_I and the rate of Fe_I–V formation, it is possible to deduce the relative diffusivity of the vacancy.

In $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ with $x < 0.1$, the diffusivity of the vacancy is slow compared to the interstitial Fe atom, in accordance with the vacancy being an extended defect [3, 4]. In Ge, the formation of the Fe_I–V pair, takes place at ~ 350 K [5] suggesting that the vacancy behaves as a point defect. Here we present data on $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ with ($0.1 \leq x < 0.3$), where the transition of the vacancy from an extended defect to point defect takes place at $T \sim 500$ K.

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Fri-A-2.5o

Dangling-bond defects in laser-crystallized polycrystalline SiGe thin films

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Keywords: SiGe,laser crystallization,grain boundary,defect band

Up to now, most research in the field of laser crystallization has focused on silicon thin-films on foreign substrates, which nowadays are widely used for large-area electronic devices such as liquid crystal displays and solar cells. Recently, the utilization of silicon alloys like silicon–germanium (SiGe) has become an important approach to fabricate novel electronic and optoelectronic devices. This growing interest is based on the tunability of the physical properties of SiGe with the alloy composition. Moreover, the production methods for SiGe are compatible with the well established Si technology. However, the basic mechanisms governing the electrical and optical properties of polycrystalline SiGe (poly-SiGe) are poorly understood compared to those of poly-Si thin-films.

The poly-SiGe thin films investigated in this study were fabricated on quartz substrates by the following steps. Initially, intrinsic amorphous silicon–germanium films (a-$\mathrm{Si}_{1-x}\mathrm{Ge}_x$:H) were deposited by glow-discharge decomposition of a mixture of disilane, germane, and hydrogen to a thickness of 100 to 255 nm. The Ge content, x, of the resulting samples was varied over the entire composition range $0 < x < 1$. In a second processing step the amorphous samples were crystallized employing a XeCl excimer laser utilizing either a step-by-step crystallization technique [1] or a single pulse irradiation.

Electron spin resonance (ESR) measurements reveal that laser-crystallized poly $\mathrm{Si}_{1-x}\mathrm{Ge}_x$ thin films with $0 < x < 0.84$ contain a dangling-bond concentration of about $N_s = 4 \times 10^{18}$ cm^{-3} that is independent of the used crystallization method. Surprisingly, the ESR signal vanishes completely for the Ge-rich alloys and instead a broad atypical signal appears that is attributed to electric dipole induced spin resonance (EDSR). In addition, samples that showed this behavior also exhibited an unexpected high and nearly temperature-independent electrical conductivity in the range of 20–100 K. Optical absorption data of Ge rich alloys obtained by photothermal deflection spectroscopy (PDS) exhibit a behavior that is characteristic for disordered semiconductors. This implies that the absorption occurs primarily at the grain boundaries. Finally, the influence of a remote hydrogen plasma-treatment on the properties of the films is presented, showing a decrease in the ESR and the sub-band-gap absorption signals. Interestingly, this is accompanied by a remarkable change in the electrical transport properties. The conductance changes from metallic to insulator-like behavior. The results will be discussed in terms of the formation of a dangling-bond defect band located at the grain boundaries in the vicinity of the Fermi level.

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Fri-A-2.6o

Origin of the optically active Er centers in $Si_{1-x}Ge_x$:Er layers grown by the sublimation MBE in germane gas atmosphere

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Keywords: SiGe, Er centers, photoluminescence

Er-doped silicon is widely recognized as the promising material to develop effective light-emitters on Si basis. The variety of device structures operating from 4.2 K to room temperature has been demonstrated nowadays. Moreover sufficient optical gain of about 30 cm^{-1} has been predicted for this material [1]. In this contribution we discuss the luminescence properties and peculiarities of Er centers formation in Si/$Si_{1-x}Ge_x$:Er structures being of interest for a laser realization. The introduction of $Si_{1-x}Ge_x$ layers in this case enables the formation of an effective waveguide with the strong optical mode localization in an active area.

The Si/$Si_{1-x}Ge_x$:Er structures were grown by the sublimation MBE method in germane gas (GeH_4) atmosphere [2]. Depending on the gas pressure, germanium content in $Si_{1-x}Ge_x$ layers can be varied between 5 and 33%. The structures with the Er impurity concentration of $(2–3)\times10^{18}$ cm^{-3} and the thickness of $Si_{1-x}Ge_x$:Er layers of 0.1–3 μm were studied. In this work we have analyzed the types of optically active Er centers being involved in the photoluminescence (PL) response of these structures. In particular, the correlation between the $Si_{1-x}Ge_x$:Er layer parameters (its molar and impurity content) and the type of optically active Er centers has been considered. It will be shown that the PL response of Si/$Si_{1-x}Ge_x$:Er structures strongly depends on the Ge content in the $Si_{1-x}Ge_x$:Er layers. The PL response related with the oxygen containing Er centers and complexes has been observed for the Si/$Si_{1-x}Ge_x$:Er structures with the Ge content $< 25\%$. Oxygen containing Er-O1 center, erbium-oxygen complexes of the low symmetry and the SiO_x:Er precipitate type centers were distinguished in these structures. The novel type of the optically active Er centers has been observed in the Si/$Si_{1-x}Ge_x$:Er structures with the Ge content $\geq 25\%$. The centers of this type are represented in PL spectra by the line series of 6508.1 cm^{-1}, 6481.6 cm^{-1}, 6468.1 cm^{-1}, 6443.5 cm^{-1}, 6423.8 cm^{-1}, 6333 cm^{-1}, 6303 cm^{-1} (center Er–Ge1), and 6501.6 cm^{-1}, 6473 cm^{-1}, 6457 cm^{-1}, 6434.8 cm^{-1} (center Er–Ge2). The last one appears in the PL spectra only at elevated temperatures ($T \geq 8$ K). Analyzing the temperature dependence, dependence of the PL lines intensity on the excitation power, as well as their reproducibility in various samples, we will show that both these line series belong to the different Er centers with various microstructure. The probable types of symmetry for these centers are D_{2d}, C_{2v}, C_s.

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Fri-B-2.1o

Impurity-band ferromagnetism in Mn-doped Ga(As, P)

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Keywords: GaAs, GaP, Mn, spintronics, ferromagnetism

The transition-metal Mn is unique in semiconductor science as the only substitutional acceptor to induce hole-mediated ferromagnetism in III–V compounds. $Ga_{1-x}Mn_xAs$ has been the most thoroughly studied among these ferromagnetic semiconductors. While the Curie temperature T_C in this prototypical system increases with increasing concentration of substitutional Mn acceptors, room temperature ferromagnetism remains elusive. An alternative, less explored route by which T_C may rise is via anion substitution in order to enhance p–d exchange between the holes and Mn acceptors. Using a combination of ion implantation and pulsed-laser melting, we have produced epitaxial, single crystalline films of ferromagnetic $Ga_{1-x}Mn_x$(As,P) alloys. In the endpoint compound $Ga_{0.96}Mn_{0.04}P$ non-metallic transport is observed, corresponding to a T_C of 64 K compared to $\sim$ 110 K for $Ga_{0.96}Mn_{0.04}As$ with a similar x, and at low temperature holes are localized in a Mn-derived band. Dilution of $Ga_{0.96}Mn_{0.04}P$ with As leads to further hole localization without changing significantly the impurity-band width and results in a modest reduction of T_C by $\sim$ 15 K. Dilution of the endpoint compound $Ga_{0.96}Mn_{0.04}As$ with 3% of P, on the other hand, leads to a precipitous reduction of T_C to below 60 K and a metal-insulator transition even as the Mn concentration is held constant. The observed suppression of T_C is explained in terms of alloy disorder induced reduction of the mean free path of holes localized in the Mn impurity band. Thus, while anion substitution may enhance p–d, hole-localization effects must be considered when developing a suitable picture for ferromagnetism in these materials.

Fri-B-2.2o

Model of 3d impurities in silicon carbide

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Keywords: SiC, transition metalls

A small cluster of silicon carbide (SiC) with the 3d transition metal (TM) impurity in substitution position was considered, the second neighbors were the cluster boundary. Interaction of the nearest neighbors was considered within bonding orbital model. The Coulomb shift of levels due to excessive charge on the atom and its neighbors was also taken into account. It was supposed, that the excessive charge of the TM impurity is neutralized within the cluster and this leads to self-consistent solution. The estimation of nearest neighbors' relaxation gives values less than 0,01 nm, and therefore the effects of structural relaxation were neglected. It was also supposed, that the Jahn-Teller effect missed.

The carried out calculations allow to reveal the basic tendencies of the energy position of TM levels, their genesis, and also give the evolution of the levels with charge state of impurities. For all the elements a deep a type resonance occurs in the valence band relevant to the interaction of TM s-orbitals with dangling bonds of vacancy. Two of TM d-orbitals do not interact with orbitals on neighbor atoms and form atomic-like e levels, whereas the three other d-orbitals undergo strong pd-hybridization. Cr and V show the most rich structure of the localized states. In the neutral state Ti does not yield local levels in the bandgap of cubic SiC and only yields resonances in the conduction band. In the acceptor state Ti forms a bonding level t_b close to the valence band edge. In opposite to titanium the levels of Co and Ni are located mostly in the valence band. In an acceptor state Co yields an antibonding level t_a close to the top of the valence band. For the TM elements from the middle of 3d-series only antibonding t_a states remain in the bandgap. Estimation of the contribution of multielectron effects has shown, that in the case of V and Cr a crossing of e and t_a levels can take place.

Also the silicon, carbide and impurity atoms excess atomic charges and localized magnetic moments are evaluated.

Fri-B-2.3o

Role of intrinsic defect in the magnetic properties of iron doped ZnO: a first principles simulation

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Keywords: magnetic impurities, spintronics, ab initio calculations

By means of density functional plane-wave pseudopotential calculations and supercell techniques we have investigated the magnetic properties of wurtzite ZnO doped with diluted concentration of iron. In particular, we perform a systematic study of the magnetic interaction of different type of complexes formed by iron impurities with intrinsic defect of ZnO, considering both neutral and charged defects, finding that the defect formation energy is strongly influenced by the presence of iron impurities. We predict what types of complexes are the more stable, we study how the complex formation depends on the growth condition of the oxide, and we compute the defect concentration as a function of temperature, giving new insight in the understanding of the magnetic properties experimentally detected in this material at room temperature. The calculation of the thermal activation energy of different complexes is compared with experimental data reported in literature.

Some of the complexes investigated, such as the $\mathrm{Fe_{Zn}}$–$\mathrm{I_O}$, present integer magnetic moment and a full spin polarization at the Fermi energy, in a similar way as already found for $\mathrm{Fe_{Zn}}$–$\mathrm{V_{Zn}}$ [1], suggesting the possibility to employ this material into future spintronic devices in which the magnetic properties can be tailored by the relative concentration of defects. According to our preliminary calculations similar properties are also displayed by doping ZnO with other transition metal elements.

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Fri-B-2.4o

Effects of MnSb clusters on magnetic and electrical properties of (In, Mn)Sb

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Keywords: diluted magnetic semiconductor, magnetic cluster

Alloying of nonmagnetic semiconductors and 3d-magnetic elements let to synthesize ferromagnets which are called diluted magnetic semiconductors. Progress in growing Mn-doped semiconductors of III–V group showed the high potential these compounds for applying in original classes of spintronic devices. A number of possibilities for the spin manipulation are opened by the embedding of ferromagnetic materials with high T_c to non-magnetic semiconductors. As high-tempe rature ferromagnetic compounds are using Mn–V compounds: MnAs, MnSb, MnP. Indium antimonide has attracted attention as material having the narrowest energy gap and the highest carrier mobility at 300 K among III–V semiconductors. The nature of the high-temperature ferromagnetism in InSb heavy doped with Mn is not hole-mediated and is connected with the presence of MnSb clusters.

To synthesis of polycrystalline InSb:Mn samples solid state reactions with fast cooling (cooling rate $\sim 10-12$ K/s) have been used. The XRD patterns of samples had only InSb peaks. The lattice constant a changed from 6.4794 Å (Mn 0.47% mass) to 6.4779 Å (Mn 1.42% mass). The decreasing of a can explain by the formation of the $\mathrm{In}_{1-x}\mathrm{Mn}_x\mathrm{Sb}$ solid solution when Mn atoms substitute In sites. No traces of the second phase compounds were observed. At the same time micro-structural analysis detected presence of MnSb inclusions with a size from 100 to 500 nm.

Measurements of magnetic and electrical properties showed essential influence of MnSb clusters on the charge transport and magnetization of the samples (Curie temperature above 580 K). The features of the resistivity curves can be connected with trapping the holes at the interface between the MnSb clusters and the InSb:Mn matrix. The "$\mathrm{T}^{-1/2}$-law" was observed at the low temperatures and the implication is that the variable-range hopping between clusters takes place.

The hole mobility is match lower value for single undoped crystals and can be improve by using the special growth technique for production directly solidified InSb–MnSb monocrystall eutectic.

Fri-B-2.5o

Manganese doped InAs/GaAs quantum dots studied by X-STM

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Keywords: manganese, quantum dots, InAs/GaAs, magnetic nanostructures

In the search for future electronic/fotonic devices, quantum dots doped with magnetic atoms are very promising candidates as building blocks for these devices since they offer the opportunity to use the electronic, magnetic and optical characteristics of such a structure simultaneously. In this work, we present results of Cross Sectional Scanning Tunneling Microscopy (X-STM) studies on Mn doped InAs quantum dots in GaAs.

Mn doped InAs quantum dots in GaAs were analyzed by X-STM at room temperature. For this sample, 2.1 ML of InAs were deposited at a low growth temperature of 450° to limit Mn segregation and to improve Mn incorporation in the dots. Each QD layer was doped with $1.0 \times 10^{11}/\ \mathrm{cm}^2$ Mn. At these low growth temperatures, an average baselength and height of the dots of 7.9 nm and 3.0 nm was observed respectively. It was found that despite the low growth temperature, strong segregation of the Mn atoms takes place. Mn segregation in GaAs has been investigated with dedicated samples showing that even at 350° segregation still takes place.

A similar sample with 2.4 ML of InAs was grown at an even lower temperature of 320°. X-STM measurements confirmed Mn densities of at least 1.4% ($8.8 \times 10^{12}/\ \mathrm{cm}^2$) per QD layer. The average baselength and height of the dots was 8.6 nm and 2.3 nm respectively and we have been able to observe Mn atoms in small dots but we were yet unable to resolve Mn in larger dots. As a next step, Scanning Tunneling Spectroscopy (STS) was performed at 77 K. Mn atoms inside QD's were resolved showing a characteristic splitting in the lateral direction of the Mn feature.

The influence of spatial confinement and strain distribution in QD's on the Mn wavefunction and binding energy has been calculated using the Effective Mass Approach. We use the Bir-Pikus Hamiltonian in cubic approximation with a Yukawa potential for Mn. The problem has been solved numerically by Finite Elements Method. Calculations have been performed both for Mn in bulk GaAs as well as InAs QD's.

Poster sessions

ICDS-25

Mon-1.1po

The role of intrinsic point defects at interphase interaction of nickel with silicon carbide under proton irradiation

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Keywords: Ni-SiC system, proton irradiation, interphase interaction model

The contact of n-SiC with the most widely used silicide-forming metal, nickel becomes ohmic (non-rectifying) at annealing temperatures exceeding 900°C. At these temperatures, the film Ni interacts with SiC to give nickel silicides: Ni_2Si, NiSi and $NiSi_2$. Irradiation with protons at elevated temperatures considerably improves the uniformity of the contact morphology and lower the formation temperature of Ni-SiC ohmic contacts from 950 to 750°C [1]. The component distribution in the system Ni-SiC have specific features: existence of an extended reaction zone, excess of carbon concentration over that of silicon at the interface with a SiC substrate, and accumulation of carbon near the surface [2].

For interpretation this observations a quantitative model of the interfacial interaction of a silicide-forming metal with single-crystal SiC has been developed. This model based on the interdiffusion of components with account Kirkendall effect and with account the volume reactions of the formation of metal silicides. The model enables a satisfactory description of the basic features of component redistribution in the system Ni-SiC under irradiation with protons at elevated temperatures. It is shown that the proton irradiation raises the diffusion coefficient of the metal by a factor of 2–4 and the rate of the chemical reactions by a factor of 10–20. Both these effects are attributed to generation of intrinsic point defects, interstitial atoms and vacancies, during proton irradiation. Excess intrinsic point defects accelerate the diffusion of metal and serve as a source of a free volume for solid state chemical reactions of the formation of metal silicides.

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Mon-1.2po

Comparative mid- and far-infrared spectroscopy of nitrogen-oxygen complexes in silicon

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Keywords: silicon, nitrogen-oxygen defects, infrared spectroscopy

Nitrogen-related defects in silicon are of great interest because of their impact on crystal imperfections due to vacancy and/or interstitial aggregates. N-O complexes are efficiently formed in N-doped Czochralski silicon after extended thermal annealing at around 600°C. They act as shallow donors (SD) and can be studied by characteristic electronic transitions in the far infrared (FIR). Recently the chemical composition of all major N–O SD defects could by clarified by FIR spectroscopy of crystals with systematic variation of the N and O content, introduced by special crystal growth techniques [1 ,2].

This work is focused on the thermal stability of N–O SDs and their vibrational properties as a counterpart to the electronic behavior. The thermal equilibrium concentration of different N–O species is established in the temperature range between 600 and 1000°C by a two-step annealing process. The concentration of NO SDs is evaluated from quantitative FIR spectroscopy. It is found that the experimentally observed decay in this temperature range is not in agreement with recent calculations of formation energies [3].

With this information on annealing temperature dependence of N–O SDs available, we examine the MIR spectra (between 650 and 1100 cm^{1}) of similar samples, however with an order of magnitude higher N content ($\sim 10^{15}\ \mathrm{cm}^{-3}$), for an identical "thermal fingerprint" of generation and decomposition, to detect and identify specific N–O SD-related local vibrational modes (LVM) amongst well-known modes of the dominant nitrogen pair (and its derivatives due to agglomeration of interstitial oxygen atoms).

Based on the similar dependence on the annealing temperature — both for the FIR and the MIR signal — we suggest that the 860 cm^{-1} absorption structure must be attributed to a LVM of the SD species N–O–3, with the $1s \rightarrow 2p_{\pm}$ transition at 240 cm^{-1}. This assignment would match frequencies calculated by Fujita *et al.* [3], using local density theory, for the NO_2 defect (i.e. N–O–3) in the O–N–O configuration.

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Mon-1.3po

Analysis of photoluminescence spectra as a detection method of tension in silicon substrates after the polycrystalline diamond deposition

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Keywords: photoluminescence, adhesion, dislocation, silicon/diamond interface

The low temperature (5 K) photoluminescence (PL) of silicon substrate in the range of 0.8–1.2 eV before and after microwave plasma assisted chemical vapor deposition of polycrystalline diamond films was studied [1]. The diamond films were deposited at the temperature of 750–850°C onto the pure ($\rho \sim 3$ kOhm·cm) dislocation — free silicon treated by mechanical polishing (MP) or by the more perfect chemical-mechanical polishing (CMP). In the PL spectra of coated silicon substrates treated by CMP, the D_1 and D_2 lines were registered related to dislocation emission [2]. We suppose that the formation of dislocations in the substrate is caused by a strong adhesion of diamond film and as a consequence by the formation of inner tensions released as dislocations. The spectra observed were in fact identical to PL spectra measured for silicon ($\rho \sim 100$ Ohm·cm) grown with the moderate dislocation density of $\sim 10^4$ cm^{-2} (as a testing material for comparison).

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Mon-1.4po

Photoluminescence of erbium-doped Si structures grown on SOI by molecular beam epitaxy

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Keywords: silicon, SOI, erbium luminescence

Creation of light-emitting devices (LED and lasers) remains important and not solved problem of Si photonics. Er-doped silicon structures have received a lot of interest as a possible material for Si-based photonic applications because the radiative transitions of the Er ion occurs at the technologically important wavelength 1.54 μm. For realization of the Si:Er laser it is necessary to produce an active Si waveguide of good crystalline quality with high enough refractive index. As was shown in the works [1, 2] Er-dopped Si structures on silicon-on-insulator (SOI) substrates demonstrate waveguide properties in near IR range and small optical gain at 1.54 μm [2]. Ion implantation of Er in SOI leads to a limitation of the wave guide parameters and generation of an additional optical losses [1, 2].

In the presented paper we report on the waveguide structures with active Si:Er layer grown on the SOI substrates by the method of sublimation molecular-beam epitaxy [3] and on the results of their luminescence properties study. In this work we have solved the problem of formation of the waveguiding active Si:Er:O layer on SOI with high crystalline quality and with one dominating emitting center *Er-1* [4]. Due to its extremely narrow line ($\sim$ 10 μeV) this center seems to be optimal (from all known erbium-related centers) for realization of maximal gain at the radiative transition $^4\mathrm{I}_{13/2}$–$^4\mathrm{I}_{15/2}$ of erbium ion. We have studied influence of the post-growth thermal treatment on the PL intensity. In the presented report we discuss the results of our studies of the PL temperature dependence, photoluminescence excitation spectra in the range 0.7–1.4 μm and the PL kinetics of the Si:Er:O/SOI structures.

It has been shown that the non-uniform width of the erbium PL line in the produced epitaxial structures (10 μeV) is at least an order of magnitude lower then the values previously reported for the Si:Er/SOI structures, and the quantum efficiency of the low-temperature erbium PL is substantially higher then in the structures produced by ion implantation. The gain value in the investigated structures has been estimated.

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Mon-1.5po

Point defects in gamma-irradiated germanium and their characterization by high-momentum electron-positron annihilation radiation

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Keywords: radiation defects, germanium, positrons

In this report we are going to present the data obtained by studying the annihilation of positrons in the ion cores of vacancy-group-V-impurity atom complexes.

After the injection into the sample the positron to be trapped by a defect is capable of annihilating with core electrons of the surrounding atoms and the annihilation radiation bears elementally specific information about the individual atomic components of the site where the event of annihilation occurs. Direct detecting the annihilation gamma-quanta to be emitted from the core region of the vacancy-group-V-impurity atom complexes in germanium has allowed one to identify these defects as the centers of the positron localization. For a variety of reasons, the evidence of such kind may not be obtained by the positron lifetime spectroscopy and by the measurements of the Doppler broadening of annihilation radiation, — the techniques which are widely used in the positron researches of defects in semiconductors.

A change of both number and positions of the ion cores occurs in the vacancy-group-V-impurity atom complexes in the course of irradiation. A special attention has been given to the revealed changes of the number of vacancies involved into the microstructure of the defects both before and after n–p-conversion of the investigated materials.

In experiments we used the samples of single crystals of oxygen-lean n-Ge<V> (V= P, As, Sb, and Bi) subjected to gamma-irradiation Co^{60} ($T_{\mathrm{irr.}} \approx 280$ K). Elementally specific high-momentum angular correlation of the annihilation radiation to be emitted from the ion cores has been registered with high precision (the angular resolution of spectrometer was $\leq 0.06°$).

In the materials before n–p-conversion there is observed a displacement of the ion cores directed towards inward of the free volume of the vacancy-group-V-impurity atom complex.

After n–p-conversion the intensity of emission of the high-momentum annihilation radiation from the subvalent shells is suppressed thus suggesting strongly a decrease of the number of the ion cores around the positron trapped by the radiation defects. This directly indicates the addition of vacancies to the vacancy-group-V-impurity atom complex in the course of gamma-irradiation. Deep hole states in the forbidden gap contribute to decreasing the electron density around the positron localized at the multi-vacancy-P-, Sb-, and Bi-impurity-atom complexes.

Mon-1.6po

Excimer laser formation of nanocrystals and impurity activation in amorphous silicon films

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Keywords: silicon, nanocrystals, impurity activation, shallow junction

Amorphous silicon represents free-ordered material having significant meaning in modern applications. It's well known that under energetic impact one should expect transition in crystalline form for a-Si. This paper represents itself the study simultaneous nucleation and impurity activation, contributions in conductivity which was seemed to distinguish difficultly. Nanocrystals look like extended defects in homogeneity doped amorphous films. So as undoped films, as boron (phosphorus) doped a-Si films were examined under nanosecond laser impact.

Research of electronic properties was provided for amorphous films with silicon nanocrystals, formed at nanosecond laser irradiation. It was discovered, that for Si-nanocrystals with dimensions about 2 nm changing of conductivity mechanism was detected with lowering of activation energy from 0.7 eV down to 0.12–0.17 eV. Calculations of temperature dependence for Fermi energy in amorphous Si-films was realized within representation of nanocrystals as multi-charged centers. Computation has demonstrated pinning Fermi energy close to values of energetic levels localized inside of nanocrystals, depending on background doping level. Electronic states in forbidden zone were taken into account, meanwhile dimensions for nanocrystals was chosen to be equal.

For the similar laser treatments regimes transition of boron and phosphorus atoms in electrical active state was detected without melting of a-Si films. That allows to conserve initial spatial distributions of B,P atoms. The activation leaded to forming of shallow p–n junctions with characteristic depth below 20–30 nm. Spread resistances as well as ampere-voltage ($I-V$), capacitance-voltage ($C-V$) characteristics for p-n junctions were studied revealing quite good electrical properties. Laser treatments at large energy density and thermal treatments leaded to full activation of boron and increase of p-n junction depth up to 400–500 nm. Full concentration of boron was registered by means of SIMS method detecting spatial distribution variation. Using Raman spectroscopy proved the activation due to observed increasing of the peak corresponding to Si-B vibrations when boron is found in tetrahedral configuration surrounded by Si atoms, i.e. in electrical active state. Plasma immersion and ion implantation were used for formation of initial samples, as well as doping during growth process, what gave variation of boron distribution depth from 20 nm to 100 nm.

Comparison with results for undoped films allows separating two contributions in conductivity. Results may be important for formation of contacts and p-n junctions with varied depth and without heating of substrates. So the fields of large-area electronics and nanoelectronics may be interesting for application of the results.

Mon-1.7po

Spatial redistribution of selenium and sulfur in silicon: Effect of surface doping with phosphorus

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Keywords: silicon, defects, diffusion of chalcogens

It was found in the present study that doping of silicon with phosphorus (P) can essentially enhance the diffusion rate of selenium and sulfur that are known to create deep donor centers in the semiconductor. The effect was revealed for wafers of p-type silicon homogeneously saturated with the deep impurity of selenium or sulfur. Doping of deep impurities was performed by a method of a high-temperature diffusion of elements from the gas phase in sealed quartz ampoules. After doping, samples became n-type; the concentration of electrically active centers of a chalcogen was in the range 3×10^{15}–3×10^{16} cm^{-3}. The subsequent doping of samples with P was carried out by both a short-term P diffusion, and the ion implantation technique. The implantation was followed by annealing of samples in vacuum. For both methods, the surface concentration of P was up to $\sim 10^{19}$ cm^{-3}.

It was established that doping with P by the specified methods leads to a strong increase of the specific resistivity ρ in the subsurface area of both Si:S and Si:Se samples. The application of a spreading-resistance profiling gave an evidence that the appreciable effect of ρ increase took place up to the depth 5–7 microns for both impurities.

Distribution of chemical elements near a sample surface was measured for Si:Se samples, which was done by the Laser Ablation Inductively Coupled Plasma Mass Spectrometry technique. The measurements indicated that the occurrence of profiles of specific resistance were connected with the depletion of a sample volume with selenium. The effect extended up to a rather large depth from a sample surface. Apparently, the similar effect occurred also for Si:S samples.

Observed regularities are interpreted as the enhanced chalcogen diffusion at studied conditions. In our opinion, the phenomenon is initiated by injection of non-equilibrium silicon interstitials Si_i into the sample volume from the subsurface layer that is highly doped with P. The increase in Si_i concentration displaces the balance between the substitutional and interstitial positions of chalcogen centers in the silicon lattice.

This is accompanied by the growth of concentration of impurity centers at interstitial sites, where their diffusion transport is enhanced. Our results confirm the hypothesis of the authors of [1], who supposed that the diffusion of S and Se in silicon proceeds mainly through the interstitial mechanism.

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Mon-1.8po

The stability of detonation nanodiamond under *g*-irradiation

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Keywords: nanodiamond, gamma irradiation, cathodoluminescence

Detonation nanodiamond (DND) is the form of synthetic diamond witch consists of the amount of crystalline diamond nanoparticles with average size near 4.5 nm. It attracts the constant attention of investigators due to its unique physical and chemical properties.

Taking into account the fact that the diamond is thermodynamically unstable under atmospheric pressure and room temperature, one can expect that DND could be easily transformed into graphite by the accumulation of the point defects, induced, for instance, by gamma irradiation. For the other hand, the idea that the contribution of the surface energy makes the diamond nanoparticles thermodynamically stable at normal conditions still exists [1].

In order to obtain the answer for this question we have irradiated the samples of DND by the high intensive Co60 gamma source (major energy lines 1.17 MeV and 1.33 MeV, intensity $8.2 \cdot 10^5$ R/min) during 600 hours. The total absorbed energy of gamma irradiation has exceeded 78 eV per carbon atom.

The comparison of the results of study the irradiated and the reference samples of DND by HRTEM, XRD and ESR techniques could not reveal any noticeable transformations in the structure or the defects content under irradiation. Only in the cathodoluminescence spectra we have observed the relative increase the intensity of two broad bands with peak energies 2.3 and 2.8 eV after irradiation. But even this modification can be related not with the structure and defects of the crystalline core, but to the partial surface oxidation of DND particles by the oxygen evolved by photolysis of water vapor. The cathodoluminescence spectra observed on the irradiated samples of DN after annealing in hydrogen at 800° prove this assumption.

The observed resistance of DND for the intensive gamma irradiation gives the additional argument for the idea of the thermodynamic stability of diamond nanoparticles at normal conditions.

The equipments of a Center Material study and diagnostics for advance technology (Ioffe Institute, St. Petersburg, Russia) have been used at investigation of DND.

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Mon-1.9po

The first principal calculation of the electronic structure of the Ge strained layers and the set of Ge islands on (001) Si film

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Keywords: Ge, Si film, electronic structure

Electronic properties of the Ge strained layers (3 mono layers from 24 atoms on the cell) on (001) Si film (2 mono layers from 16 atoms on the cell) and the set of Ge pyramidal islands (3 mono layers from 7 atoms on the cell) on Si film are investigated by **our** computer program package based on the density functional theory and psevdopotential to obtain quantum-mechanical ground state electronic configuration. These atom systems are participants of the process of the conversion from the 2D epitaxial growth of the strained heterostructures to the 3D nano islands growth. As a result studies it was appeared significant space localization of the electronic density in the Ge islands as compared with the Ge continuous strained film. So the facts are as follows the trace of electronic density is still observed on the distance of 3.6 Å from the surface of the Ge film whereas this distance from the Ge islands top is only 2.4 Å. As for the electronic energy spectrum for the set of Ge islands on Si film the valence bands overlap and their top falls.

Mon-1.10po

Electron properties of free-standing wires of porous silicon: ab initio calculation.

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Keywords: free-standing silicon wires, electron properties, ab initio calculation

We are performed a Monte–Carlo simulation of fabrication processes of porous silicon by electro-chemical etching under 300 K of (100) single silicon and resulted a set of free-standing wires. We are not obtained rebuilding of break bonds as like on the

surface. Next we are performed ab initio calculation for elaboration of electron properties of free-standing silicon wires. For this the Car-Parrinello molecular dynamics and ab initio norm-conserving pseudopotential were used. The calculation algorithm means using of atomic basis (it reflects features of the investigating system) which certainly ought to have inverse symmetry. The atomic basis of the primitive tetragonal unit cell of the superlattice represented an infinite silicon free-standing wires with a square cross section at side with 5.43 Å and (100) orientation.

An examination of the maps of valence electron density distributions and valence electron spectrum obtained with the help of author program code can explain properties of considered atomic objects. It was indicated that an each atom on surface the wire with a slight thickness had different electron state. This result show anisotropy of electron properties of atoms along free-standing wire surface even if cross section of wire was homogeneous on whole length and explain of wide bar of luminescence not only by means of scatter of parameters of cross section of free-standing wire.

Mon-1.11po

Spin relaxation and coherence for shallow donors in Si

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Keywords: donors in Si, pulsed EPR, relaxation mechanisms, ESEEM

Since the original Kane suggestion [1] to use phosphorous donors in a Si lattice as qubits for quantum information processing (QIP), many studies have been performed to check whether this system could be practically employed for quantum computation, and actually positive proofs have already been collected [2]. In particular, the most important physical property for this purpose, the electron spin phase memory time, has been proved to reach values which could allow efficient quantum computation (i.e. the implementation of quantum error correction [3]). Thus, the main mechanisms leading to decoherence, such as instantaneous diffusion, spectral diffusion, and spin-lattice relaxation time [2, 4, 5] must be investigated carefully. However, it is still unclear whether the phosphorus donor is the best candidate for a Si-based implementation of quantum computation.

We report a comparative pulsed-EPR investigation on both spin-lattice (T_1) and spin-spin (T_2) relaxation times for different group-V shallow donors in Si, such as P, As and Bi, as function of temperature and magnetic field. We will also discuss new details on the spin-lattice relaxation processes for the donors.

Finally, we will focus on the peculiar case of the Bi donor (^{209}Bi: I=9/2), and in particular on the super-hyperfine interaction with the ^{29}Si nuclear spins dispersed into the Si lattice, probed by electron spin echo envelope modulation spectroscopy (ESEEM), providing information on the donor wave-function.

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Mon-1.12po

Dislocation luminescence and electrical properties of dislocation network produced by silicon direct wafer bonding

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Keywords: dislocation luminescence, bonded wafers

Going wireless for data transmission will definitely be a breakthrough in the next generation microprocessors development. The dislocation-related luminescence (DL) in silicon is known to be perfectly suitable with contemporary optoelectronic devices. That is why it is often considered as a possible source of light radiation to be used for on-chip LEDs [1]. Although being studied for more than four decades the vast majority of intrinsic properties as well as the mechanism of DL in silicon and related effects are still not definitely determined.

The technology of direct wafer bonding coupled with SmartCut^{TM} process is already industrial and well compatible with modern silicon technology. The technology allows to produce uniform dislocation networks at the bonding interface with specified types and densities of dislocations lying at a defined depth.

In the present work electrical and optical properties of the set of Schottky diodes made on bonded silicon wafers with the depths of the bonded interface varying from 50 nm to of about 2 um was investigated. Usage such kind of the samples allowed to change the occupation of electron states changing the bias voltage applied to the Schottky diodes. The occupancy of the states was monitored by $I-V$, $C-V$ and DLTS measurements and the dependence of the intensity of DL on the occupancy was established. The influence of electric field on the spectral positions DL-bands was also investigated.

It was found that the electric field effect observed in the present work exceeded that was reported previously [2] by more than hundred times and could not be interpreted as a Stark effect. Besides, correlations between the DL intensity and particular features on IV and CV were found. The estimation of the electron energy levels responsible for DL in silicon was made on the base of analysis of correlations found.

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Mon-1.13po

Correlation between defects and magnetism in Mn-implanted SiC

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Keywords: dilute semiconductor, defects, magnetism

X-ray diffraction (XRD) and channeling Rutherford backscattering (RBS/C) were combined to assess the defects in Mn-implanted SiC. Two polytypes 3C-SiC(100) and 6H-SiC(0001) were implaned with Mn at 80 keV for different fluences. Thermal stability of implantation-induced defects was also investigated by annealing the samples. It is shown that the type of substitutional site of Mn (Si or C) and defects environment of Mn play a crucial role on magnetism in Mn-implanted 3C-SiC. It is found that Mn has a preference for Si site which in turns contributes to a large enhancement of magnetic moment per Mn atom at room temperature (RT) from 0.23 to 0.65 m_B. This was also supported by ab-initio calculations.

For 6H-SiC, a strong correlation between defects and strain depth profiles is observed with no sign of magnetism at RT. The absence of magnetism in Mn-implanted 6H-SiC can be related to the low carriers' concentrations as deduced from micro-Raman spectroscopy (mRS). This is reflected in the absence of the Plasmon-phonon mode in mRS for 6H type.

Mon-1.14po

A new spin one defect in cubic SiC

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Keywords: divacancy, EPR, 3C-SiC

In this report the results from an EPR study of high dose neutron irradiated 3C-SiC bulk crystals are presented. Cubic SiC single crystals were grown by thermal decomposition of methyl-trichlorosilane in hydrogen. All the crystals under study were unintentionally doped n-type with carrier concentration in 10^{17} cm^{-3} range. After fast neutron irradiation with a dose of 10^{19} cm^{-2} a new defect, labeled Ky5, has been revealed in the EPR spectra in addition to the dominant spectrum of the negatively charged silicon vacancy, the T1 center. Angular variation of the Ky5 spectrum indicates its origin from a spin $S = 1$ defect. This spectrum can be detected in darkness in the whole temperature range 4.2–295 K with practically unchanged parameters confirming a triplet ground state of the Ky5 center. Its spin Hamiltonian parameters are isotropic $g = 2.004$ and axially symmetric D tensor aligned along crystal directions, $D = 443 \times 10^{-4}$ cm^{-1}. The angular dependence of the hyperfine structure could not be analyzed for Ky5 center due to its relatively broad EPR linewidths, about 0.67 mT. Three times narrower lines are observed at about half-field range representing forbidden $\Delta M_S = 2$ EPR transitions where hyperfine splittings are found for some crystal directions. Based on the symmetry and closeness with spin Hamiltonian parameters in 6H-SiC [1] and 4H-SiC [2] the Ky5 center has been tentatively assigned to the neutral divacancy in cubic SiC. The annealing experiments are briefly discussed.

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Mon-1.15po

Study of oxide precipitates in silicon using X-ray diffraction techniques

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Keywords: silicon, oxide precipitates, X-ray diffraction

Structural quality of semiconductor wafers and epitaxial layers is an important parameter substantially influencing their electrical properties and the performance of fabricated integrated circuits. A reliable control of the defect nucleation and growth during the semiconductor technology is an important issue, since the defects may affect detrimentally the electric parameters of the semiconductor structures, but they can also be beneficial, because they can getter out impurities, especially heavy metal atoms.

Si wafers pass through the series of thermal operations during production technology of integrated circuits where the oxygen precipitation plays an important role. The dynamics and kinetics of this process has been associated mostly with the interaction of oxygen atoms and vacancies during Si ingot growth in recent years. Series of papers investigate physical models [1–3] which describe growth of bulk micro defects (BMD) and its space distribution as along the ingot axis as in radial direction for various growth rates. These models of BMD evolution during the ingot growth are formulated in a complex way, so that they involve diffusion effect, crystal growth rate, temperature gradients and mutual interaction between self-interstitials, vacancies and oxygen simultaneously.

We have used two different x-ray diffraction techniques to characterize oxygen precipitates in Czochralski grown silicon. The first one is a reciprocal space mapping in the Bragg diffraction, which is used to determine the deformation field around precipitate. This method however does not give the information about precipitate concentration.

The other method was simultaneous measurement of the diffracted and transmitted beam intensity in the Laue diffraction [4]. This method could give also concentration of the oxygen precipitates in the Czochralski silicon, which was experimentally justified.

The X-ray results of both methods are compared to the simulation of the precipitation process and to the interstitial oxygen measurement using infrared absorption spectroscopy and optical microscopy of etch pits.

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Mon-1.16po

VOH centre in Si: formation and thermal stability study

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Keywords: silicon, defects, hydrogen, DLTS, irradiation

Electrically active defects induced by fast neutron irradiation and subsequent annealing in n-type CZ-grown Si crystals have been studied by means of deep level transient spectroscopy (DLTS). Three electron traps with the activation energies for electron emission of 0.16, 0.24 and 0.42 eV were observed upon fast neutron irradiation. Traps E(0.16) and E(0.24) are assigned to vacancy-oxygen and double negative charge state of the divacancy, respectively. The most dominant trap E(0.42) is assigned to the single negative charge state of the divacancy. Upon annealing at low temperatures, while the intensities of the vacancy-oxygen and divacancy-related traps are decreasing, a new level emerges at 0.31 eV. This trap is the result of the hydrogen interaction with vacancy-oxygen pair. It is assigned to the VOH centre, and could be used as an indicator of hydrogen presence in silicon. The thermal stability of VOH centre has been found to be very high. In this work, formation rate as a function of the neutron fluence, as well as the thermal stability of the VOH centre has been studied in detail.

Mon-1.17po

Divacancy-oxygen defect in fast neutron irradiated CZ-Si

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Keywords: silicon, defects, DLTS, irradiation

Electrically active defects induced by neutron irradiation in P-doped Si crystals have been studied by means of capacitance transient spectroscopy. Several electron traps have been observed immediately upon irradiation. In this work we have focused on the E(0.24) trap which is assigned to the double acceptor state of the divacancy. As expected this trap anneals out at 220°C but its disappearance is immediately followed by the appearance of the new trap. The new trap has the activation energy for electron emisson of 0.23 eV. It is suggested that interstitial oxygen atoms are traps for the released divacancies. This interaction results in formation of the divacancy-oxygen defect which is responsible for the E(0.23) defect. A correlation between the accumulated dose of fast neutron irradiation and the formation rate as well as thermal stability of the divacancy-oxygen defect has been investigated.

Mon-1.18po

Divacancies in NTD–FZ–silicon for stable silicon resistivity at 20–160°C

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Keywords: silicon, divacancies, resistivity, power electronics

Conductance of silicon versus temperature was investigated in dependance on concentration of divacancy point defects. Flattening of temperature dependance for resistivity was achieved by means of radiation-thermal treatments. Initially high resistivity silicon ingots were used in experiments, which were undergoing neutron irradiation for n-type doping in a course of nuclear transmutation process. Electron irradiation was used for generation of point defects and thermal treatments were applied for annealing of some kind defects remaining divacancies in the bulk of silicon. Point defects concentrations before and after annealing were controlled by means of DLTS method. Temperature dependance of resistance were measured in range of temperatures 20, 180°C. For description of observed dependencies electronic states of divacancies were taken into account during calculation of conductivity. Multielectron nature of divacancies were assumed in the model as well as multicharge statistics was applied for evaluation of Fermi level, free carrier concentration and conductivity of silicon versus temperature. Mobility of carriers was estimated using semi empirical model described in [1]. Experimental curves for silicon resistivity were measured both before and after electron radiation and thermal annealing. In temperature range 20–160°C deviation of resistance became lesser as much as 10% of nominal value due to point defect introduction. Different curves for initial wafers reflect irregularity of resistance. Calculations of conductivity were provided to be in qualitative agreement with experiment results when only divacancy electronic spectrum was taken into account. Increasing of resistivity in high temperature range about 160°C was assumed to be possibly explained by presence of acceptor-type level near middle of forbidden gap. Involving certain concentration of acceptors possibly V_2O complexes in model was allowed more exactly to describe experimental temperature dependencies. Comparison of two models describing charge filling statistics for divacancies was compared. One model was based on multielectron statistics for hierarchy of deep levels in forbidden gap, meanwhile, other replace divacancy by three one-electron levels. Both models well corresponds to each other, quantatively describing free carrier concentrations versus temperature.

On basis of found regimes of electron radiation and subsequent thermal treatments power resistors were manufactured demonstrated improved characteristics of resistance. Stable resistance in temperature range 20–160°C was achieved. The optimum ratio free carrier concentration and deep levels was found for stabilization of resistance.

The powerful silicon resistors will find wide application in power electrical engineering, carrying out functions of protection, management and regulation. Such resistors are optimal for use with modern powerful semiconductor devices: diodes, thyristors, IGBT-modules etc. Obtained results may be interesting and for other semiconductor devices, which will require temperature stability for characteristics.

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Mon-1.19po

Self-assembling conditions of 4C10Sn nanoclusters in Ge: (C, Sn)

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Keywords: self-assembling, nanoclusters, isoelectronic impuruties

Self-assembling (SA) of 4C10Sn nanoclusters in Ge:(C, Sn) was predicted in [1]. Carbon and Sn are substitutional isoelectronic impurities in Ge. Therefore, Ge:(C, Sn) are ternary Ge-rich $C_xSn_yGe_{1-x-y}$ alloys. The covalent radii of carbon and Sn are smaller and larger, respectively, than that of Ge. Isolated carbon and Sn atoms dilate and shrink, respectively, a crystal lattice of $C_xSn_yGe_{1-x-y}$ alloy. The dilation and shrinking compensate each other after SA and, therefore, SA decreases the crystal lattice strains. Thus, SA of 4C10Sn nanoclusters in Ge-rich $C_xSn_yGe_{1-x-y}$ is preferable from the strain energy standpoint. The equality conditions of the free energies of random alloys and alloys in which all Sn atoms are located in 4C10Sn nanoclusters were obtained [1]. However, SA in Ge-rich CxSnyGe1-x-y when a fraction of Sn atoms are situated in 4C10Sn nanoclusters are not developed yet.

The SA conditions when a fraction of Sn atoms are in 4C10Sn nanoclusters are represented by the phase diagram of Ge:(C, Sn) in the dilute limits of the carbon and Sn contents. This fraction of Sn atoms is a cluster order degree. The phase diagram is obtained by the minimum condition of the free energy of mixing. The maximal cluster order degree depends significantly on the carbon content. The alloys with $x = 0.01$ and $x = 0.001$ have the maximal cluster order degree 0.86 and 0.23, respectively, at $y = 0.024$ and $y = 0.0075$, respectively, and temperature of 500°C. At this temperature the successful molecular beam epitaxy growth of C_xGe_{1-x} alloys up to $x = 0.032$ was demonstrated [2]. Thus, the Ge-rich $C_xSn_yGe_{1-x-y}$ alloys with the significant cluster order degree may be obtained if $x > 0.4y$. At this content condition

SA of 4C10Sn nanoclusters becomes more preferential from the thermodynamics standpoint than SA of 1C4Sn nanoclusters described in [3].

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Mon-1.20po

On the charge states of point defects in irradiated germanium

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Keywords: germanium, irradiation, point defects

For a long time, properties of point defects in Ge were out of the main stream of defect studies in semiconductors. Recently some technical applications of Ge and Ge-rich SiGe alloys regained close attention to investigations of intrinsic defects and impurity-related complexes in this material. A real breakthrough in DLTS and theoretical studies of point defects in Ge has been made over several years [1–4]. As a result, the modeling of defects in Ge is progressing rapidly. However, a striking inconsistency appears in interpretation of electrical properties of defects, especially their charge states. By way of example, the E-center (the vacancy-group-V impurity atom) is reportedly a double acceptor in Ge [1, 2]. This seems to be at variance with the earlier data on Hall effects measurements; see for instance review paper [5]. It is possible to reconcile the obtained DLTS and Hall effect data suggesting that the E-center is a single acceptor with two atomic configurations. The stable configuration is determined by the Fermi level position at thermal equilibrium or by injection conditions in the opposite case. The electron trapping properties of E-centers in DLTS experiments on irradiated n-Ge are thought to be determined by an energy barrier associated with electrically neutral E-centers with strongly distorted surroundings but not by their negatively charged states as is assumed. Another example is dealing with charge states of the so-called Ge–$P1$ defects studied in [6] and interstitial gallium atoms tentatively identified in [4]. Again, there is a conflict with Hall effect data [7] concerning the identification of radiation-produced defects and their charge states under thermal equilibrium. This report will also be supplemented with a short discussion of impurity-related defects in irradiated p-Ge as well as n-Ge subjected to n–p conversion under irradiation.

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Mon-1.21po

Titanium and nickel in Si: a first-principls study

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Keywords: theory, silicon, nickel, titanium, hydrogen

Ti and Ni are common 3d transition metal (TM) contaminants in Si, especially in photovoltaic material. The isolated TM species have been identified by techniques such as DLTS, EPR, and ENDOR. The NL29 EPR spectrum has been assigned to Ti^+ at an interstitial site with T_d symmetry. Substitutional Ti and interstitial Ni have not been directly observed in n- or p-type material, but substitutional Ni has been seen by EPR in n-type Si and photo-EPR in p-type Si. Interstitial Ti and substitutional Ni introduce levels in the band gap that reduce the lifetime of minority carriers. Ti and Ni also interact with hydrogen to form {TM,H} complexes, which affects their electrical activity. Both {TiH} and {NiH} complexes have been observed by DLTS. In this paper, we report preliminary results of theoretical studies of isolated Ti and Ni (both interstitial and substitutional) and their interactions with hydrogen. Our first-principles, density-functional based calculations are done using the SIESTA method. The configurations, electronic structures, activation energies for diffusion, and binding energies are calculated and the positions of the gap levels of the various defects are estimated, using the marker method, in supercells ranging in size from 64 to 216 host atoms.

Mon-1.22po

First principles method for calculating thermal conductvities in semiconductor supercells

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Keywords: non-equilibrium MD, thermal conductivity, silicon

The conventional density-functional-based first-principles method to calculate properties of impurities in supercell is extended to allow the calculation of thermal conductivities. The "usual" approach for calculating thermal conductivities (Green–Kubo formalism) is based on equilibrium molecular-dynamics (MD), and involves very slow-converging autocorrelation functions. These necessitate the use of empirical potentials in exhausting MD runs. The new approach uses temperature-controlled non-equilibrium MD, without thermostat, and is entirely of the "first-principles" type and therefore capable of handling impurities. The key is to reduce the thermal fluctuations, and this is achieved by "preparing" various parts of the supercell in thermal equilibrium at different temperatures, then monitoring how the heat flows through the system. Comparisons between calculated thermal conductivities $k(T)$ in Si supercells and the ones measured in Si nanowires will illustrate the technique. Preliminary results for k vs. impurity content will be presented.

Mon-1.23po

High resolution deep level transient spectroscopy of p-type polycrystalline diamond on p-type silicon

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Keywords: Laplace DLTS, diamond, defects, polycrystalline

We have applied high resolution Laplace Deep Level Transient Spectroscopy (LDLTS) at temperatures up to 600 K to thin polycrystalline semiconducting diamond films containing different amounts of boron, deposited on conducting p-type silicon. The technique has an energy resolution of approximately 5 meV, in contrast to conventional DLTS where the resolution can be as poor as 50 meV. To the best of our knowledge, examining defects in semiconducting diamond at these temperatures is a new application of the LDLTS technique. We have also directly measured trap capture cross-sections by DLTS.

The boron-doped diamond films were grown by hot filament chemical vapour

deposition at a process pressure of 20 Torr using 1% CH_4/H_2 as the process gases plus B_2H_6 as a variable, but controlled, gaseous source of boron. The single crystal (100) Si substrates were manually abraded before deposition using 1–3 μm diamond grit. Rhenium was used for the filament material, since Re does not act as a sink for carbon or boron species. The filament temperature was kept constant at 2400°C, and the substrate temperature was maintained at approximately 900°C. A growth time of 8 hours gave a diamond film thickness of 3–4 μm. The boron concentration in the diamond film ranged from approximately 7×10^{18} cm^{-3} to 2×10^{20} cm^{-3}. Schottky contacts were fabricated on the diamond film and Ohmic contacts on the Si. Assuming a low ionisation rate of the boron in the diamond, the Si resistivity was chosen in order that the majority of the depletion region was contained in the diamond.

Conventional DLTS was carried out on the diode and a combination of peaks was observed, with some broader than others. LDLTS was then carried out at the temperatures correlating to these peaks. There are several different emission rates at 170 K and a similar result was obtained at a range of temperatures. Activation energies could not be found from the LDLTS data, since emission rates did not consistently reduce with temperature, yielding an inaccurate Arrhenius plot. This is attributed to the presence of strain fields in the sample. Capture cross-section measurements also show that these peaks exhibit a time-dependent capture cross-section, which is indicative of carriers being trapped at large electrically active defects. We show that a combination of LDLTS and direct capture cross-section measurements can be applied to semiconducting diamond to understand whether defects possess single or multiple energy levels, and whether the trapping is at an isolated point defect or at an extended defect. The results are discussed in terms of boron segregation to grain boundaries.

Mon-1.24po

Use of DLTS measurements to determine defect cluster parameters in ion and neutron irradiated semiconductors

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Keywords: DLTS, silicon, clusters, ion implantation, modelling

DLTS is an important technique for defect characterization in semiconductor structures. Its application to point defects is well known and described in many reviews and textbooks. However the correct treatment of DLTS data is not well elaborated for structures containing defect clusters. Knowledge of defect cluster parameters (for example, the number of defects in a cluster and its physical size) is often important to understand impurity and defect related process in semiconductors and semiconductor structures. At present two characteristic features of cluster-type defects in silicon are well established. Firstly, there is often a particular temperature dependence of the DLTS peak heights ($S_{\text{peak}}(T_{\text{peak}})$) and a closely related is that there is an difference in the peak height of the divacancy peaks [1–4]. Secondly, a key feature is the "stretched exponential" kinetics that needs to be applied to understand the filling of clustered traps [3–4]. Both these features are caused by the potential barrier for charge carriers around defect clusters.

The purpose of this paper is to elaborate an approach for the determination of the cluster parameters using the temperature dependence of DLTS peak height. We have performed numerical simulations of the potential distribution around a spherical cluster which allow us to deduce $S_{\text{peak}}(T_{\text{peak}})$ dependence related to potential barrier. It has been shown that using semiconductors with different doping level we can distinguish contributions of isolated and cluster-type defects.

Silicon diodes irradiated with different particles (neutrons, He and Xe ions) were used to obtain experimental validation of the approach used for the modeling. The obtained data shows that the correct interpretation of experimental DLTS spectra requires us to take into account the l-effect [5], occupancy of defects with low capture cross-section [6] and peak superposition for defects obeying the Meyer–Neldel rule. It has also been shown that for all the irradiation particles the core of the clusters consists of radiation defects which have different properties from di- and tri-vacancies.

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Mon-1.25po

Electron paramagnetic resonance spectroscopy of lithium donors in monoisotopic silicon

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Keywords: magnetic resonance, monoisotopic silicon, shallow donors

Electron paramagnetic resonance (EPR) spectra are reported for the lithium-related donors in monoisotopic silicon. In silicon of natural abundance of isotopes the line width of resonances are caused by unresolved hyperfine interactions with the magnetic nuclei of ^{29}Si isotope. In [1, 2] the contribution of ligand superhyperfine interaction to the line width of paramagnetic shallow and deep centers in silicon by numerical calculation have been analyzed. The results have shown linear behavior of the line width for all centers at low concentrations of magnetic nuclei and square-root character for high concentrations. In this work high resolution spectra of lithium donor centers in monoisotopic silicon, enriched by ^{28}Si isotope (99.99%) with very narrow lines which confirm calculations [1, 2] are reported. Three types of samples are studied: two samples are ^{28}Si enriched floating zone silicon with lithium concentration about 10^{16} cm^{-3} and 10^{18} cm^{-3} consequently, and one sample is crucible-grown silicon with natural abundance of isotopes and lithium contamination about 10^{18} cm^{-3}. Only single line is observed in natural silicon sample. This line was earlier described in [3]. In monoisotopic silicon sample with low concentration of lithium the trigonal EPR spectrum, with well resolved ^{7}Li hyperfine structure is recorded in temperature range 3.5–20 K. This spectrum was earlier attributed to LiO complex in [4]. At high concentration of lithium in monoisotopic silicon two types of spectra are observed. The trigonal one has the same feature as for low concentration of lithium with g-values: $g_{||} = 1.9974$ and $g_{\wedge} = 1.9989$. Another spectrum consists of two lines and has tetragonal symmetry with $g_{||} = 1.9992$ and $g_{\wedge} = 1.9983$. This spectrum is more intensive than trigonal one and has no resolved hyperfine structure due to time averaging of the hyperfine interaction. Only single EPR line of axial symmetry about [001] with $g_{||} = 1.9997 \pm 0.0001$ and $g_{\wedge} = 1.9987 \pm 0.0001$ has been observed in [5] in silicon under strong uniaxial compression along [001] or tension along [110] which was identified as due to isolated lithium in silicon. We can attribute our tetragonal spectra to single donor electron state. Nevertheless, high lithium concentration which is closed to Mott transition range and unresolved ^{7}Li hyperfine structure give rise to suggest that donor electron undergo the hopping motion and the hyperfine interaction is averaged by this motion. For trigonal spectrum that is caused by LiO center the electron states are more localized and the width for some lines of spectrum have very small values dH $\sim$ 0.03 G. This is less than can be predicted from square root behavior and confirms the linear dependence of the hyperfine contribution to the line width.

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Mon-1.26po

Nonuniform boron precipitation in Si at the Ostwald Ripening stage

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Keywords: precipitate, boron, silicon, Ostwald Ripening

It is known, that the Ostwald Ripening theory can be applied to the number of defect related phenomena. They are an impurity precipitation, the growth of {113}-defects and dislocation loops in Si and void swelling in metals. The Ostwald Ripening fundamentals were given by L. Lifshitz and V. Slyozov for a uniform ensemble of precipitates in solids [1]. The purpose of this work is to apply the Ostwald Ripening theory to describe a nonuniform distribution of boron precipitates induced by high-dose boron implantation into highly- boron doped Si with concentration $C_{\mathrm{Bo}} = 2.5 \times 10^{20}\ \mathrm{cm}^{-3}$, after annealing at $T = 900°\mathrm{C}$.

The developed numeric model includes the boron precipitates randomly distributed in 3D space and surrounded with solution of substitutional boron atoms. The equilibrium concentration of solute boron atoms close to the precipitate surface is given by the Gibss-Thompson equation [1]. The precipitate growth/dissolution rate is considered equal to the diffusion flow through the precipitate surface. The diffusion task for the solute boron concentration in-between precipitates is solved numerically at the uniform time-3Dspace mesh. In the beginning boron precipitates are distributed randomly at the space mesh nodes in accordance with the implanted boron profile. Because of well-known G. Watkins reaction: $\mathrm{I}+\mathrm{B}_s \rightarrow \mathrm{B}_s\mathrm{I} \rightarrow \mathrm{B}_i$, the starting solute boron distribution can be assumed to be equal the initial C_{Bo} distribution minus the as implanted interstitial (I) distribution. This leads to a zero concentration of substitutional boron atoms around R_p (mean project range of implantation) and almost unchanged initial concentration C_{Bo} at the both edges of implanted layer. Thus the precipitates at the edges are the overcritical ones and start to grow by consuming boron atoms from the solution. At the same time precipitates around R_p are the subcritical ones and tend to dissolve by emission the boron atoms at first. The second assumption we have made is that the subcritical precipitates start to shrink from edges toward R_p step by step. The subcritital precipitates close to the edges start to dissolve first and provide a local excess of substitutional boron atoms. This makes the subcritital precipitates, located next to them toward R_p and starting later, to become overcritical. Such a wave-like process of the precipitate shrinkage and growth from edges toward R_p is supposed to be a reason for several maximums and minimums formation, observed at boron profiles in [2]. The third assumption in our model concerns the effective diffusion coefficient of boron atoms in the region of precipitate ripening. This coefficient should be much higher then the classical one due to enhanced diffusion by a self-interstitial flow from growing precipitates toward shrinking ones.

With all these three assumptions above, the Ostwald Ripening model is able to describe the nonuniform boron profiles, obtained by SIMS in [2]. The developed model correctly predicts the number of maximums at the boron profile, but the positions and amplitudes of calculated maximums should be refined for better consistence with experiment.

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Mon-1.27po

Characterization of major In-grown stacking faults in 4H-SiC epilayers

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Keywords: 4H-SiC, stacking faults, photoluminescence mapping

SiC can crystallize in over 200 different polytypes. The multiplicity of structures is the consequence of the very low energy necessary to locally change the stacking sequence in any of the crystalline forms of SiC. For that reason, the planar defects, stacking faults (SFs), are the common defects in 4H-SiC. They manifest as hetero-polytype structures of limited thickness in 4H-SiC, which appear spontaneously during the growth or a later processing step such as doping, annealing, oxidation or implantation or, even, in electrically stressed p-i-n diodes [1]. SFs give strong negative impacts on the device performance and its long-term stability. In order to suppress the deleterious effects of SFs on 4H-SiC device structures, the formation of these SFs must be understood so that a plan for controlling them can be formulated. And meanwhile, a highly practical analysis method is imperative to easily and quickly characterize the SFs in the epilayers. The aim of this paper is to spatially profile the SFs in 4H-SiC epilayers using the micro-photoluminescence (micro-PL) mapping method carried out at room temperature and to reveal the stacking sequences of identified SFs using high-resolution transmission electron microscopy (HR-TEM). SFs in 4H-SiC form quantum-well-like electronic states which can be observed by luminescence [2]. Three different kinds of in-grown SFs have been successfully identified in the samples based on the micro-PL spectra. Each kind of SFs shows the distinct PL emission with a peak wavelength located at 500, 480, and 460 nm, respectively. Micro-PL intensity mapping at each of these wavelengths (band energy) has been performed to spatially profile the shape and location of each SF. In order to identify the stacking sequence of each in-grown SF, the samples are etched in molten KOH at 500°C for 5–10 min. This step produces two etching pits corresponding to two basal plane dislocations (partial dislocations) and a groove corresponding to the intersection of SF with the epilayer surface for each SF. The TEM specimens are cut from the part of the SF where the defect intersectes the surface. The stacking sequences of these three in-grown SFs have been revealed by HR-TEM observations, as (6,0), (3,5), and (4,4) in the Zhdanov's notation, respectively, which apparently differs from the perfect 4H-SiC, (2,2). That means three kinds of in-grown SFs identified in the samples are double Shockley SF (500 nm), triple Shockley SF (480 nm), and quadruple Shockley SF (460 nm), respectively. The formation mechanisms of these in-grown SFs are also discussed at the conference.

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Mon-1.28po

Laser-induced extended defects in compositionally graded SiGe layers

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Keywords: SiGe, laser treatment, TEM

Thin layers of crystalline silicon-germanium (SiGe) alloys are attractive for thin-film electronic devices (e.g. TFT), photodiodes, infrared photodetectors and next generation of solar cells. One of the major advantages of alloying Ge with Si is the enhanced optical absorption of the alloy in comparison to pure Si. Laser crystallization of amorphous SiGe alloys is a promising method for preparation of crystalline SiGe layers on foreign substrates.

In this study, thin amorphous or microcrystalline SiGe layers were CVD deposited in a compositionally grading manner on (001)-Si wafers at temperatures between 300 and 450°C. The thickness of the layers varied between 50 and 300 nm. The samples were then crystallized with a pulsed Nd:YAG laser operating at a wavelength of $\lambda = 1064$ nm, a pulse length of 15 ns, an average energy density between 0.5 and 1.9 J/cm^2, and a repetition rate of 25 Hz. Structural properties were characterized by transmission electron microscopy (TEM) and atomic force microscopy (AFM). Composition variations of the SiGe samples were measured using Rutherford backscattering spectrometry (RBS).

According to TEM, amorphous or microcrystalline as-deposited layers showed, after laser annealing at different energy density, textured columnar grain polycrystalline or dislocated/twinned single crystalline microstructure. AFM images reviled noticeable surface roughness depending on the pulse energy of laser treatment. RBS spectra showed that depth redistribution, alloying and surface segregation of Ge takes place at high energy of laser pulse. Reliable phonoconductivity values are extracted as a function of energy density of laser annealing. The results are discussed within the model of liquid-phase recrystallization.

Mon-1.29po

The optical spectra of structure defects in the diamond

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Keywords: theory experiment, modeling

The photoluminescence and absorption spectra of the two systems with the main lines 415.2 nm and 741.0 nm of natural diamond crystal of types Ia at 77–300 K was investigated. The spectra consists from the main line and wide band in the short-wavelength (for the absorption) and long-wavelength (for the photoluminescence) spectra range. The nature of these spectra is the electron-phonon interaction. The diamond crystal is the most convenient object for such investigation. The width of forbidden band is 5.5 eV. Diamond crystal has a big extent of one-phonon spectra. It is 1333 cm^{-1} and has small value of the Stokes shift.

For system 415.2 nm the structural spectra are typical. The Van–Hov features of quasilocal oscillations were observed in the region of one phonon spectra (the shift from main line less than 1333 cm^{-1}). Deviation of the photoluminescence and absorption spectra from mirror symmetry was found. (The frequencies of quasilocal oscillations, the stokes shift and types of the Van-Hov differ).

The photoluminescence and absorption spectra of second system 741.0 nm are less structural (smaller frequencies of quasilocal oscillations, greatest stokes shift and different types of the Van-Hov features). The deviation of the photoluminescence and absorption spectra from mirror symmetry also found.

For studied system one phonon spectra was calculated and they were compared with the spectral distribution of one phonon spectra frequencies. The reason of deviations is discussed.

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Mon-1.30po

Luminescence of Xe-V defect in diamond

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Keywords: diamond, Xe-V defect, luminescence

Ion implantation doping is widely used to modify semi-conducting properties of diamond for advanced electronic and optoelectronic applications. Many implanted ions create in diamond optically active defects having emission lines in broad spectral regions, including visible and near-infrared. These optical centers may be used in advanced photonics and optical communication applications like single photon emitters [1] or diamond light emitting diodes [2]. Another advantage of ion implantation is the possibility to control the dose and the energy of ions, which gives a robust tool for device fabrication. On the other hand, ion implantation creates a number of radiation defects which influence properties of optical emission from the center.

We will report on micro-Raman and photo- and electroluminescence studies of Xe-ion implanted diamond crystals. Artificial and natural diamonds were implanted with Xe-ions within the wide dose range of $10^{10}-5 \times 10^{14}$ ion/cm^2. Our interest in the Xe-V defect originated from the fact that this center is one of a few having sharp emission spectra in the infrared spectral region. At low temperatures, the photoluminescence spectra featured the single zero phonon lines at 811.7 nm and a weak phonon sideband [3]. The room temperature luminescence consists of a zero phonon line at 813 nm and a weaker line at 794 nm. The Xe-V defect in diamond was previously considered theoretically as a potential n-type donor [4]. It was concluded that due to its large size, the Xe ion generates stresses and yields a stable configuration in the off center divacancy site. Our luminescence studies support the calculated structure: vacancies are involved in the formation of this defect [3], it contains a single Xe ion, and Xe-V is a $\langle 111 \rangle$ oriented trigonal defect. With purpose to observe a single defect luminescence, we performed confocal micro-luminescence mapping of the transitional area between the Xe-ion implanted (dose of 10^{10} ion/cm^2) and non-implanted regions based on changes in the 813 nm line intensity. This approach allowed us to study a luminescence profile at different doses through the implantation boundary and detect as low as a few defects per μm^2.

The damages induced by ion implantation at different doses were characterized by Raman spectra and relationships between the diamond phase and the graphitic phase for different doses of ion implantation will be discussed. Micro-Raman mapping of the transitional region between diamond and graphitic phases based on the Raman peak positions for diamond (1332 cm^{-1}) and graphite phase (G-band at 1600 cm^{-1}) was demonstrated.

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Mon-1.31po

Vacancy clusters created via low temperature irradiation in 6H-SiC

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Keywords: vacancy clusters, silicon carbide, magnetic resonance, fine structure

Since dopant atoms hardly diffuse into SiC, ion implantation is the preferred doping method, which results in various radiation-induced defects. High temperature annealing is required to reduce unwanted by-products. Valuable information of the annealing process can be gained from the unannealed samples, which provide good insight in the conditions before the annealing process. It is quite intuitive that the omnipresent vacancies introduced by the radiation are compensated by the creation of interstitials. In this context it is common consensus, that mobile split-interstitials, either intrinsic ones like the carbon split-interstial $(\text{CC})_C$ or those in connection with dopants, play a central role in the beginning of the annealing process. Although being highly important, these defects are controversially discussed and some of them could still not conclusively be assigned to experimentally observed electron paramagnetic resonance (EPR) spectra (e.g. [1]). In unannealed 6H-SiC samples that were electron irradiated at room temperature, the EIn/EI3 [1, 2] of $(\text{CC})_C$ remain the dominant EPR spectra. However, besides V_{Si}^{-}, further S=1 triplet spectra are observed. Some of them are well-known from irradiated p-type material and are most probably vacancy-related. At least one of them (EIm) of unknown microscopic origin was not reported before and has the strongest fine structure constants observed so far in SiC ($D = 652 \times 10^{-4}$ cm^{-1}). A positive sign of D demonstrates that the spin-orbit contribution to the zero-field splitting exceeds by far that of the spin-spin coupling. Moreover, the intense EPR-lines with isotropic g-tensor ($g = 2.0018$) allows the observation of resolved hyperfine (hf) lines due to 4 silicon ligands. Already after low temperature annealing the EIm spectrum is vanished and instead the well known P6/P7 spectra [3, 4] appear. Assuming recombination with the mobile $(\text{CC})_C$ split-interstials, this annealing behavior suggests vacancy clusters like $V_CV_{Si}V_C$ as initial defects created via low temperature irradiation. This tentative assignment of the EI*m* spectrum is supported by the EPR parameters calculated from first principles, the hf parameters, as well as the elements of the g-tensor. Furthermore, the exceptionally high zero-field splitting D can be qualitatively understood by the occurance of additional close-lying defect levels resulting in comparatively large second-order spin-orbit coupling in the vacancy clusters.

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Mon-1.32po

Formation of Frenkel pairs and diffusion of self-interstitial in Si under normal and hydrostatic pressure: quantum chemical simulation

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Keywords: Frenkel pair, self-interstitial, diffusion, hydrostatic pressure

The effect of stress on diffusion in silicon has recently taken on more importance for microelectronics. To increase mobility of charge carriers in semiconductor transistors with dimensions $\leq$ 90 nm the special procedures for forming of strain regions are used (so-called strain engineering). Stress effects on diffusion have been blamed for significant deviations in the device characteristics for both n-type and p-type metal-oxide semiconductor transistors. On the experimental side, contradictory results for the qualitative influence of stress on boron diffusion further motivate a fundamental investigation of stress effects on diffusion. Generally, the process of diffusion of dopant is connected with formation and generation of native point defects — self-interstitial atoms and vacancies. However, experimental data on coefficients of diffusion of self-interstitial atoms and vacancies in strained crystals are practically unknown. In the present work we present the results of quantum chemical (semiempirical (NDDO-PM5, PM6) and ab-initio (SIESTA) methods) simulation of effects of hydrostatic pressure on energy of formation of a separated Frenkel pair and energy of formation of vacancy and self-interstitial in Si crystal. The detailed analysis of process of diffusion of self-interstitial at hydrostatic pressure is presented also. It is found, that hydrostatic pressure lead to decreasing of energy of formation of a separated Frenkel pair. And decreasing of energy of formation of Frenkel pair is determined by decreasing of energy of formation of vacancies while energy of formation of self-interstitials practically not changes. For the self-interstitial in charge state I^0 ($Z = 0$) the more stable configuration is the split $\langle 110 \rangle$ (dumbbell) configuration. The tetrahedral configuration is not stable, an interstitial atom being shifted from T position in a new position T1 on a distance $\Delta d = 0.2$ Å. The hexagonal configuration is not stable in NDDO approximation. In charge states $z = +1, 2$, and also in excited triplet and singlet states the equilibrium configuration is the tetrahedral (T) configuration. Hydrostatic pressure does not lead to change of an order of stable configurations of the self-interstitial. The diffusion barrier and pre-exponential factor for diffusion of the self interstitial in charge state $z = 0, +2$ have been evaluated and are $\Delta E_a(I^0) = 0.59$ eV; $\Delta E_a(I^{++}) = 1.15$ eV; $D_0(I^0) = 5.7 \times 10^{-4}$ cm^{2}s^{-1}. Hydrostatic pressure decreases the diffusion barrier and slightly influences on the pre-exponential factor. The activation barriers for self-diffusion of vacancy ($\Delta E_{sd}(V^0) = 4.28$ eV), self-interstitial ($\Delta E_{sd}(I^0) = 5.02$ eV), energy of formation self-interstitial ($E_f(I^0) = 4.43$ eV), vacancy ($E_f(V) = 3.78$ eV) and Frenkel pair (E_f(Frenkel) $= 3.59$ eV) were evaluated and are in a good agreement with experimental ones.

Mon-1.33po

Amorphous silicon clusters embedded in crystalline silicon and the space charge sign inversion problem

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Keywords: amorphous silicon, type inversion, radiation damage, DFT

It is a well-known empirical fact that n-type oxygen-containing silicon in radiation detectors undergoes a type inversion to p-type under hadron or electron bombardment. This effect, also known as the Space Charge Sign Inversion, is a limiting factor in the lifetime of radiation detectors, especially those in harsh radiation conditions such as the LHC or the prospective CLIC particle accelerators in CERN. Despite much research into the problem, the phenomenon is not yet fully understood.

We use a novel approach towards the problem by studying the electronic density of states of amorphous silicon clusters embedded in otherwise crystalline silicon. These systems emulate the amorphous zones that are formed in the silicon when the material is subjected to energetic particle bombardment. We use classical molecular dynamics simulations for first creating the ionic configurations of the systems. Then, we determine the electronic structure of these systems by using plane-wave, pseudopotential density functional theory calculations.

Our results show that the introduction of amorphous zones into the silicon causes the formation of abundant localized electronic states within the band gap of the material. These states are likely to reduce n-type conductivity, and they possibly also enhance p-type conductivity, thus accounting, at least partially, for the observed type inversion. The validity of the method is also assessed and found to be sufficient for at least a semi-quantitative description of the systems.

Mon-1.34po

Control of impurity diffusion in silicon by IR laser excitation

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Keywords: diffusion, IR excitation, resonance

Control of impurity diffusion is an important element in the device technologies of the present days. Usual thermal processes have an inherent disadvantage that not only the intended species but also all impurities involved are equally affected. This imposes many restrictions on the device process. In order to remove such restrictions, it is desirable to diffuse the specific species only. One of such attempts is use of infrared (IR) excitation [1]. The idea is that every impurity has its own local vibrations in the host crystal. The frequency is dependent of impurity species. Irradiation of IR laser with the resonant frequency could cause excitation of the local impurity modes, which results in the selective enhancement of the diffusion of that impurity.

Unfortunately, there is a well-known and big problem for this aim, that is, there is no suitable IR laser sources. The missions of the theoretical study are to confirm this effect by simulations, and, if effective, to derive the conditions where this effect appears. This makes it possible to design the laser experiment, if appropriate light sources are available.

The resonant effects of impurity modes have been studied by first-principles MD simulations [2]. An external electric field with an IR frequency is applied to the impurity atom only. We observe that IR excitation is effective for O and B impurities, while is ineffective for P. Based on the MD simulations, we are able to design the IR excitation experiment in order to observe an appropriate effect on atom migrations. The needed power of IR laser depends on the lifetime of the local mode under investigation. The lifetime of phonons is basically predictable by ab initio calculations [3, 4]. For those modes of sufficient long lifetime, a design of a real experiment is given in this study.

Based on these FP–MD simulations, we have drawn the first draft of experiment in SPring-8 facility. We report a first-time attempt of diffusion control of impurities by IR excitation, by using an intensive synchrotron radiation facility, BL43IR of SPring-8. Although the result is discouraging, the plan, experimental setup, irradiation experiment, and the result on the impurity diffusion, are described in detail, in hoping improvement of experiment in the future. It is suggested that the input power employed in the present experiment is not enough to observe the intended results.

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Mon-1.35po

Photoluminescence from triplet states of isoelectronic bound excitons at interstitial-carbon-interstitial-oxygen defects in silicon

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Keywords: silicon, C-line, triplet state, photoluminescence, isoelectronic center

We have observed photoluminescence (PL) from triplet states of isoelectronic bound excitons (IBEs) at hole-attracting interstitial-carbon-interstitial-oxygen (C–O) defects in silicon (Si). The isoelectronic defects can act either as an electron trap or as a hole trap [1]. Once the primary particle is captured by the short-range defect potential, the second particle with opposite charge is attracted by the long-range Coulomb potential of the effective-mass-like states, so forming the IBE. C–O defects are known as hole-attracting isoelectronic defects [2]. Because of the low symmetry of the C–O defects, the orbital angular momentum of the hole must be quenched. Therefore, the excitons bound to C–O defects possess singlet-triplet states [2]. However, luminescence from the triplet states has not been reported the past. The present work reports detection of luminescence involving the triplet states of C-O defects for the first time using a bulk ^{nat}Si ([^{28}Si] = 92.2%, [^{29}Si] = 4.7%, [^{30}Si] = 3.1%) crystal, and isotpically enriched bulk ^{28}Si ([^{28}Si] = 98.07%), ^{29}Si ([^{29}Si] = 99.23%), and ^{30}Si ([^{30}Si] = 98.74%) single crystals.

PL measurements from C-O defects in ^{nat}Si show not only a strong 789.66 meV line (C-line) [3] but also a 787.03 meV line, which we call C_T-line. The energy difference between these lines (ΔE) is 2.63 meV and this is consistent with the previous time-resolved PL measurement that yielded $\Delta E = 3.2$ meV [4]. In addition, our PL measurements show the energy shift of C_T-line due to the different silicon-isotopic compositions and its trend is the same as that of C-line. This fact indicates that C_T-line is not a phonon replica of C-line but is a no-phonon line just like C-line. We have also performed Zeeman PL spectroscopy. It shows that C_T-line splits into three peaks under magnetic field indicating that C_T-line is composed of three degenerate states. Moreover, its peak position does not depend on the angle between the magnetic field direction and crytalograhic orientation. No dependence on the angle implies for the quenched angular momentum. Thus, we conclude that C_T-line is the photoluminescence from the triplet state. It should be noted that the excited triplet state of C–O defects, as well as of divacancy (V+V) and vacancy-phosphorus (V+P) defects, were predicted by analysis the experiments on optical nuclear polarization in silicon [5]. Later, the excited triplet states were found by electron paramagnetic resonance for (V+V) and (V+P) [6], but not for C-O defects so far.

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Mon-1.36po

Dynamics of reorientation of single lattice vacancy in silicon

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Keywords: silicon, vacancy, Jahn-Teller effect, reorientation

Recently, elastic softening of crystalline Si at low temperatures below 20 K has been observed by ultrasonic measurements [1]. It has been argued that this softening is due to single lattice vacancy. However, the mechanism of the softening proposed has some contradictions to previous understandings [2] especially in Jahn-Teller (JT) energy and the symmetry of JT distortion of vacancy. In order to solve these contradictions and to elucidate the softening mechanism, we have studied the vacancy using first-principles calculations.

First-principles molecular dynamics simulations which we performed show that the reorientation of the JT distortions can easily occur for V+, and we have suggested that the dynamics of the reorientation may be related to the softening [3]. Therefore the barrier height of the reorientation called reorientation energy is very important. For V+ the reorientation energy is evaluated in the range between 50 K and 300 K. This value is in good agreement with an experimental value of 13 meV [2]. On the other hand, for V0 the reorientation energy is higher than 300 K which also agrees with the experimental value of 230 meV. However, accurate values and the detailed path of the reorientation have not been calculated yet.

In present work, we calculate the reorientation energy in more detail and clarify the reorientation path. For this searching, we adopt Force–Inversion method. In addition, we present the adiabatic potential surface around JT distortions.

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Mon-1.37po

Electron spin resonance of palladium-related defect in silicon

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Keywords: palladium, silicon, defect structure, electron spin resonance

The properties of transition-metal (TM) impurities in Si have been studied intensively for long. The defect structures, the electronic levels, and the local vibrational modes of various TM-related defects have been identified by measurements of electron spin resonance (ESR), deep-level transient spectroscopy (DLTS), and optical-absorption spectra. In particular, the valuable information on the defect structure can be obtained by ESR measurement. Observation of the ESR of palladium (Pd) and platinum (Pt) was reported by Woodbury and Ludwig [1]. The ESR signal of Pd in n-type Si is anisotropic. It is indicated that Pd in Si is a defect of orthorhombic (C_{2v}) symmetry. It is thought that the Pd atom with the negative charge state (Pd^-) and spin equal to 1/2 occupies at a substitutional site distorted by displacement of Pd along $\langle 100 \rangle$ direction. In this study, we have found a different Pd-related defect from a substitutional Pd with (C_{2v}) symmetry by ESR measurement. The ESR signal of the Pd-related defect shows different g-value and symmetry from those of a substitutional Pd. The samples were prepared from P-doped CZ Si. Palladium was evaporated on one side of sample, which was sealed in quartz capsule with Ar gas at a pressure of 0.2 atmosphere and annealed at 1250°C for 24 h, followed by quenching in water. ESR measurements were performed at 12 K with an X-band spectrometer. The ESR signal due to substitutional Pd in the negative charge state (Pd^-) was observed in the sample. The signal is composed of a center line and six satellite lines due to ^{105}Pd isotope with nuclear spin $I = 5/2$ and natural abundance 22.2%. The anisotropic g-values of g[-110] = 1.91, g[001] = 2.05, and g[110] = 1.97 for a substitutional Pd obtained in this study are comparable to previously reported g-values [1] and the anisotropy indicates that the substitutional Pd is the defect of orthorhombic (C_{2v}) symmetry, as reported by Woodbury and Ludwig [1]. In addition to the ESR signal due to the substitutional Pd, we have found new ESR signal in the sample. The new signal also shows the hyperfine structure of Pd. Therefore, it is though that the new signal is originated from Pd-related defect. The new ESR signal has anisotropic character of monoclinic (C_{1h}) symmetry. The calculated g-values are $g_1 = 1.97$, $g_2 = 2.03$, $g_3 = 2.16$, and the g_1 axis is along $\langle 110\rangle$ direction. The g_2 and g_3 axes are perpendicular to the g_1 axis. The g_2 axis is rotated from $\langle 100\rangle$ to $\langle 111\rangle$ direction at the angle of 51°. The Pd-related defect might be an interstitial Pd or a complex of Pd and other impurities.

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Mon-1.38po

The photoluminescence of the thermo-treated silicon

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Keywords: Si, photoluminescence, thermodonor, thermodefect

Thermal treatments during Si crystals and layers growth lead to electro-active defects (oxygen thermodonors) formation [1]. At the present work the influence of the thermal defects and thermal treatments on the near-edge photoluminescence (PL) [2] is investigated.All the initial Si crystals regardless of conductivity polarity, oxygen contamination, growth method show the broad near-edge PL with maximum at $E = 1.084$ eV. The doping level increment leads to the PL band fusion which is may be caused by gap band decrement.

Starting from the assumption about the bulk defect influence on the PL intensity, the thermal treatments in the dry nitrogen ambient at the temperatures $T = 300$–1050°C were carried out. Such a defect may act as the center for non-radiating recombination or as the trap for nonequilibrium carriers. The PL intensity growths in the $T = 400$–550°C region. As the temperature increases, the PL decreases in the region $T = 600$–650°C and has a rather growth at the $T = 700$°C. The PL vanishes at $T = 900$°C and higher. In order to control the PL behavior after the $T = 1050$°C treatment the thermal-treated sample was repeatedly annealed at the same temperature region 300–1050°C. The sample show the same regions of PL intensity growth and decreasing but at the greatly less level.

The presence of thermal oxide grown at $T = 1100$°C on the silicon surface leads to the PL intensity increment. Removing of the oxide leads to PL intensity decrement, which agrees with previous data on PL dumping by annealing. This effect shows the passivating role of oxide on the silicon surface.

The PL depth profile after thermal treatment at $T = 1050$°C show PL intensity decrement in whole crystal volume. This may be caused by uniformly generated centers for non-radiating recombination.

On the basis of our experimental data one can assume generation of the thermal defects during the crystal growth and treatments which leads to generation of the traps for nonequilibrium carriers. Devastation of traps leads to radiating recombination giving contribution to the near-edge PL at 1.084 eV.

The coincidence of the thermal intervals for the defects annealing and reconstruction with thermal intervals for oxygen thermodonors (I and II types) generation and annealing [1] permit us to suggest the traps formation by oxygen thermodonors with Ec-(0.09 . . . 0.15 eV) level [3]. Within the framework of our interpretation the observed PL acts as the check method for Si crystal characterization on the presence of the oxygen thermodefects.

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Mon-1.39po

Oxygen diffusion diffusion in $Si_{1-x}Ge_x$ alloys

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Keywords: SiGe, oxygen, diffusion

Oxygen is the main technological impurity in Si and $Si_{1-x}Ge_x$ alloys grown by Czochralski method. It takes part in formation of a great number of defects during irradiation and thermal treatments. Many defects (all types of thermal donors,

V_nO_m defects) are created at thermally stimulated diffusion of oxygen. In $Si_{1-x}Ge_x$ alloys the rate formation of such defects is known to be suppressed in comparison with Si. One of the main motives of this effect may be the changing of oxygen diffusivity in $Si_{1-x}Ge_x$.

A few papers were published till now in which the diffusion of oxygen in $Si_{1-x}Ge_x$ alloys was discussed. Some authors made a conclusion that Ge reduces diffusion of oxygen, and other assert that accelerates. In this paper we present new data concerning the oxygen diffusion in $Si_{1-x}Ge_x$ alloys. The diffusivity has been determined from the study of recovery kinetics of stress induced dichroism in the 1107 cm^{-1} oxygen absorption band. Ge content in samples investigated was $x = 0.01 - 0.05$.

It has been found that the recovery kinetics in $Si_{1-x}Ge_x$ alloys consists of two stages, fast and slower. The oxygen atom in $Si_{1-x}Ge_x$ lattice is known to connect with Si atoms and avoids formation of Ge–O bonds [1]. But with increasing Ge content a considerable part of oxygen is known to have Ge atom as the second neighbor. We suppose that two stages observed in recovery of the stress induced dichroism are bound up with diffusion of oxygen being in two configurations. One stage observed in dichroism recovery in $Si_{1-x}Ge_x$ alloys brought into correlation with the diffusion of oxygen surrounded by Si atoms, and the other with diffusion of oxygen having Ge atom as the second neighbor. The values of oxygen diffusivity for oxygen in these two configurations have been determined. It has been shown that with increasing Ge content oxygen diffusivity is reduced for both configurations.

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Mon-1.40po

Interstitial oxygen in Ge doped with tin

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Keywords: germanium, tin, oxygen

In recent years, the investigation of the properties of germanium has become a matter of considerable interest particularly concerning extremely scaled integrated circuits. The Ge doped with Sn or Si can be promising materials for the construction of ultra fast devices. The presence of defects and impurities in semiconducting materials is known to impact the device performance. In this work the influence of tin doping with concentration of $N_{Sn} = (1-4)10^{19}$ cm^{-3} on the behavior of ν_3 vibrational mode of oxygen (Ge–O–Ge quasimolecule) have been studied. The ν_3 vibrational mode of oxygen in Ge is known to consist at low temperatures of series of ~ 30 absorption bands due to different isotopic combinations of Ge atoms (^{70}Ge, ^{72}Ge, ^{73}Ge, ^{74}Ge and ^{76}Ge) in quasimolecule and of the coupling of ν_3 with the low energy symmetric bending ν_2 mode [1]. It has been found that in Ge doped with Sn three additional series of absorption bands appear besides the ν_3 mode. The higher is the Sn content in Ge, the stronger is additional absorption. Additional absorption is absent in oxygen lean Ge:Sn samples. The structure in each series of found bands is similar to isotopic structure of ν_3 vibrational mode of oxygen. But at a difference with the ν_3 mode the fine structure due to coupling of it with the low energy symmetric bending ν_2 is not observed in each found series of bands. The isotopical structure in new series of bands remains up to temperatures 130 K. At temperatures T>130 K the spectra in each series likewise to ν_3 mode become a wide structureless band shifted to the low-frequency region. The found series of absorption bands are ascribed to the ν_3 vibration of interstitial oxygen disturbed by tin atoms located in the first, second and third neighbourhood of Ge–O–Ge quasimolecule.

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Mon-1.41po

Comparative analysis of the radiation defects accumulation in n-Si and n-SiGe, used for the discrete thyristors manufacturing on the initial stage of irradiation, using estimation of the probability of A-, E-, K-centers formation

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Keywords: radiation defects, n-SiGe, probability, estimation

The opportunity of n-SiGe usage for the increasing of low-power transistors and thyristors radiation hardness is known [1, 2]. The features of accumulation of radiation defects in a material of wide thyristor n-base on the initial stage of an irradiation, determining degradation processes of the electrophysical characteristics of the device require an additional study.

For the definition of P_{iV} (probability of the vacancy capture by various impurities) were used the empirical equations, describing accumulation of the radiation defects and well known system of the kinetic equations, describing reactions between dot defects [3, 4], formed in CZ n- Si and n-SiGe ($N_{Ge} = 5 \times 10^{19}$ cm^{-3}, $\rho = 35$ Ohm×cm, concentration of oxygen in the initial wafer 7×10^{17} cm^{-3}, carbon 2×10^{16} cm^{-3}) at action of an irradiation on test p$^+$n diodes, manufactured by boron diffusion (depth of p$^+$n junction 5 microns) by the flow of a-particles with energy 4 meV. Quantity of the defects was measured by DLTS method. Obtained results were express by formulas using STATISTICA7.0. Features of the received results are the following. The numerical value of P_{ASiGe} changes within the first second of an irradiation from 10^{-14} till 10^{-18}, and the change of P_A for the same time makes from 10^{-18} till 10^{-25}, i.e. 3 order is higher. Probability of the E-centres formation undergoes the similarly changes. The accumulation of radiation defects correlates not with absolute value of P_{iV}, but with its relative meaning. In too time the probability of K- centre makes 10^{-49} and within the first second of an irradiation does not change. At high dozes of an irradiation ($10^7 \ldots 10^{12}$ cm^{-2}) $P_{\mathrm{KSi}} = 10^{-65} \ldots 10^{-73}$, that is essentialy less $P_{\mathrm{KSiGe}} = 10^{-50} \ldots 10^{-55}$. The received results are explained by the special features of n-SiGe [5] technologies.

The developed approach to the numerical estimation of radiation defects accumulation in n-base of discrete semiconductor devices allows to project technology of space application products.

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Mon-1.42po

Certain features of hydrogen behavior in crystalline silicon

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Keywords: hydrogen, single-crystal silicon, polycrystal silicon, macropores, crystallization

Study of hydrogen behavior in silicon is promising in terms of analysis of crystallization processes development single crystals properties manipulation new instrumental technologies development [1]. Hydrogen may be found in silicon both as interstitial and as void in free state. The determined hydrogen concentration values are rather high: $\sim 3 \times 10^{18}$ cm^{-3} and $\sim 5.5 \times 10^{18}$ cm^{-3}for single crystals grown by Czochralski method and float zone method accordingly and $\sim(1 \ldots 3) \times 10^{18}$ cm^{-3} for polycrystal silicon grown by different methods [2]. In cast polycrystal silicon the hydrogen content may reach $\sim 1.3 \times 10^{19}$ cm^{-3} due to presence of residual water vapors in the atmosphere of the molding facility and capture of hydroxyl groups from the quartz container. Consequently in order to manufacture cast silicon products which are free from internal voids the package of measures aimed at melt degassing was developed.

Monoatomic hydrogen in silicon is able to passivate electrically active impurities defects deep-level impurities (Cu Ni Fe Au Ag Pt etc.) [3]. There were implemented the processes of growing of phosphorus-doped single-crystals up to the concentration of $N_p \sim 5 \times 10^{14}$ cm^{-3} in the argon flow in the argon flow admixed with monoatomic hydrogen (0.16…0.02) volume % and in the helium flow. The pressure in the growing vessel varied within the range of 0.13…133 kPa. In the single crystals grown in the mixture of Ar+H we observed lower oxygen concentrations and significantly higher values of non-equilibrium charge carriers lifetime $-\tau_{\min}$ ~400…500 μs in comparison with $\tau_{\min}$ ~150…160 μs for single-crystals grown in the argon flow and $\tau_{\min}$ ~180…190 μs for single-crystals grown in the helium flow. With pressure increment in the vessel the increase of $\tau_{\min}$ values was observed but the production of dislocation-free single-crystals was hindered due to capabilities of the vacuum system of the crystal growing furnace. It should be noted that the effect of $\tau_{\min}$ increase in single crystals grown in the mixture of Ar+H is instable in terms of time. In the process of storage within 3–5 months under room temperature $\tau_{\min}$ progressively decreased to the level specific for single crystals grown in the flow of pure argon.

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Mon-1.43po

The features of electro-optical memory effect for 1.54 micron electroluminescence of an Er doped Si diode

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Keywords: Si, Er, electroluminescence

Since more than twenty years Er-doped silicon attracts considerable interest as a promising material for silicon photonics. In this work we present the results of the time resolved study of electroluminescence (EL) of n+Si/n-Si/n-Si:Er/n-Si/p+-Si structures in which the Er doped active layer was positioned relative to the p-n junction in the space-charge region. The main attention is focused on the investigation of electro-optical memory effect, or stored electroluminescence effect (SEL), which has been observed in these structures [1]. A long time after termination of the forward-bias pulse we observed stored EL (SEL) of Er3+ ions, by application of a reverse biase to the diode structure. It is important that in all experiments: i) the voltage of the reverse bias pulses that excite SEL $U \sim 10\,\mathrm{V}$ was below the breakdown voltage, so the SEL effect cannot be explained by the EL signal arising at avalanche breakdown of the reverse-biased p-n junction; ii) SEL of Er3+ ions was observed only if the reverse bias pulse was preceded by a forward-bias pulse. The experimentally observed peculiarities suggest that the memory effect characteristic of the electro-optical conversion is associated with availability in the structure of deep traps for free carriers. During the forward bias pulse the traps fill up with the carriers. At negative bias the carriers get free from the traps and are able to excite Er ions by impact excitation, if the electric field is high enough. In the report we discuss the mechanism of SEL excitation, as well as the reason of high SEL efficiency (more than an order of magnitude higher as compared with forward-bias EL). Also we discuss the origin of the deep traps, responsible for the SEL effect.

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Mon-1.44po

Self-diffusion in $Si_{1-x}Ge_x$ isotope heterostructures and its composition dependence

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Keywords: self-diffusion, silicon, germanium, isotope heterostructures, activation enthalpy

Diffusion of Si and Ge in $Si_{1-x}Ge_x$-isotope heterostructures with Ge contents $x = 0$, 0.05, 0.25, 0.45 and 0.70 was investigated in a temperature range between 690°C and 1270°C. The concentration profiles of the stable Si- and Ge-isotopes were recorded by means of time-of-flight secondary ion mass spectrometry. Analysis of the experimental profiles shows that the Si and Ge diffusion coefficients in elemental Si agree within experimental accuracy. However with increasing Ge content the diffusion of Ge gets increasingly faster compared to that of Si. An Arrhenius type temperature dependence of diffusion is observed for all compositions with slightly lower values for the activation enthalpy of Ge compared to Si. The more pronounced Ge diffusion indicates that with increasing Ge content the diffusional jumps of Ge atoms become more successful compared to those of Si. This trend is explained with an increasing contribution of vacancies to self-diffusion in $Si_{1-x}Ge_x$ with x. In contrast to earlier results the composition dependence of the activation enthalpy of self-diffusion reveals an upward bowing. A similar composition dependence is reported for Sb diffusion in SiGe [1] and is predicted theoretically for the stability of phosphorus-vacancy and arsenic-vacancy pairs in SiGe [2]. The nonlinear behavior seems to be a general trend and accordingly mainly a consequence of the SiGe alloy system.

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Mon-1.45po

Extremely sharp electroluminescence from Er-doped silicon

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Keywords: erbium, silicon, electroluminescence

Erbium-doped silicon is considered as a promising way to a silicon-based light-source because of a narrow and temperature stable emission line at 1.5 μm, arising from the incomplete $4f$ shell of the Er^{3+} ion. A new impulse to research into erbium-doped silicon was initiated by fabrication of Si:Er layers with preferential formation of so-called Er-1 center [1]. Grown by the sublimation molecular beam epitaxy, these layers demonstrate ultra narrow emission lines in photoluminescence spectra with total width down to 10 μeV at 4.2 K [2].

In this letter, we present the first data on electroluminescence (EL) from p^+/n-Si:Er diodes with Er-1 emitting center. EL spectra were recorded with spectral resolution down to 0.05 cm^{-1}. We find emission lines with total width down to 0.2 cm^{-1} (25 μeV) at 30 K — the narrowest lines ever observed in Si:Er EL spectra. To compare, in conventional Si:Er diodes line width is ~ 2 cm^{-1} for Er-O1 and more than 100 cm^{-1} for SiO_2-like precipitate center. So, formation of optically active centers with such a narrow emission line offers the challenge of achieving ~ 500 times higher value of absorption cross section, as compared to Si:Er structures with SiO_2-like Er-related centers used so far, and the possibility of laser action. It is all the more important, that all optically active Er^{3+} ions contribute to a single type of emitting centers, maximizing possible optical gain. Another advantage of these structures is very efficient electrical pumping of Er^{3+} ions. At 30 K, measured value of the excitation cross-section is 4×10^{-15} cm^2. It is close to the highest observed in c-Si:Er at both optical and electrical pumping [3]. Due to ultra narrow emission lines and a high excitation cross-section of Er^{3+} ions, such diode structures are promising for realization of an electrically-pumped silicon-based laser.

For Er-1 center, temperature dependence of EL intensity is investigated, and time-resolved measurements of the EL response are performed within the temperature range of 30–140 K. In the diode structures, it is possible to separate deexcitation processes in the electrically neutral region and in the depleted region of the diode. In the first case, it is found, that prevalent non-radiative deexcitation process of Er^{3+} ions is Auger deexcitation due to shallow (20–30 meV) impurity centers. However, in the depleted region of the diode the decay time is independent on temperature, meaning that virtually all deexcitation processes are suppressed. Features of electrical pumping efficiency are discussed.

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Mon-1.46po

Evolution of defect structure in 4H-silicon carbide single crystals

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Keywords: micropipe, polytype inclusion, small-angle boundary

Defect structure of silicon carbide ingots, grown by PVT seeded technique, is extremely complicated, and type and total amount of defects generated during growth or inherited from the seed are different depending on the growth direction. Defect distribution in 4H-SiC single crystals in dependence on seed orientation and basic growth parameters was investigated by selective KOH etching, optical microscope imaging and X-ray topography. Focusing on the main mechanisms of structural degradation hampering growth we have consistently considered (0001)-plane growth (C-growth), (10-10)- and (11-20)-plane growth, modified us so-called RAF growth process presented in [1] and C-growth process with an enlargement of ingot diameter.

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Mon-1.47po

Structural study of Ge-nanocrystals embedded in Al_2O_3 films

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Keywords: Ge nanocrystals, magnetron sputtering, defects in nanocrystals

It is well known that, as a result of quantum-confinement effects, the emission colour of semiconductor nanocrystals (NCs) can engineered by simply changing their size [1]. This is the main reason why they have a high potential for applications in optoelectronic and nano-electronic devices. Metal–Insulator–Semiconductor (MIS) structures using Si and Ge NCs have been reported to show good memory effects and low power operation at room temperature [2]. One of the most common structures used for memory or LED purposes is the metal or poly-Si/SiO_x/Si structure with Si NCs embedded in the SiO_x layer. SiGe nanocrystals embedded in alumina or stacked dielectrics were shown to improve the performances of the flash memory based devices [3].

In this work, Ge NCs embedded in alumina were prepared using the RF-magnetron sputtering technique. The grown films were annealed in order to improve the cristallinity of the Ge phase and achieve control over the NCs size [4]. Ge NCs of suitable size and good crystalline quality were demonstrated by different techniques, including, Raman spectroscopy, grazing incidence X-ray diffraction (GIXRD), grazing incidence small angle X-ray scattering (GISAXS) and high resolution transmission electron microscopy (HRTEM). NCs shape, size distribution and the spatial arrangement were determined by GISAXS, while Raman, HRTEM and diffraction measurements provided detailed data about the NCs composition and their inner structure. The results of analysis show formation of spatially correlated NCs within the deposited layer. Spatial arrangement is 2D hexagonal lattice with certain degree of disorder. NCs have narrow size-distribution, while their average size, the composition of Ge heterostructure and degree of spatial correlation can be controlled by deposition and annealing parameters.

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Mon-1.48po

Identification of the di-nitrogen [001]-split interstitial (H1a) in diamond

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Keywords: diamond, point defects, piezeospectroscopic parameters

Many synthetic diamonds are found to contain a substantial concentration of dispersed nitrogen in isolated substitutional sites due to its presence in the growth environment. Irradiation of diamond produces interstitials and vacancies [1] which can act as acceptors, modifying the charge state of nitrogen [2] which when annealed, can lead to the formation of new defects in the lattice; H1a is one such example found in irradiated and annealed diamond with a concentration of nitrogen [3]. Differences are seen in the production of H1a in type Ib material with dispersed nitrogen and type Ia material, where nitrogen atoms have migrated into nearest neighbour pairs (A-centre). Isotopic substitution investigations show the vibration to involve a unique nitrogen atom and two carbon atoms [4, 5], resulting in the proposal of a distorted bond-centred nitrogen model [6]. The weakness in this prediction was in supporting the annealing data considering the two material types. Revised modelling instead proposed a di-nitrogen [001]-split interstitial structure which better predicted many of the experimental trends seen [7]. Subsequently, production of H1a, a mode at 1450 cm^{-1} in ^{14}N diamond, is believed to occur through the capture of an interstitial (I) by an A-centre or by the capture of an I by substitutional nitrogen (N_s), producing interstitial nitrogen which is then captured by a second N_s.

Uniaxial stress has been shown to be an excellent technique for probing the electronic strength and symmetry of defects. It is shown that the splitting pattern of H1a is characteristic of an A→E transition of a tetragonal D_{2d} defect. Following the notation used by Mohammed *et al.* [8], the values of the parameters A1, A2, B and C, are found to be 0.54(9) cm^{-1} GPa^{-1}, 1.39(5) cm^{-1} GPa^{-1}, 0.10(9) cm^{-1} GPa^{-1} and 2.75(9) cm^{-1} GPa^{-1} respectively. Therefore, the 1426 cm^{-1} absorption feature in ^{15}N enriched diamond labelled H1a, is assigned to a doubly degenerate local vibrational mode of a tetragonal defect. Considering the many predicted models for H1a, the result is that the di-nitrogen [001]-split interstitial structure proposed by Goss *et al.* is the only plausible model for the centre.

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Mon-1.50po

On the parameters of vacancies' formation in the carbon-subgroup crystals

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Keywords: vacancy, enthalpy, entropy, volume formation

The parameters of formation of vacancies in the semiconductor crystals of elements of the carbon subgroup (C-diam, Si, Ge, a-Sn) are calculated by method, whish described in work [1]. It is shown that consideration of atom delocalization brings about an increase in the values of enthalpy (h_v) and entropy (s_v) and the volume (v_v) of the vacancy formation. At low temperatures, the parameters of vacancy formation depend heavily on temperature, with the entropy of vacancy formation becoming negative: $s_v < 0$. The reasons of negative value of s_v were discussed in work [2]. The temperature dependences of vacancies parameters were studied at the isobaric ($P = 0$) heating from $T = 0$ to the melting temperature (T_m).

For diamond the next values are received at T = 300 K and 1200 K, respectively
$g_v = 1.982$ eV, $h_v = 0.395$ eV, $s_v/k_b = -61.38$, $v_v/v_a = 0.178$;
$g_v = 3.544$ eV, $h_v = 2.991$ eV, $s_v/k_b = -5.351$, $v_v/v_a = 0.717$.

The experimental and theoretical (in parenthesis) estimations are $h_d = 3.68$–5.25 eV [3]. Here, g_v is the thermodynamic potential (or free Gibbs energy) of the vacancy formation, k_b is the Boltzmann constant, $v_a(T)$ is the volume of an atom in a crystal.

For Si the next values are received at $T = 300$ K and $T_m = 1685$ K, respectively
$g_v = 2.611$ eV, $h_v = 1.892$ eV, $s_v/k_b = -27.79$, $v_v/v_a = 0.645$;
$g_v = 3.135$ eV, $h_v = 2.901$ eV, $s_v/k_b = -1.607$, $v_v/v_a = 0.896$.

The experimental and theoretical (in parenthesis) estimations are $h_d = 2.13$–4.5 [3], 2.5–4.7 [4].

For Ge the next values are received at $T = 300$ K and $T_m = 1212$ K, respectively
$g_v = 2.265$ eV, $h_v = 2.027$ eV, $s_v/k_b = -9.193$, $v_v/v_a = 0.820$;
$g_v = 2.422$ eV, $h_v = 2.302$ eV, $s_v/k_b = -1.345$, $v_v/v_a = 0.895$.

The experimental estimations are $h_d = 1.97$–2.7 [3], 2.0–3.1 [4];$s_v/k_b = 8$–10 [4].

For a-Sn the next values are received at $T = 100$ K and $T = 240$ K, respectively
$g_v = 2.106$ eV, $h_v = 1.434$ eV, $s_v/k_b = -77.95$, $v_v/v_a = 0.779$;
$g_v = 2.412$ eV, $h_v = 2.212$ eV, $s_v/k_b = -9.671$, $v_v/v_a = 1.076$.
The theoretical estimations are h_d =(2.3–3.45) [1].

It is shown that, at low temperatures the use of the Arrhenius equation for determination of the energy parameters of the vacancy formation is not correct. In the case of diamond, the use of the Arrhenius equation is incorrect even at $T < 500$ K.

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Mon-1.51po

On the self-diffusion parameters for the carbon-subgroup crystals

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Keywords: self-diffusion, enthalpy, entropy, Gibbs energy

For the first time, without any fitting parameters, by method, described in work [1], the self-diffusion parameters were calculated for the semiconductor crystals of elements of the carbon subgroup: C-diam, Si, Ge, a-Sn. It is shown that an account of quantum's effects in the delocalization of atoms brings about that under low temperature (smaller Debye temperature) the self-diffusion parameters (h_d is enthalpy, s_d is entropy, v_d is volume) have the strong temperature dependence moreover self-diffusion entropy is negative: $s_d < 0$. With growing of the temperature the function s_d moves over to the positive region of values. The temperature dependences of self-diffusion parameters were studied for crystals of IVa subgroup elements at the isobaric ($P = 0$) heating from $T = 0$ to the melting temperature (T_m).

For diamond the next values are received at $T = 300$ K and 1200 K, respectively
$g_d = 2.323$ eV, $h_d = 0.493$ eV, $s_d/k_b = -70.80$, $v_d/v_a = 0.222$;
$g_d = 3.922$ eV, $h_d = 3.731$ eV, $s_d/k_b = -1.839$, $v_d/v_a = 0.895$.

The experimental and theoretical (in parenthesis) estimations are $h_d = 6.8 \pm 1.6$, and (9.1) eV [2].

For Si the next values are received at $T = 300$ K and $T_m = 1685$ K, respectively
$g_d = 3.100$ eV, $h_d = 2.361$ eV, $s_d/k_b = -28.58$, $v_d/v_a = 0.805$;
$g_d = 3.289$ eV, $h_d = 3.620$ eV, $s_d/k_b = 2.280$, $v_d/v_a = 1.118$.

The experimental and theoretical (in parenthesis) estimations are $h_d = 4.65–4.77$ [3].

For Ge the next values are received at $T = 300$ K and $T_m = 1212$ K, respectively
$g_d = 2.673$ eV, $h_d = 2.530$ eV, $s_d/k_b = -5.534$, $v_d/v_a = 1.024$;
$g_d = 2.590$ eV, $h_d = 2.872$ eV, $s_d/k_b = 2.704$, $v_d/v_a = 1.117$.

The experimental and theoretical (in parenthesis) estimations are $h_d = 2.95–3.14$ eV [3].

For a-Sn the next values are received at $T = 100$ K and $T = 240$ K, respectively
$g_d = 2.566$ eV, $h_d = 1.789$ eV, $s_d/k_b = -90.15$, $v_d/v_a = 1.024$;
$g_d = 2.880$ eV, $h_d = 2.760$ eV, $s_d/k_b = -5.801$, $v_d/v_a = 1.117$.

The theoretical estimations are $h_d = (2.87–4.31)$ eV [4].

Here, g_d is the thermodynamic potential (or free Gibbs energy) of self-diffusion, k_b is the Boltzmann constant, $v_a(T)$ is the volume of an atom in a crystal.

It is shown that, at low temperatures (lower of Debye temperature), the use of the Arrhenius equation to determine the self-diffusion energy is not correct.

This work was supported by RFBR (Project No. 09-08-96508), and by Programs of the Presidium of RAS (Project No. 12.1.19).

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Mon-1.52po

Primary defect transformations in high-resistivity p-type silicon irradiated with electrons at cryogenic temperatures

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Keywords: silicon, radiation defects, electron irradiation

There are several DLTS studies of defect behavior in silicon irradiated at cryogenic temperatures with different particles: electrons [1–3], protons [2, 4], alpha-particles [2], ions [5]. However, there is no consistent picture describing all the available experimental data [1–4] which partly even appear to be contradictory. This situation stimulates further investigations of effects of low temperature irradiation.This paper presents some new findings on the formation and annealing behavior of radiation-induced primary defects in silicon irradiated with 6 MeV electrons at low temperature (78 K). The samples studied were n^+–p structures with a hole concentration in the base region of about $4–12.5\times10^{12}$ cm^{-3}. Such a low hole concentration allowed to minimize the injection annealing of primary defects upon irradiation by using the electron beam of low intensity and to consider the reactions of primary defects with boron as minor ones.

Immediately after irradiation several DLTS peaks were detected in the spectra recorded in the temperature range 78–100 K. Some of the peaks have been identified on the base of their DLTS signatures and annealing characteristics. First of all a peak related to a trap with an activation energy of $E_a = 0.135$ eV was observed. It appeared immediately after irradiation and annealed at 200–220 K. Its amplitude strongly depends on the rate window used for the registration of the DLTS spectra giving indication that the defect could be a negative-U center. All these properties allow to identify this peak as related to the isolated vacancy [1, 6].

To monitor the mobile interstitial Si atoms (I_{Si}) we use a peak related to interstitial carbon C_i ($E_a = 0.29$ eV). We have found that this peak begins to appear only after thermal annealing at temperatures higher than 300 K. However direct current injection resulted in complete transformation of I_{Si} to C_i already at 78 K.

Other peaks have distinct annealing stages at temperatures of 110–130 K, 150–170 K and 240–260 K. And similarly to I_{Si}, they can be annealed by current injection at 78 K. It is suggested that a broad peak with $E_a = 0.15-0.17$ eV and annealed at 110–130 K can be attributed for close Frenkel-type defects ($mV+nI_{Si}$ where $m, n > 1$).

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Mon-1.53po

A TEM study of in-grown stacking faults in 3C-SiC layers grown by CF-PVT on 4H-SiC substrates

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Keywords: 3C-SiC, CF-PVT, stacking faults, twin boundaries

Silicon carbide has long been investigated because it possesses high thermal conductivity, high hardness and Young's modulus, high critical electric field and radiation resistivity [1]. Among the large variety of SiC polytypes the cubic one, having the lowest band gap energy (2.4 eV), has several advantages over the most commonly used hexagonal (4H-SiC and 6H-SiC) polytypes. It exhibits isotropic properties and has the highest electron mobility [2]. However, the growth of 3C-SiC epilayers and bulk material of crystalline quality appropriate for device development is still an issue. The presence of structural defects such as dislocations, stacking faults (SFs) and twin boundaries can seriously degrade the device performance. The nature of such defects and their generation mechanism is still not well understood.

In the current work a transmission electron microscopy study on the generation of SFs and SF induced inclusion during different stages of 3C-SiC growth by CF-PVT method (Continuous Feed Physical Vapour Transport) on 4H-SiC substrates is presented. A transition region of about 100 nm between the 4H-SiC substrate and 3C-SiC layer, where cubic and 4H-SiC sequences follow after each other is observed. The most common thickness of the 3C sequence is made of six Si-C bilayers separated by an average of six bilayers with the 4H sequence. Moreover in the near interface region (below 1 mm) the occurrence of twin boundaries (TBs) and multiple SFs, like 2SFs, 3SFs and 4SFs is observed. They rarely originate directly at the interface, but they are found to start on TBs in some cases. Later during the CF-PVT growth process, at a thickness above 5 mm the density of SFs in the (111) and (-111) gradually increases. The (-111) SF density is the higher which leads to the formation of large 6H-SiC inclusions, extending to very large lengths. The detailed description of the SFs, through simulations, and their interaction with dislocations and twin boundaries will be also presented.

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Mon-1.54po

Defect structure of $Si_{1-x}Ge_x$ ($x < 0.1$) single quantum walls in the range of 5–70 nm thicknesses grown by molecular beam epitaxy on (001) Si with Si cap layer

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Keywords: SiGe, defects, nanostructures, x-ray diffractometry

Evolution of defect structure of $Si_{1-x}Ge_x$ ($x < 0.1$) single quantum wells (QW) in the range of 5–70 nm thicknesses with the use of high resolution x-ray diffractometry, reflectometry and low temperature luminescence was studied. QW up to the thickness of 30 nm grown by molecular beam epitaxy at 700°C is characterized by the lowered Ge concentration in comparison with that in a gas phase near to growth surface. In such a QW only insignificant inhomogeneity in Ge distribution along the growth surface is observed. In thicker QW both Ge concentration and its inhomogeneity distribution is increased. This leads to decreasing of satellite reflection intensity on the rocking curves as well as of diffuse scattering from the cap layer Si on the two-dimensional diffraction patterns. Diffuse scattering from QW is observed only in the pulses counter approached down to the distance of 120 mm (as compared to the standard distance 320 mm) in diffractometer PANalytical X'PERT PRO MRD. This diffuse scattering is observed only for one system of asymmetric reflections {113} and {224} whereas for three other systems of the same reflections — is absent. A transverse scanning of reflectometric maxima reveals one additional peak misorientated by 0.1–0.25 deg. from the basic peak. This allows us to suggest the increased Ge concentration near to combined growth steps with formation of a wavy surface like a sandy dune. When the substrate misorientation is less than 0.1 deg. from plane (001), the direction of waves is close to [110], but not always precisely coincides with it. Photoluminescence of such QWs at low temperatures and low excitation density represents the emission of localized and delocalized exitons typical for a system with the disorder presence.

With increase of Ge concentration from 5% up to 7% for the same QW thickness of 70 nm the diffraction picture changes radically. In the sample with 7% Ge the diffuse scattering is completely absent, but there is a peak displacement from the QW which is typical for the samples with misfit dislocations on the substrate/layer SiGe boundary in two dimensional patterns near to asymmetric reflections. We observed also a case of dislocations appearance in the top part of QW without their appreciable presence on the bottom boundary. In this case misorientation of cap Si layer peak is observed. Disappearance or an appreciable decrease of diffuse scattering intensity in both cases allows us to assume that the dislocations appearance in the top or bottom part of QW results in dissolution of already existing inhomogeneities and simultaneously suppresses a photoluminescence in such QWs. The reflectometry data allow us to draw a conclusion that the misfit dislocations appearance promote interlayer diffusion in comparison with the dislocation-free samples.

Mon-1.55po

Homogenization of CZ Si wafers by Tabula rasa annealing

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Keywords: Czochralski silicon wafers, oxygen precipitates

Under the homogenization of Si wafers one usually understands a temperature process, which suppress the evolution of structural artifacts determined by the growth history of Si ingot. These defects are furthermore present in Si wafers and are called Crystal Originated Particles (COPs) [1]. This homogenization process is also called as Tabula Rasa (TR) [2]. COPs is a common name for structural defects of nanometer size which include clusters of vacancies, interstitials, nuclei of oxygen precipitates and its various combinations. These defects are further characterized by a specific lateral concentration distribution as on the Si wafer surface as along the ingot growth. It is determined by the growth rate, temperature gradients and also by cooling conditions after the crystal pulling and other growth parameters. An important feature of COPs is the fact that they are not experimentally observable without submission of the Si wafer to any further temperature process.

The nucleation processes in Si wafers during annealing have the same physical base as the ones in Si ingots, but they proceed under substantially different boundary conditions, distance of wafer surfaces, rate of temperature changes etc. These differences significantly influence the nucleation of vacancies and interstitials in Si wafers [3]. It was shown that the vacancies and interstitials in Si wafers have a negligible influence on self-precipitation in comparison to Si ingots if the cooling rate of Si wafers is smaller than 5 K/s [3].

The aim of this work is to investigate the nucleation processes of oxygen precipitates in Si wafers on experimental and theoretical level and to optimize the process of TR specifying its critical phase, temperature and the period of annealing and cooling during TR.

For the experimental verification of theoretical results based on the classical theory of nucleation [4] we use infra-red (IR) spectroscopy, optical microscopy and X-ray diffraction techniques in order to obtain parameters of the oxygen precipitates grown during three-stage annealing after application of TR. The investigated samples were subjected to various TR processes, including the elimination of TR for one series due to comparison, and further annealed in three stages. From IR spectroscopy we could determine the decrease of interstitial oxygen concentration, the shape and stoichiometry x of the SiO_x precipitates [5]. Measurements of precipitate density by etching technique were done by optical microscopy.

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Mon-1.56po

Interaction of self-interstitials with interstitial carbon-interstitial oxygen center in irradiated silicon: an infrared absorption study

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Keywords: silicon, irradiation, self-interstitial, carbon, oxygen

The evolution of radiation-induced carbon-oxygen related defects [1] with the fluence of MeV electrons and upon the subsequent isochronal annealing (75–400°C) in Si crystals with different carbon and oxygen content has been studied by means of Local Vibrational Mode (LVM) spectroscopy. In particular, the generation kinetics of the bands at 998 and 991 cm^{-1} is considered in detail and an additional support for their previous assignment [2] as arising from the $I_2C_iO_i$ and $I_3C_iO_i$ complexes is found.

An annealing behaviour of the LVMs related to the C4 (IC_iO_i) defect has been studied in detail as well. In all the samples studied the bands at 940 and 1024 cm^{-1} are found to disappear at about 200°C while 3 new LVM bands, at 724 cm^{-1} (O-related) and at 952 and 973 cm^{-1} (both C-related) are emerging. Further increase in annealing temperature up to 250–275°C results in a transformation of the latter bands into a new set of LVM bands at 969 cm^{-1} (O-related) and at 951 and 977 cm^{-1} (both C-related). These bands disappear at about 300–325°C. The ratios of all the bands intensities as well as their transformation rates do not depend on the oxygen and carbon content in the material nor on the kind of irradiation (2 and 10 MeV electrons, fast neutrons) and a dose. These facts confirm the previous conclusion [3] that all the above-mentioned LVMs arise from the C4 defect being in different configurations (ICiOi, IC_iO_i*, and IC_iO_i**), and are not consistent with a suggestion [4] that they can be related to defects of different kind.

It has been pointed already in Ref. 3 that the LVM bands related to ICiOi* (at 724, 952 and 973 cm^{-1}) display unusual temperature dependence: they are clearly observed in the absorption spectra measured at low temperatures and are not detectable in the room temperature spectra. In the present work the temperature dependence of the band intensities in the range 20–300 K is studied and the results obtained are presented.

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Mon-1.57po

Unique defects in heavily boron-doped silicon single-crystals grown by Czochralski method

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Keywords: silicon, boron, dislocations

Heavily doped silicon (Si) crystal is widely used as a base material for large-scale integrated circuit devices, etc. Recently, atomic configurations and electrical characteristics of dopant atoms in such heavily doped crystal are attracted interest from practical and physical viewpoints. Boron (B) is commonly used as a p-type dopant in Si crystal, but there are limited works concerning the structural nature of B atoms in heavily-doped one; i.e., formation of silicon-boride precipitates [1] and B clusters [2], which would affect the electrical properties. This paper reports novel grown-in defects in heavily B-doped Si grown by the Czochralski (Cz) method, presumably related to B, revealed by transmission electron microscopy (TEM).

A bulk single crystal of Cz–Si with the B concentration of 2×10^{20} cm^{-3} was grown from a melt of commercial high-purity poly-Si and granuated B with a purity of 99.5%, charged in a high-purity silica crucible in a high-purity carbon heater, in a high-purity argon atmosphere at 20 torr (more than 99.9995%) [3]. The B concentration was estimated using resistivity measurements and inductively coupled plasma atomic emission spectroscopy, and the results agreed within an accuracy of 6% [3]. No dislocation was detected in the crystal by X-ray topography and the etch pit method, as well as TEM.

Differing from undoped Cz–Si and Cz–Si doped with dopants except B, TEM revealed wavy planar defects with the number density of about 10^{10} cm^{-3}. The lateral size of a defect was up to a few tenth micrometers, and the thickness was about 5 nm. A defect consisted of small segments (submicrometer in size) lying on {112} and {113} planes, and it expanded, on average, on a {111} plane. A defect gave rise to diffraction spots, that were not observed previously [1], and dark-field TEM taken with a spot revealed that a segment of the defect is an agglomerate of nanocrystals (less than 5 nm in size). A set of lattice planes in the nanocrystals was parallel to a {220} plane in the Si matrix, and the interplanar separation of the planes (0.185 nm) was close to that for {220} plane in Si (0.192 nm). The estimated separation was close to the bond length of B atoms in silicon-boride or B clusters, suggesting that the defect is related to B.

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Mon-1.58po

Structural characteristics of dislocations in heavily phosphorus-doped silicon

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Keywords: silicon, phosphorus, dislocations

Dislocations are of considerable importance in semiconductor technology, since they are frequently introduced during crystal growth and device fabrication, and they affect the mechanical property, as well as electronic one, of semiconductor devices. Impurity atoms also affect the property via their segregation on dislocations, even though the impurity effect has not been fully elucidated. This paper reports transmission electron microscopy (TEM) study of dislocations in silicon (Si) heavily doped with phosphorus (P), which is a common dopant in Si.

Si single crystals with the P concentration of 3×10^{18} cm^{-3}, grown by the Czochralski method, were compressively deformed at elevated temperature 1073 K for about 30 min (up to the strain of about 10%) in a high-purity argon flow atmosphere, to introduce fresh dislocations. Subsequently, some specimens were annealed at the same temperature for 3 or 10 h without stress. Then, as-deformed specimens as well as deformed and subsequently annealed ones were cooled slowly by removing the heat source.

A weak-beam TEM ($s = +1.4 \times 10^{-2}$ A^{-1}) revealed that, almost all dislocations in as-deformed specimens were dissociated into partial dislocations. The observed dissociation width for dislocations close to the edge orientation or that close to the screw one was, respectively, 7.5 nm or 4.5 nm, and the stacking fault energy was estimated to be 50–70 mJ m^{-2}, as previously reported [1]. On the other hand, dislocations in annealed specimens were constructed over long segments of the dislocation line. The number density and total length of constructed segments increased with increasing annealing time; about 40% of the dislocations were constructed at annealing time of 10 h. Three-dimensional TEM and convergent-beam electron diffraction revealed that, all constructed segments of a dislocation climb out of the slip plane toward the compression side of the dislocation. In pure Si, similar construction process is not observed at 1073 K but observed at 1623 K [2]. Also, the dissociation width for dissociated segments increased with increasing annealing time; the width in a specimen annealed for 10 h was about 120% that in an as-deformed specimen (the stacking fault energy was reduced to 40–60 mJ m^{-2}), presumably due to the increase of P concentration around dislocations [3]. One possible explanation is that, P atoms accompanied with vacancies migrate rapidly and segregate around dislocations; agglomeration of vacancies induces climb of the dislocations.

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Mon-1.59po

Effects of irradiation induced lattice defects on standard trench and fine pattern trench IGBT characteristics

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Keywords: IGBT, electron irradiation, degradation, interface, defects

A comparison is made of irradiation damage in standard trench and fine pattern trench IGBTs (Insulated-Gate Bipolar Transistors). 2-MeV electron irradiation was performed at room-temperature with anhe electron fluence ranging from 10^{14} to 10^{15} e/cm^2. Two different types of IGBTs are studied. The first one has a trench structure with a trench depth of 4.2 μm and a trench width of 1.4 μm and a gate oxide thickness of 25 nm. The second one has a trench structure with a trench depth of 3.0μm and a trench width of 0.89 μm and a gate oxide thickness of 13.5 nm. For both types of device, the breakdown voltages is 400 V. It is shown that for the fluence range that was studied, the electron fluence dependency of the voltage shift due to the radiation-induced interface traps (ΔV_{it}) and the voltage shift due to the radiation-induced oxide traps (ΔV_{ot}) are different. On the other hand, the leakage current dependence on irradiation fluence is very similar. Detailed experimental results illustrating the relationship between the induced lattice defects and the device degradation will be presented together with a physical model which allows to explain the observations.

Mon-1.60po

Comparison of electron irradiation effects on diodes fabricated on silicon and on germanium doped silicon substrates

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Keywords: CZ-SiGe didode, electron irradiation, degradation, lattice defect

With the increasing implementation of microelectronics components and circuits in nuclear reactors, high-energy particle accelerators and artificial satellites, the development of semiconductor devices, which can operate in a radiation-harsh environment, is extensively taking place worldwide. There are several reports that Si_xGe_{1-x} devices are more radiation hard than Si devices [1]. In the present paper, the degradation of diodes prepared on Si and $\sim 10^{19}$ cm^{-3}Ge doped Si substrates is compared after 2-MeV electron irradiation.

The p-on-n diodes under study were manufactured at IMB-CNM following a well-established fabrication process [1]. This includes 1mm-thick field oxide growth, oxide patterning, boron and phosphorous diode and backside implantation, implant annealing, contact opening, metal deposition, patterning and annealing. The starting materials included 110^{19} cm^{-3} germanium-doped Czochralski-grown (CZ) Si and Ge-free control CZ Si wafers. The final diodes had an active area of 5 mm×5 mm.

Diodes were irradiated at room temperature by 2-MeV electrons using fluences between 1×10^{14} and 1×10^{17} e/cm^2 using the electron accelerator at Takasaki Japan Atomic Energy Agency. Before and after irradiation, the current/voltage (I/V) and capacitance/voltage (C/V) characteristics of the diodes were measured with applied voltages ranging from -2 to 2 V and 0 to -2 V, respectively. DLTS measurements was performed to study the deep levels introduced by the electron irradiation.

After irradiation, both types of diodes degrade as revealed by increasing reverse current and decreasing capacitance. For electrical property, the degradation is nearly same for both diodes. This means that there is few effects on radiation damage for same fabrication process of diode. However, it is observed that for C/V measurement degradation of CZ-SiGe diode is few less than that of CZ-Si diode. According to previous reports, the introduction of Ge may increase the radiation-hardness of the material by the interaction of the Ge atoms with the vacancies and interstitials created by the electron irradiation [2].

During the conference, a detailed analysis of the radiation-induced deep levels will be reported based on the study of diode characteristics together with the recovery behavior of the diode characteristics by thermal annealing and lifetime degradation to confirm the degradation mechanism.

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Mon-1.61po

Model of hopping dc conduction via boron atoms in moderately compensated diamond crystals

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Keywords: boron doped diamond, dc hopping conductivity, activation energy

It is well known that in the dark the hopping conduction of the boron doped diamond is observed at the essentially higher temperatures and concentrations of boron than in the silicon and germanium crystals doped with this acceptor impurity at the comparable compensation ratios. But for a long time structural imperfection of boron doped p-type diamonds does not allow to determine surely the hopping dc conduction parameters and their dependence on the concentration of boron atoms and their compensation. Due to the progress in the technologies of synthesis of the high-quality homoepitaxial crystalline diamond films with controlled doping, the experimental data on hopping dc conduction σ_h via boron atoms were obtained [1–3], which are available for comparison with theoretical models. However the quantitative description of the hopping transport of holes via boron atoms in diamond crystals is still lacking.

We elaborated the model [4], where the hopping conduction of holes via gallium atoms in crystalline germanium with compensation ratio $K = 0.35$ was quantitatively considered in agreement with the experiment. Using this approach here we consider diamond crystals in which boron atoms with concentration N and compensating impurity with concentration KN form a nonstoichiometric simple cubic lattice with translational period $R_\mathrm{h} = [(1 + KN]^{-1/3}$ in crystalline matrix. We take into account only hole hops of length R_h between acceptors during accidental alignment of their energy levels due to the thermal fluctuations. Averaging over random orientation of impurity lattice relatively to the direction of the external electric field is carried out as well. It is taken into account that energy levels of boron atoms are normally distributed due to disorder created by the Coulomb interaction only of the nearest ions at the distance R_h.

Band conduction σ_p of holes in the valence band is equal to hopping conduction σ_h via boron atoms at some temperature T_j. The temperature T_j dependence on the concentration N of boron atoms was obtained as in [5] from the dependences of logarithm of conductivity $\sigma_\mathrm{p} + \sigma_\mathrm{h}$ on the reciprocal temperature $1/T$ for different N at $0.05 < K < 0.5$ according to the works [1–3]. It is turned out that the numerical dependence T_j vs N has been described by the ratio $T_j \approx 2N^{0.11}$ where $[T_j] = K$ and $[N] = \text{cm}^{-3}$.

Our calculations of the pre-exponential factor σ_3 and activation energy ε_3 of hopping conductivity σ_h as functions of the concentration of boron atoms agree well with experimental data [1–3] at the temperature $T_\text{h} = T_j/2$ for moderately compensated ($K \approx 0.25$) diamonds.

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Mon-1.62po

Shallow hydrogen-related donors in the epitaxial silicon, implanted whith proton

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Keywords: shallow hydrogen-related donors, proton implantation, ion distribution

Formation of the shallow hydrogen-related donor in proton-implanted epitaxial silicon at the subsequent thermal treatment are investigated in the present work.

Schottky diodes fabricated on epitaxial n-Si ($r = 1.05$ and 1.8 W cm) are used. The samples were implanted with 300 keV H^+ ions through the metallic (Ag–Ni–Mo) contact at the room temperature. The range of doses was $F = (1 \times 10^{13} – 6^{\times} 10^{15})\ \text{cm}^{-2}$. The mean of the annealing temperature was between 275 to 475°C for 20 minutes. The distribution of shallow donor species in diodes was measured by standard $C-V$-method at 1.2 MHz frequency.

At least two different types of hydrogen-related donors were simultaneously formed in the temperature range (350–475)°C at the large doses (F$\sim 10^{15}$ cm^{-2}). First of them have bistable property. They were annealed at the $T \approx 475$°C completely. Concentration of untransformed donors was invariable in temperature range (350–475)°C. In the dose range 10^{13}–10^{14} cm^{-2} H-donors of first type were formed only. They maximum concentration coincides with maximum distribution of the implanted ions. H-donors of second type were formed in the dose range 10^{14}–10^{15} cm^{-2}. Maximum concentration was displacement close to implanted surface, where is maximum of radiation defects concentration. Mechanism of this displacement is discussed.

Mon-1.63po

TEM observations in Si: an attempt to link deformation microstructures and electrical activity

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Keywords: dislocations, plastic deformation

Dislocations which have been produced by plastic deformation of silicon in a temperature range of 550°C–750°C close to the brittle to ductile transition have been studied by a number of spectroscopic techniques giving puzzling results. It has been shown that the extended defects, associated to dislocation trails formed behind moving dislocations in the slip plane and revealed by chemical etching, exhibit an electrical activity using Electron Beam Induced Current (EBIC). This EBIC contrast of the defects in the dislocation trails is also associated to the absence of any EBIC contrast on the dislocations themselves [1]. The defects formed in the dislocation trails were assumed to be associated with agglomerates of intrinsic point defects formed during the dislocation motion. Dislocation-related DLTS signals have been also found when dislocations traveled a significant distance which strongly depend on dislocation velocity [2]. These DLTS signals were interpreted as resulting from some core defects and atomic impurities accumulated on the dislocations during their slow motion.

The interpretations of these defect signatures interest several scales i.e. microscopic (dislocation core structure defects) and mesoscopic (the collection of microscopic defects in trails in the wake of moving dislocations). It is of importance trying to relate those signatures to the actual dislocation microstructures of these deformed materials. As a matter of fact the deformation microstructures of silicon deformed in those conditions have not been investigated so much up to now. In an effort to shed some light between the spectroscopic measurements and the actual dislocation microstructure, TEM observations have been conducted on Si samples deformed in this range of temperature.

Dislocation microstructures show an unexpected large number of dislocation dipoles as well as numerous small dislocation loops distributed along crystallographic directions or waving around dislocations. These microscopic features will be discussed in relation with the possible different core structures of dislocation in silicon [3] as well as the occurrence of dislocation trails.

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Mon-1.64po

Impact of silicon substrate germanium doping on diode characteristics and on thermal donor formation

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Keywords: Ge doping, thermal donors, Czochralski silicon, magnetic Czochralski silicon, float zone silicon

Germanium-doped silicon is of potential interest for application inmicroelectronics. In particular, it has been reported that silicon-germanium solid solutions at low germanium contents, as well as $Si_{1-x}Ge_x$ epitaxial layers, exhibit higher radiation resistance than Si [1–3]. The improved radiation-hardness is attributed to the role of germanium atoms as centres of annihilation of radiation-induced primary defects [1, 3]. Moreover, it has also been reported that doping silicon with germanium leads to a reduced formation of oxygen-related thermal donors (TDs) [4–6]. This may be of particular interest for processing of silicon radiation detectors, where temperatures in the range of 450°C may be reached during back-end and post-metallization annealing. It is believed that Ge can pair with oxygen and vacancies to form stable complexes, while reducing the oxygen flux leading to the small oxygen clusters related to TDs [6]. However, the generation of thermal donors may significantly depend on the involved temperatures and thermal history of the material [7]. In this way, recently it has been observed that the formation of thermal donors in germanium-doped Czochralski silicon may be even higher than in control silicon by the application of a rapid thermal annealing pre-treatment [8].

In order to shed some further light on the behaviour of germanium-doped Czochralski (CZ) silicon material, two n-type CZ crystals were pulled, one doped with with a Ge concentration of about 1×10^{19} cm^{-3}), the second one without Ge doping. Both crystals were grown under the same pulling conditions, giving rise to similar final resistivity and interstitial oxygen content. As a difference to previous works, in which unprocessed material was generally used, here p-on-n diodes were fabricated on polished wafers prepared from both crystals following a well-established fabrication process [9]. For comparison, devices processed on additional silicon materials with different oxygen contents (high resistivity (HR) standard and oxygenated float zone (FZ), as well as HR magnetic CZ (MCZ) silicon) were also included in the study.

The diodes were subjected to a matrix of thermal treatments with temperatures ranging from 250°C to 450°C, annealing times between 0.5 and 5 h and using N_2/H_2 or N_2 annealing ambients. The impact of silicon substrate germanium doping on diode characteristics and on thermal donor formation has been analysed by means of capacitance-voltage, current-voltage and microwave photoconductance decay recombination lifetime measurements. The formation of thermal donors was only observed for the materials with the higher oxygen contents (CZ Si, CZ Ge-doped Si and HR MCZ). Changes in free carrier concentration start to be observed for $T \geq 400°\mathrm{C}$ in HR MCZ and $T = 450°\mathrm{C}$ in CZ Si and CZ Ge-doped-Si. The changes are increasing with increasing annealing time, with some donor profile near the surface and some increase in reverse currents. Interestingly for device applications, less thermal donor generation is indeed found for the case of the Ge-doped material. The obtained results should be taken into account when defining potential applications of Ge-doped materials.

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Mon-1.65po

EPR, ESE and pulsed ENDOR study of the nitrogen donor pairs on quasi-cubic lattice sites in 6H SiC

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Keywords: EPR, ESE, pulse ENDOR, 6H-SiC, nitrogen pairs

The recent high frequency electron paramagnetic resonance (EPR), field-sweep electron spin echo (FS ESE) and pulsed electron nuclear double resonance (ENDOR) study of the 4H SiC and 6H SiC wafers showed that depending on the nitrogen (N) concentration the n-type 4H-SiC and 6H SiC wafers revealed, besides a triplet due to nitrogen residing on the quasi-cubic sites (N_c) and unresolved triplet due to N on hexagonal site (N_h), additional N triplet lines labelled N_x with g-tensor corresponding to the average value of the N_c and N_h spectrum: $g(N_x)\approx \frac{1}{2}[g(N_c) + g(N_h)]$ in 4H SiC [1] and $g(N_x)\approx \frac{1}{2}[g(N_{c2}) + g(N_h)]$ in 6H SiC [2]. It was found that the N_x triplet lines have half of the hf splitting of the N_c center in 4H and 6H SiC. The N_x triplet lines was attributed to the distant N donor N_c-N_h pairs on inequivalent lattice sites which are coupled to S = 1 centers with very small zero-field splitting [3]. In this work we used D-band EPR, X-band FS ESE and pulsed ENDOR to study the highly compensated n-type 6H-SiC wafers with donor concentration of about $(N_D - N_A)\approx 10^{16}$ cm^{-3} to verify whether the N donor pairs occur between two quasi-cubic sites in the case when the nitrogen atoms on the hexagonal site were ionized and the numbers of the paramagnetic nitrogen atoms at the two quasi-cubic positions became already very different. The D-band EPR and X-band FS ESE study of the highly compensated n-type 6H SiC wafers show besides the well known hyperfine (hf) triplet lines of ^{14}N on the two quasi-cubic (N_{c1}, N_{c2}) sites with the intensity ratio of $I_{Nc1}/I_{Nc2} = 0.7$ three additional N triplet lines of comparatively low intensity. X-band Davies pulsed ENDOR spectra measured in the 6H SiC sample have shown intense ^{14}N ENDOR signals of N_{c1}, N_{c2} centers and new lines attributed to the nitrogen centers N_1, N_2, N_3 with the isotropic hyperfine splittings: 21.037 MHz; 26.426 MHz; 29.771 MHz, respectively.

Analysis of the angular dependences of the nitrogen EPR and FS ESE spectra in 6H-SiC wafers showed that the g-tensors of the N_2 and N_3triplet lines coincide with those of nitrogen on quasi-cubic N_{c2} site. The g-tensor of the third N_1 triplet lines corresponds to the average value of the N_{c1} and N_{c2} spectrum: $g(N_1)\approx \frac{1}{2}[g(N_{c1}) + g(N_{c2})]$. On the base of the obtained data it was suggested that the observed new nitrogen triplet lines with A_{iso} = 21.037 MHz is due to the spin coupling between nitrogen on two quasi-cubic N_{c1} and N_{c2} sites while two others are due to nitrogen pair formed between nitrogen atoms on one quasi-cubic N_{c2} site. To confirm this suggestion the further investigation of the spin state of the nitrogen triplet lines by using the nutation frequency experiment are in progress.

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Mon-1.66po

Defect structure of zinc doped silicon revealed by X-ray diffuse scattering method

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Keywords: X-ray diffuse scattering, reciprocal space map, silicon, transition metal impurity, deep levels

Silicon containing impurity of transitive metal zinc is traditionally used for development of IR-converters [1]. Usually Si was doped by Zn during high-temperature diffusion annealing with the subsequent quenching. Recently in such material the micron size microdefects (MDs) were observed. These MDs were assumed to be dislocations and/or zinc precipitates. In present work these MDs were investigated by X-ray Diffuse Scattering (XRDS) method using high-resolution X-ray diffractometer. We investigated n-type Si(111) samples with Zn concentration $N_{\mathrm{Zn}} = 1 \times 10^{14}$ cm^{-3}. The samples sizes were $(5.0 \times 5.0 \times 0.8)$ mm^3. The X-ray diffraction studies were performed on a TRS-1 diffractometer. Reciprocal space maps (RSM) were measured using a Bruker D8 Discover diffractometer. For detailed study of MDs in Si<Zn>(111) samples the distribution of XRDS intensity $I(q_x, q_z)$ in the neighbourhood of a reciprocal lattice point (111) was measured. Here q is a deviation of scattering vector $\mathbf{Q}$ from reciprocal lattice point $\mathbf{q} = \mathbf{Q} - \mathbf{H}$. Components of vector $\mathbf{q}$ along a sample surface q_x and a normal to it q_z are connected with experimentally measured angles for sample $\Delta\theta_{\mathrm{sam}}$ and for analyzer $\Delta\theta_{\mathrm{an}}$ from exact Bragg angle θ_B.

To analyze RSM shape the dynamic scattering effects were removed using an original procedure [2]. The gravity centre of the contours is shifted towards negative values of q_z. It provides evidence that the MDs are of vacancy type. The shape of the contours corresponds to the scattering caused by plane defects (like dislocation loops). The characteristic size of the MDs was estimated from the value of q_x, where

I(q_x) dependence changes from Huang-type (I$\sim q_x^{-1}$) to asymptotic type (I$\sim q_x^{-3}$). This value was about 2 μm.

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Mon-1.67po

Dislocation photoluminescence in plastically deformed germanium

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Keywords: germanium, dislocations, photoluminescence, point defects

In plastically deformed germanium dislocation photoluminescence (DPL) is detected over the energy range 0.43–0.60 eV and its spectral distribution is determined by the deformation conditions [1–3]. There are many non-resolved lines in the DPL spectra attributed to dissociated 60° dislocations of "relaxed" morphology. The DPL spectra were deconvolved into Gaussian lines, which could emanate from both regular segments of dissociated 60° dislocations with various stacking fault widths Δ (band-like states) and some defects on dislocations (localized states) [2, 3]. According to [1], the d8 line with $E = 0.513$ eV (at 4.2 K) corresponds to regular segments of 60° dislocations with the equilibrium stacking fault width Δ_0. A decrease of the d8 line intensity is accompanied by emergence of some other lines with increasing dislocation density and after annealing of deformed samples at temperatures above 600°C [3].

In this paper we intend to clarify the process promoting the spectral redistributing of the DPL intensity. Germanium single crystals were plastically deformed at temperatures below 520°C and cooled down to room temperature with various rates. The significant deviations from the point defect equilibria occuring under plastic deformation give rise to a number of deformation-induced point defects (PD) registered by the Hall effect technique [4]. A short annealing of deformed samples at temperatures above 420°C leads to a measurable decrease of the PD concentration, the achievement of the point defect equilibrium being determined by the interaction of deformation-induced PD with dislocations.

The isochronous and isothermal annealing of deformed samples was perfomed over a wide temperature range 130–750°C. It was found that the important changes in the DPL spectra correlate with a considerable decrease of the deformation-induced PD concentration. The results obtained suggest that the interaction of the PD with dislocations affects the spectral distribution of dislocation photoluminescence. The possible mechanism of the effect is discussed.

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Mon-1.68po

A new structure of Cu complex in Si and its photoluminescence

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Keywords: theory, group IV and compounds, isotope effect, photoluminescence

A problem of Cu complex has been for a long time a controversial issue. The main evidence for the Cu complex in Si comes from a sharp zero-phonon (ZP) line in photoluminescence. Actually, this line is a composite line of Γ_3 and Γ_4 exciton peaks. Since J. Weber's systematic analysis of this line was made more than 20 years ago [1], it has been believed that the Cu complex is a Cu pair with the local symmetry of C_{3v}. Recent first-principles calculations support this, for example by Estreicher *et al.* [2]. Only Nakamura aroused suspicion on this interpretation [3]. But, Nakamura's criticism has received little attention in this community.

The situation has been drastically changed since Thewalt's experiment appeared [4]. In their series papers, they performed isotope shift experiment on the ZP line with quite higher resolution than ever seen; the resolution is more than simple resolving Γ_3 and Γ_4 exciton peaks. They discovered complicated ways of splitting of these excitons, which is difficult to interpret by the old pair model.

Recently, we have theoretically studied Thewalt's experiment by a Cu_4 model [5]. First-principles calculations which the authors performed show the stability of the Cu_4 complex over Cu pair. More importantly, the authors are able to provide a reasonable account for the complicated splitting of Γ_4 exciton peak by using a non-totally symmetric phonon mode. This model seems to require selection rules between excitons and the associated phonons. A similar way of splitting had been discovered in Li_4 complex in Si more than 20 years ago [6], but there was no successful explanation.

Therefore, their model has potential of wide applicability over defect physics and theory of photoluminescence.

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Mon-1.69po

Thermo-physical and physico-chemical behaviour of thermal donors in cs-silicon

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Keywords: CZ-silicon, thermal donor, physico-chemical equation

Thermo-physical and physico-chemical are two co-existent and integral aspects encountered during the process of thermal donor formation. Annealing of the CZ-Si samples leads to the redistribution of impurities and charge transfer. Quite a few physical processes take place simultaneously, which can well be represented with the help of physico-chemical equations. As an illustration, $(C\text{-}H)_i$ and oxygen atom, both in interstitial positions, may get associated either with a single interstitial oxygen atom resulting in the formation of $(C\text{-}H)_i\text{-}O_{2i}$ or $(C\text{-}H)_i$ may be associated with an interstitial dimer again meeting the same fate as above. $(C\text{-}H)_i\text{-}O_{2i}$ so formed has every likelihood to be associated with interstitial dimer resulting in the formation of $(C\text{-}H)_i\text{-}O_{4i}$. $(C\text{-}H)_i\text{-}O_i$ may acts as a pre-cursor of $(C\text{-}H)_i\text{-}O_{2i}$. Interaction between $(C_i\text{-}O_i)$ and hydrogen is equally possible, resulting in the formation of $(C_i\text{-}O_i)\text{-}H$, $(C_i\text{-}O_i)\text{-}H_2$ and $(C_i\text{-}O_{2i})\text{-}H$. All these help in the formation of thermal donors. A possible model is also proposed. A logical support of experimental findings to theoretical concepts and vice-versa leads one to conclude that the field is still wide open to be supplemented by other studies to ascertain the authenticity of various possibilities.

Mon-1.70po

Effect of the band-gap problem of density functional theory on intrinsic defects in germanium

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Keywords: germanium, DFT, hybrid potential, intrinsic defects

One shortcoming of Density Functional Theory (DFT) calculations based on the Local Density Approximation (LDA) or Generalized Gradient Approximation (GGA) is its failure to reproduce well the band gap of semiconductors and insulators. In the case of germanium a closing of the band gap is even observed for well-converged DFT calculations [1], predicting thus a wrong metallic ground state. This deficiency of DFT is attributed largely to discontinuities in the derivative of the exchange-correlation energy. The LDA indeed often fails to describe systems with localized (strongly correlated) d and f electrons and underestimates the binding energy of these states that pushes up the valence-band maximum, leading to a reduction in the calculated band gap. The LDA+U approach aims to correct for this by adding an orbital-dependent term, in a (screened) Hartree-Fock like manner, to the LDA potential. Another way to overcome the lack of band gap problem is the application of a certain fraction of exact (Hartree-Fock) exchange within DFT via a so-called hybrid functional. This approach and the LDA+U approach is illustrated using require computationally demanding simulations. Their effect on the calculated intrinsic point defect properties is therefore treated separately.

Properties of intrinsic point defects were investigated in previous work using DFT LDA+U calculations [2, 3] to calculate the formation and migration energy of vacancies and self-interstitials, in combination with both experimental and theoretical data available in literature [4].

The present paper focuses on DFT calculations using hybrid potential HSE06 [5] which leads to a band gap and gives a good estimate for the activation energy of self-diffusion in germanium. In the present paper results obtained from standard (LDA and GGA) and corrected (LDA+U and hybrid) potentials are compared and discussed.

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Mon-1.72po

Iron diffusion in silicon under external stress

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Keywords: external stress, group I–IV and compound, experiment, diffusion, iron impurity

Recent investigations by means of Mössbauer spectroscopy have shown that iron atoms exist on interstitial sites and substitutional sites, after deposition [1–3]. A wafer of silicon, even of ultrahigh purity, commonly contains impurities and crystal defects such as vacancies and dislocations. Such a defect must be accompanied by a strain field, which affects the atomic diffusion properties in Si. In spite of the important role played by a stress-induced diffusion, however, the diffusion of transition metal impurities in Si under a stress has never been studied until now. In the present study, we introduce ^{57}Fe probe into FZ-Si sample and measured Mössbauer spectra of ^{57}Fe-dissolved Si under an external stress for the first time.

Stress-strain curve of FZ–Si are measured using strain gauges fixed on both sample surface when compressive stress is applied to a Si sample along the [011] direction of Si using an Instron-type tensile testing machine. Maximum yield of strains on both sample surfaces is +0.07% on tensile side and -0.13% on compressive side, respectively. This suggests that the bending stress is applied to a Si sample. A 3nm thick layer of ^{57}Fe are deposited on FZ–Si, and subsequently annealed at 1273 K to dissolved ^{57}Fe in Si. The Mössbauer spectra under stress ranging from 0 MPa to 44 MPa can be fitted with two Lorentzians components, corresponding to substitutional Fe and interstitial Fe. The line widths for the both components broadened when a tensile stress was applied on the ^{57}Fe-deposited side. The line broadening is directly proportional to the diffusion. The diffusivity of the interstitial Fe is estimated to be about 2.6×10^{-9} cm^2/s from the line broadening observed at 44 MPa. The value turns out to be substantially larger than the generally accepted diffusivities at room temperature.

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Mon-1.73po

Precipitation of GeAs in heavily As-doped Ge crystal during Czochralski growth

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Keywords: germanium, arsenic, precipitation

Recently, germanium (Ge) has made a comeback into advanced semiconductor industries as a substrate for GaAs solar cells and high speed Ge-MOSFET ULSI devices [1]. For latter applications, heavy doping by ion implantation has been studied as a key technology to form shallow junctions in a channel, source and drain [2]. However, heavy doping in Czochralski (CZ) grown Ge crystal is poorly known. Generally, in Ge crystal growth, Sb is used for n-type dopants, but high concentration of Sb more than 10^{18} cm^{-3} is difficult to be established because of its small segregation coefficient. The segregation coefficient of arsenic (As) is known to be larger than that of Sb. We found that the effective segregation coefficient of As decreases with increasing in As concentration [3]. This paper reports precipitates observed in heavily As-doped CZ-Ge crystal growth and its formation mechanism is discussed.

Ge polycrystals weighing 150 g were charged in a silica crucible 50 mm in diameter with GeAs alloys as the dopants. Using $\langle 111 \rangle$ or $\langle 001 \rangle$ oriented Ge seed, Ge crystals 1 inch in diameter were grown by the CZ method at a pulling rate of 4 or 10 mm/h at 1 atm under Ar gas flow. Wafers cut from the grown crystals were mechanically polished and preferentially etched. Defects in the crystals were revealed by the etching. As contents in the wafers were quantitatively measured by electron probe microanalysis (EPMA).

When As concentration in the crystal exceeded 9×10^{18} cm^{-3}, plate-like precipitates with about 1 mm in width were observed in Ge grown crystals. They were identified to be GeAs by EPMA. GeAs precipitated along $\{111\}$ for $\langle 111 \rangle$- and $\{001\}$ or $\{111\}$ for $\langle 001 \rangle$-grown crystals, respectively. Straight ditches appeared above such precipitates and As concentration gradually increased toward the precipitates. We conclude that constitutional supercooling occurred and unstable As-rich droplets were formed in the crystal. As concentration in such droplets increased along a liquidus in Ge-As phase diagram [4] during the crystal growth, finally the droplets freezed as GeAs. Ge matrix below all GeAs precipitates were probably solidified by the lateral growth along $\{111\}$ facet planes before GeAs was formed.

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Mon-1.74po

Dislocation generation due to thermal shock in Si crystal growth

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Keywords: silicon, dislocation, shear stress

In Czochralski (CZ) Si crystal growth, dislocations are generated in a Si seed after dipping in Si melt due to thermal shock. During the crystal growth, if such dislocations are eliminated insufficiently, they propagate into the grown crystal across the interface between the seed and the grown crystal, and lead to polycrystallization. We reported that the dislocation generation due to thermal shock can be suppressed effectively by using a heavily B-doped Si seed [1]. This result has been supported by finding that the critical shear stress of Si crystal at 800°C is enhanced by heavy B doping [2]. In the present study, generation and suppression of dislocations due to thermal shock in CZ–Si crystal growth under different dipping temperature are investigated. The dependence of critical shear stress on B concentration at the melting point of Si is experimentally estimated.

<001> oriented heavily B-doped Si single crystals of $7 \times 7 \times 70$ mm^3 in size were used as the seeds. Such a seed was dipped into the Si melt in a silica crucible. The temperature difference during seed dipping, ΔT, was selected 30, 45 and 82°C by controlling the crucible position in the CZ furnace. Then, the seed and the crystal were pulled up after dipping at a pulling rate of 0.5 mm/min. The concentrations of B in the grown crystal were selected to avoid generation of dislocations due to lattice misfit [1]. The grown samples with the seed and grown crystal, cut parallel along (110), were examined by X-ray topography.

When a seed with a B concentration of 2×10^{18} cm^{-3} was used, dislocations due to thermal shock were generated in the seed in the case of $\Delta T = 45$°C but not in $\Delta T = 30$°C. Similarly, such dislocations were generated in the seed with B concentration of 1×10^{19} cm^{-3} in the case of $\Delta T = 82$°C but not in $\Delta T = 45$°C. These results indicate that a larger temperature difference at the dipping causes larger thermal stress to the seed. Critical shear stresses of B-doped Si crystal with B concentration of 2×10^{18} and 1×10^{19} cm^{-3} at the melting point of Si can be estimated to be around 8 and 13 MPa, respectively. A model for generation and propagation of dislocation due to thermal shock under different temperature conditions will be discussed.

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Mon-1.75po

Morphological features affected by constitutional supercooling during Czochralski growth of Si and Ge crystals

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Keywords: silicon, germanium, constitutional supercooling, cellular structure, precipitation, heavy doping

Heavy doping in semiconductors becomes important for manufacturing high performance of electronic devices. In Czochralski (Cz) crystal growth, B, P and Sb are adopted in Si while Ga, P and Sb in Ge for heavy doping with a concentration beyond 10^{18} cm^{-3}. It is also known that constitutional supercooling occurs in heavily impurity doped Si and Ge during the growth [2]. The phenomenon is promoted under the conditions as higher dopant concentration, faster growth rate, lower temperature gradient at the growth interface and smaller segregation coefficient of dopants [3, 4]. Since such constitutional supercooling leads to irregular growth interfaces and precipitation, finally resulting in polycrystallization, the phenomena should be well clarified for single crystal growth. The present paper reports morphological features of crystallinities where constitutional supercooling is developed in Si and Ge crystals heavily doped with various impurities in concentrations higher than 10^{18} cm^{-3} together with relevant growth conditions.

Rectangular cellular structures were observed in advance of appearance of irregular growth interfaces in [001] pulling axis growth of Si heavily doped with B, Ga, As and Ge. Such structures were characterized as a pyramidal shape in the (110) cross section parallel to the growth axis. Finally all Si heavily doped with such impurities became polycrystals. In advance of polycrystallization precipitation of SiAs was observed in As-doped Si crystals.

Contrarily, cellular structure were not observed clearly and only irregular growth interfaces were observed in the growth of Ge heavily doped with Ga along [111] direction. In As doped Ge, though there were not either cellular structures or irregular growth interfaces, GeAs precipitates were observed.

Thus, crystalline morphologies are in a variety dependent on the matrix, dopant and growth conditions.

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Mon-1.76po

Isotope study of far IR absorption of bistable centers in hydrogen-implanted silicon

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Keywords: hydrogen-related bistable donor, nanostructures

Far IR study of high-purity crystalline silicon implanted by protons and deutrons at low ion beam current density and room temperature was performed. Isotope analysis shows that a set of new absorption bands in the 100–1000 cm^{-1} range are connected to bistable hydrogen-related centers. It is found that the behavior of the bands correlates with that of the high-order IR bands observed in the near IR absorption spectra of neutron-irradiated silicon. The bands are tentatively associated with nanostructured interstitial defects oriented along the $\langle 110 \rangle$ axis.

Mon-1.78po

Deactivation mechanism of ion-implanted arsenic in germanium

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Keywords: germanium, arsenic, deactivaton, precipitation

Ge (germanium) is a promising material for overcoming the scaling limit of silicon (Si) devices because of the higher carrier mobility in Ge than that in Si. One of the major issues in Ge devices is the high contact resistance due to the difficulty in obtaining high concentrations of active n-type dopants that are ion-implanted into Ge. In this study, we investigated the deactivation mechanism of ion-implanted arsenic (As) in Ge.

As ions (90 keV, 2×10^{14} cm^{-2}) were implanted into Ge substrates and Ge isotope superlattices (SLs). The Ge SLs are composed of alternating layers (15 nm) of ^{nat}Ge and ^{70}Ge with a ^{nat}Ge cap layer (100 nm) on the top. The samples were annealed at 450–550°C for 1–48 h. The peak concentration of implanted As is about 4×10^{19} cm^{-3}, which is half of the solid solubility of As in Ge [1]. In the depth profiles of annealed samples, however, we observed immobile As species, which are generated in the early stage of annealing and decrease with time. We confirmed that this immobile As is electrically inactive from our simulation that takes into account

the V^{2-} contribution [2] because As diffusion would be overestimated if immobile As were electrically active.

This As deactivation can be attributed to the formation of neutral As-vacancy complexes [3] and to As precipitation. The formation of As-vacancy complexes in the early stage is less likely because the solid phase epitaxial regrowth of the amorphous region should almost totally eliminate supersaturated vacancies in the implanted region. On the other hand, the simulation that takes As precipitates into account well reproduces the simultaneous Ge-self and As diffusion profiles with consistently using the thermal Ge self- and As diffusivities. This result indicates that implanted As tends to precipitate due to non-equilibrium effects even if the As concentration is below the solubility limit. In conclusion, As precipitation is a major cause of the deactivation of ion-implanted As in Ge under the implantation conditions employed in this study.

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Mon-1.79po

Structural and optical properties of nanocrystalline 3C-SiC layers

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Keywords: silicon carbide, crystal lattice, luminescence

Silicon carbide exhibits luminescence in the visible frequency range although it is the indirect-band-gap semiconductor. Recently it has been shown that nanocrystalline 3C-SiC [1, 2] may emit light in the ultraviolet frequency range with relatively high efficiency [3]. These findings stimulate new investigations of light emitting properties of different silicon carbide modifications.

We studied the properties of cubic silicon carbide layers produced by chemical conversion of the surface of Si(001) and Si(111) wafers in hexane (C_6H_{14}) vapors at temperatures 700–1000°C. The morphology and structure of the layers were studied by white light interferometry (WLI), atomic-force microscopy (AFM), -ray diffractometry, and transmission electron microscopy (TEM) of plan-view and cross-sectional specimens. The photoluminescence of the samples was excited by a femtosecond laser (266 nm).

In the technological procedure used, the silicon carbide layers are formed through the carbonation of the silicon surface in a hydrocarbon atmosphere accompanied by recrystallization of the layer structure. Transmission electron diffraction (TED) patterns as well as TEM images of the plan-view specimens revealed a polycrystalline structure of SiC layers consisting of nanocrystals of 40–100 nm in diameter. At the same time, a macrostructure consisting of large domains is observed in the 3C-SiC/Si(111) layers. These domains are faceted by $\{111\}$ planes to produce specific microrelief (growth figures) on the layer surface. For the grown layers, a set of interplanar distances has been derived from the TED patterns, which values correspond exactly to that for cubic silicon carbide (F43m lattice symmetry). We present the comparative analysis of the structural and luminescence properties of silicon carbide layers. The nature of the lines observed in the photoluminescence spectra is discussed.

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Mon-1.80po

Spin-Peierls transition in the Ge:As semiconductor impurity system in the vicinity of the insulator-metal phase transition

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Keywords: germanium, spin-Peierls transition

The effect of an elastic spontaneous distortion of the crystal lattice of a doped semiconductor Ge:As was observed near the insulator–metal (IM) phase transition. The effect was discovered in a study of the electron spin resonance at electron concentrations $0.8 \leq n/n_C \leq 1$ ($n_C = 3.7 \times 10^{17}$ cm^{-3} is the critical electron density for the IM phase transition) at low temperatures $T \leq 100$ K [1]. A study demonstrated that the phenomenon can be understood in terms of the Peierls model of a spin transition in the disordered spin system of the semiconductor.

Compared with ordered crystalline materials in which the spin-Peierls transition is observed, the effect in the Ga:As system has specific features resulting from the chaotic spatial distribution of impurities.

The spin-Peierls transition gives rise to a new type of defects in doped uncompensated or weakly compensated n-type semiconductor in the form of a domain structure. Separate domains in this structure differ in the deformation orientation along one of the [110] directions. Introduction of compensating Ga impurities by neutron transmutation doping eliminates this effect and gives rise to isotropically distributed microdeformations caused by electrostatic forces [1, 2].

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Mon-1.81po

Electroplasticity pure and alloyed silicon

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Keywords: semiconductors, electroplasticity, dislocations, self-organization, dissipative structures

On microlevel plasticity material are defined characteristic individual dislocations, mobility which more sensitive to influence of the direct current getting through sample. Use the directed flow of the charged carriers as controlling parameter of excitement dislocation systems of the crystal allow to affect and on morphology, and on nature of the sharing the fault structure. These structures what the experiments show, possess more ranked and uniform orientated morphology, than got by other classical methods (for instance, method hot plastic deformation). In work is studied in comparative plan change springy-plastic characteristic pure and alloyed single-crystalline silicon samples, in condition of the passing of the constant electric current through sample (electroplastic deformation), on change the form crooked compressions s(e) got experimental. As object of the study in work were used pure samples p-type with resistivity $\rho_1 = 35$ kΩ·cm and is come alloyed gallium before concentration of the holes 10^{16} cm^{-3} sample p-type conductivities with resisitivity $\rho_2 = 17$ Ω·cm. The single-crystalline silicon samples of rectangular shape 15å9å6 mm^3, which rib complied with crystallographic directions [112], [111], [110] accordingly, were deformed under constant shear stress 25 MPa and at temperature interval 750–800°C during 30 min. From dependency of the value to deformation from mechanical strain s(e) is noticed, as qualitative differs the move crooked for both sample. For alloyed samples characteristic of significant resistance of the crystal deformed unlike pure samples. The difference in purity sample tells also on such deformed parameter such as elastic strength, yield strength and on the general value of the deformation. Beside clean sample importance values of the limit to bounce and limit to fluidity far less, than beside alloyed sample. Except this value of the deformation clean sample much exceeds the value to deformation alloyed sample. At the temperature of the test $T = 750-800°$‘ curves of the compression in both events are characterized not only absence “teeth” of yield, low start stress, but also different coefficients hardening unlike data, got in work [1].

The morphology and particularity of the distribution dislocation structures for both sample noticeably differed. The surface pure sample was characterized by presence of single system bands of the slide. Beside alloyed sample on surfaces existed mutually orthogonal of the system bands of the multiple slide. The reason of the reduction to mobilities dislocations in alloyed silicon is, much more likely, springy interaction dislocations with impurities, bring about formation impurity cloud on dislocations. In consequence of permeability of the bands of the slide dislocations begin to emerge in dug the sources deformed hardening. Probably, such mechanism structure forming silicon depending on its purities wholly can become perspective.

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Mon-1.82po

Dynamic nuclear polarization of ^{29}Si via spin $S = 1$ centers in isotopically controlled silicon

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Keywords: silicon, isotopes, extited triplet states, dynamic nuclear polarization

Large electron- and nuclear-spin polarization is required for future development of silicon-based spintronics and quantum information devices [1]. The low thermal equilibrium ^{29}Si nuclear spin polarization, typically $\sim$0.0001%, is one of the significant bottlenecks for the reduction of the background nuclear spin fluctuation and initialization of nuclear spin quantum bits. The electron spin polarization P_e of the paramagnetic defects in the photoexcited triplet state which is not determined by the Boltzmann distribution but by the difference in the lifetime of the $M_S = \pm 1$ and $M_S = 0$ states allows to get stronger DNP degree than the traditional spin $S = 1/2$ paramagnetic centers.

We report the results of the experiments on Dynamic Nuclear Polarization (DNP) of ^{29}Si nuclei under saturation the Electron Paramagnetic Resonance (EPR) transitions of the photoexcited spin $S = 1$ states of the oxygen+vacancy $(O+V)^{0*}$ complexes [2] (EPR spectrum labeled Si-SL1) in irradiated ^{29}Si isotopically controlled silicon.

The effect of isotope ^{29}Si abundance on the line width and hyperfine structure of the Si-SL1 EPR spectra was observed. It was shown clearly that the decrease of the ^{29}Si abundance leads to the transformation the DNP mechanism from the "differential" to "resolved" solid-effect accompanied with the increase of DNP degree. High steady-state ^{29}Si nuclear polarization 6.4% due to "resolved" solid-effect was achieved in silicon crystals with the ^{29}Si isotope abundance below 4.7%. The maximal values of the DNP degree obtained at the temperatures of 4–20 K decreases when the temperature of samples increases from 20 to 120 K in accordance with the decrease of the Si-SL1 EPR signal intensity. It was shown that the DNP degree can be increased 6 times at the magnetic field orientation along $\langle 111 \rangle$ crystal axis when the EPR lines corresponding to 6 different orientations of (O+V) centers in silicon lattice are overlapped due to inhomogeneous broadened Si-SL1 EPR lines. It indicates that the nuclear spin polarization more than 30% will be able to be achieved.

Furthermore, the DNP degree induced by saturation the hyperfine structure EPR lines of triplet centers was demonstrated, which does not follow the symmetric first derivative EPR line shape, showing the additional contribution to DNP process. The model taking into account additional transitions in the electron-nuclear spin system and explaining the observed asymmetry of DNP is suggested.

The nuclear spin polarization 6.4% we obtained is a factor of 5×10^4 larger than thermal equilibrium polarization and is the promising approach to more than 5% for the silicon nuclear-spin based quantum computers.

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Mon-1.83po

Ion Drift in Si and Ge Schottky barrier diodes

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Keywords: hydrogen passivation, shallow donors, Ge, Si

The dissociation energy of dopant-ion pairs in semiconductors is determined by a new experimental technique. In contrast to the standard reverse bias annealing process, the capacitance time response of a reversed biased Schottky barrier diode is measured at elevated temperatures. The dissociation enthalpy of the dopant-ion complex determines the density of mobile ions, which drift throughout the space charge region. From the analysis of the capacitance transients the dissociation energy of the dopant-ion pairs is determined directly. The power of the new technique is demonstrated on hydrogenated boron doped p-type silicon. The dissociation energy is found to be 1.25(2) eV, which is in excellent agreement with previously published results. Hydrogen ion drift was established in Ge for the first time and the dissociation energy of 1.38(8) eV could be determined for Sb–H pairs.

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Mon-1.84po

Improved AMOLED with aligned polycrystalline silicon thin-film transistors by laser annealing and chemical solution treatments

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Keywords: AMOLED, polycrystalline silicon, thin-film transistor

In this study, low-temperature polycrystalline silicon (LTPS) thin-film transistors (TFT) were prepared for the active-matrix organic light-emitting displays (AMOLED). The excimer laser annealing (ELA) recrystallization technique was employed with a chemical solution treatment process to improve the TFT characteristic uniformity and the AMOLED display image quality. The characteristics of the poly-Si array thin films were influenced by XeCl ELA optic module design, TFT device channel direction, and laser irradiation overlap ratio. The ELA system module provided aligned poly-Si grain size of 0.3 μm by the homogenization lens design. The poly-Si TFT exhibited improved electrical properties when the laser irradiation overlap ratio was 97.5%, due to the highly aligned poly-Si grain arrangement. The chemical solution treatment process included a dilute HF solution (DHF), ozone water (O_3), and buffer oxide etching solution (BOE). The second ELA process has been helpful in improving the uniformity of TFT characteristics. The surface condition became smoother, and the variation in the current that drove AMOLED was reduced. The PMOS TFT showed better field effect mobility of 87.6 cm^2/Vs, and the threshold voltage was -1.35 V. The off current (I_{off}) was 1.25×10^{-11} A, and the on/off current ratio was 6.27×10^6. The display streak mura caused by the manufacturing process has been greatly reduced as well. In addition, the image quality of the AMOLED display was highly improved using the 2T1C structure design without any compensation circuit.

Mon-1.85po

An application of gold diffusion for defect investigation in silicon

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Keywords: Si, Au, diffusion, vacancy, interstitial

For successful use of defect engineering a control of defect concentration and their spatial distribution is needed. But in a case of low electrical activity and low concentration of defects only few methods can be applied for control their concentration and spatial distribution. One of suitable techniques is a study of Au diffusion in silicon. In defect-free Si Au diffuses via the kick-out mechanism and its concentration in the middle of defect-free wafers can be described rather well by exponential dependence in the temperature range from 700 to 1000°C. The deviation of gold concentration from the dependence predicted by the kick-out model could be explained by the presence of sinks for self-interstitials, vacancy type defects or by self-interstitial generation during gold diffusion annealing. Therefore, the concentration of substitution gold is very sensitive to the concentration and distribution of traps for self-interstitials and to the self-interstitial generation. Moreover a study of gold profile allows to clarify in some cases the nature of defects The concentration of gold in the substitution position can be easy controlled by the Deep Level Transient Spectroscopy (DLTS).

In the present work an application of gold diffusion for defect investigation in Si is demonstrated by the experiments carried out on silicon containing different types of defects. The efficiency of gold diffusion experiments for monitoring the concentration and spatial distribution of these defects is shown.

In the case of vacancy type defects the gold concentration could be much higher than that in defect-free Si and its depth profile is characteristic for trap limited diffusion. Such profiles were observed in nitrogen-doped FZ Si and in Cz Si after rapid thermal annealing. That allows to obtain the concentration of vacancy related centers and their depth distribution. Some data concerning gold interaction with vacancy-nitrogen complexes were presented. The application of gold diffusion measurements for the characterization of defect introduced under ion implantation is illustrated by the experiments carried out on H and He implanted samples, in which nanocavities are produced.

The effect of sinks for self-interstitials on gold diffusion was studied in the plastically deformed Si. The dislocation efficiency as a sink for self-interstitials is estimated from the gold diffusion experiments and it is shown to be limited. In samples with the high enough dislocation trail density and relatively low dislocation density the gold concentration is about two orders of magnitude higher than that in defect-free crystals. Moreover, our estimations show that the gold concentration obtained from the DLTS data is at least ten times higher then the value, which could be estimated for dislocations themselves even under an assumption about their infinite efficiency. Hence, we could declare that the gold diffusion in silicon plastically deformed at low temperatures is mainly determined by the defects in the dislocation trails and additional data about their nature can be obtained.

Mon-1.86po

Characteristic aspects of elastic softening due to vacancies in boron-doped FZ silicon observed by low-temperature ultrasonic measurements

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Keywords: vacancy, silicon, softening, boron, ultrasonic

Since the vacancies strongly affect the oxygen precipitation in silicon crystals, the vacancy concentrations should be controlled precisely to achieve high production yield in device manufacturing. We recently showed an innovative method of measuring the vacancy concentration, in which we observe the low-temperature elastic softening due to the vacancies by means of the ultrasonic measurements [1, 2]. The magnitude of the softening gives the vacancy concentration [1]. Regarding the nature of the softening, we found the following two important aspects: (1) The *softening behavior* is different for the different charge state of the vacancy [1, 2], although the softenings by the neutral and positively charged vacancies are described both by a formula $C(T) = C^{(0)}[1-\Delta/(T-\Theta)]$ [2]. (2) The softening by the positively charged vacancy vanishes when we apply the magnetic field, whereas that by the neutral vacancies is insensitive to the magnetic field [1, 2]. The purpose of this study is to confirm reproducibility of the softening characteristic of the positively charged vacancy.

We prepared an ingot of B-doped FZ silicon crystal having a resistivity of 2.8 Wcm and a diameter of 100 mm. The crystal was grown by SUMCO TECHXIV CORPORATION. Also in the present experiment, we observed the steep softening that suddenly appears at around 4 K in the absence of the magnetic field, which is similar to the softening we observed previously for the B-doped silicon grown by Shin-Etsu Chemical Co. Ltd. We thus conclude that the steep softening appearing at 3–6 K is characteristic of the positively charged vacancy. Further, as in our previous experiment, the softening observed for the present B-doped FZ silicon disappeared when we applied the magnetic field of 3 T, confirming that the magnetic-field-dependence of the softening is also inherent in the positively charged vacancy. Trials of theoretical explanation of the magnetic-field-dependence are now in progress. In summary, we have confirmed the nature of the elastic softening characteristic of the positively charged vacancies: (1) the steep softening that suddenly starts at around 3–6 K, and

(2) the magnetic-field-dependent softening that disappears for the applied magnetic field of nearly 3 T.

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Mon-1.87po

Grown-in disloctions in heavily phosphorus-doped Czochralski silicon

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Keywords: dislocation, inpurity, silicon

Silicon epitaxial wafers have been widely used in the fabrication of electronic devices which require the substrate resistivity as low as possible. For n-type Czochralski silicon (CZ–Si), heavily phosphorus (P)-doping is currently the pathway to achieve the lowest resistivity. Chiou has investigated the growth of heavily P-doped CZ crystal and pointed out that dislocations were generated at the center of the crystal about 50 mm above the solid/melt interface when the tang-end of a growing crystal reached a doping limitation of P concentration. In our practices, we have also found that there are grown-in dislocations in certain wafers cut from the portion near the tang-end of apparently dislocation-free heavily P-doped CZ–Si ingot. Therefore, to investigate the origin of the grown-in dislocation is of practical importance. In this work, the grown-in defects in the wafers cut from the portions near the seed and tang-ends of an apparently dislocation-free heavily P-doped CZ–Si ingot were comparatively investigated by preferential etching and transmission electron microscopy (TEM). It was found that oxygen precipitates, dislocations and stalking faults were present in certain wafers cut from the portion near the tang-end of the ingot. It should be noted that the grown-in dislocations did not cause the crystal growth of heavily P-doped CZ–Si to lose dislocation-free structure. In order to reveal the origin of the grown-in dislocations, a wafer free of grown-in dislocation, which is also cut from the portion near the tang-end of ingot, was subjected to an anneal at 1200°C for 2 h. It was found that there were dislocations in this annealed wafer. The dislocations were likely induced by the growth of certain grown-in oxygen precipitates during the high temperature anneal. It is believed that the heavy P-doping significantly enhances oxygen precipitation during the crystal growth. The large-sized grown-in oxygen precipitates will induce dislocations during the cooling process of crystal growth, which actually includes a high temperature anneal.

Mon-1.88po

DLTS study of the oxygen dimer formation kinetics in silicon

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Keywords: silicon, oxygen dimers, radiation defects

The oxygen dimers are believed to play a decisive role in the oxygen transport in silicon below 700°C. However, such important parameters as the dimer concentration, diffusivity, and diffusion length are still a matter of speculations. For instance, the diffusion experiments [1, 2] provide only a combination of dimer concentration and diffusivity. An independent combination of the parameters can be obtained from a study of the dimer formation and dissociation kinetics. In this contribution the kinetics of dimer formation around 500°C is investigated by measuring the concentration of the radiation defects for which the oxygen dimers are a precursor [3, 4].

An increase of the dimer concentration to the equilibrium value during annealing at $\sim$ 500°C is studied in the Cz-grown silicon wafers which have been preliminary quenched from higher temperatures to reduced the initial dimer concentration. The samples annealed for various time are subsequently irradiated with MeV-electrons, and the concentration of deep-level centers is measured by the DLTS technique. Amount of the radiation defects related to oxygen dimers is found to exhibit the expected trend being increased with the annealing. However, the annealing time, which is required to reach a saturation of the defect concentration at a given temperature, is observed to be at least several times longer than that expected from the simple model of dimer formation/dissociation and commonly assumed parameters. These data could indicate the existence of a barrier for the oxygen dimer formation. The results are discussed in comparison with the infrared absorption data.

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Mon-1.89po

Minority-carrier-enhanced dissociation of the boron-hydrogen pair in silicon

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Keywords: boron-hydrohen pairs, minority carriers

Hydrogen incorporation is well known to result in a strong passivation of the shallow-acceptor impurities in silicon. Thermal dissociation of the boron-hydrogen pair (and other hydrogen-acceptor complexes) was thoroughly studied around 400 K. It was further observed that the reactivation of passivated boron is strongly enhanced by photo excitation [1]. This phenomenon was ascribed to the photo-stimulated formation of the electrically inactive hydrogen-hydrogen pairs, that precludes the re-trapping of dissociated hydrogen by other boron atoms. However, experiments show that in some cases excitation of the electronic subsystem stimulates the penetration of hydrogen and its interaction with point defects [2]. Therefore, further studies of the boron reactivation process under photo excitation is required.

In this contribution, modification of the strongly non-uniform depth profiles of boron-hydrogen pairs preformed by chemical etching and reverse-bias annealing is investigated during anneals at temperatures 300–340 K. It is observed that the trap-limited hydrogen diffusivity is strongly enhanced in the presence of minority carriers (electrons) created by the back-side photo excitation. In contrast to the known effect of photo excitation [1], nearly all hydrogen atoms retain the electrical activity under the used conditions. The results are attributed to the enhanced dissociation of the individual boron-hydrogen pair due to the minority-carrier control of the charge state of incompletely dissociated hydrogen atom in the vicinity of boron. Parameters of the hydrogen energy levels estimated from these experiments are discussed.

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Mon-1.90po

Some features of a microdefect revealing in single-crystal silicon by the preferential etching technique

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Keywords: silicon crystal, microdefect, defect-contrast etching

On the way to extremely miniature silicon devices with the components of nanometer scale increasing requirements are imposed to structural perfection of surface and bulk of single-crystal silicon. The most perfect modern dislocation-free silicon single crystals are known to contain intrinsic and impurity microdefects (MDs) of different types with sizes varying from nano- to micrometers. MDs influence on electronic, optical and mechanical properties of devices of different function, as a rule, towards deterioration of their performance. The atomic structure of the majority of these objects is unknown. Improvements in delineation technique of such defects, investigation of their individual physical and chemical properties are important challenges in the course of upgrading of growth technique of silicon single crystals and developing new fabrication technologies of the promising micro- and nanodevices [1, 2]. Among the modern detection techniques of a fine structure of silicon crystals such as optical, electron, x-ray modes of microscopy, spectroscopy, topography and tomography, preferential defect-contrast (DC) etching technique stands out for its sensitivity, a widespread use and an apparent simplicity of realization. DC-etching is known to be based on the visual and microscopic analysis of morphology features of the crystal surface etched in the certain DC-etchants [2, 3]. After such a treatment the surface relief is composed of hillocks and/or pits, which are the traces of MDs existed in the etched-off crystal layer. Details of the DC-etching process, which is enigmatic in many respects, have been insufficiently studied and have not an adequate explanation in modern phenomenological and molecular theories of crystal dissolution [3]. The purpose of our work was to obtain new experimental information on the process of MDs delineation and identification in bulk of dislocation-free silicon single crystal by DC-etching technique and to search additional possibilities for increase in sensitivity and selectivity of the technique. We closely examined shape and size of MD etch traces on Si (001) surface induced by the individual MDs which were chosen to investigate, as well as evolution features of the traces during the crystal etching in $HF–CrO_3–H_2O$ and $HF–K_2Cr_2O_7–H_2O$ systems.

Our experiments showed essential differences of delineation properties of the etchants with respect to different defects when the sort of oxidizer and relative concentration of solution components were varied. The obtained experimental results suggest the following conclusions. The “etch magnification effect” (EM-effect), i. e. magnifying of size of etch traces (hillocks of various shape) up to several tens of micrometers from MD-ancestors of nanometer size with increasing of etch depth was observed in all investigated etchants for all types of revealed MDs. The shape of MD trace and character of EM-effect depend on MD type and composition of DC-etchant. It has been suggested to use these dependences for fine identification of MDs. Some numerical characteristics of EM- effect relating to microdefects of different types are proposed for application to improve selectivity of the discussed technique of defect delineation. We emphasize that the presence of EM-effect is the evidence of an insufficient adequacy of a widespread MD classification by the size of their traces [4, 5] because this effect is responsible for formation of the traces of different sizes from identical microdefects if the latter were located at various depth in the etched-off layer of the crystal. It was determined that the concentration of CrO_3 in the most effective DC-etchants of HF–CrO_3–H_2O system is in the range from 5.0 to 8.0 M. The concentration of $K_2Cr_2O_7$ in the most effective DC-etchants of HF–$K_2Cr_2O_7$–H_2O system is about 0.11 M.

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Mon-1.91po

Simultaneous doping of SiC by Al and N impurities

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Keywords: SiC, impurities, distortions

Three atomic shell cluster of Si–C–Al–N was treated as a set of chemical bonds with tetrahedral coordination. Chemical bonds energies were determined in tight binding approximation, taking into account second neighbors interaction and atomic positions relaxation.

As it was expected, Al atoms substitute Si atoms and cause lattice dilatation and formation of acceptor level. N atoms substitute C atoms and lead to shorter interatomic distances and appearance of donor level. In both cases there was large contribution of chemical component in substitution energy due to presence or absence of extra electron. Crystal lattice relaxation partially compensated the increase of chemical energy. Metallic contribution to the bond energy also was evaluated. Simultaneous doping of SiC by Al and N atoms without formation of Al–N bonds, i.e. the case of

$Si_{1-x}Al_xC_{1-y}N_y$ alloy, did not lead to decrease of substitution energy, because the wave functions of dopants were localized and their interaction was small.

Al-N bond chemical energy was almost equal to bond energy in pure silicon carbide. It means that alloys in Si–C–Al–N system have quasibinary character $(SiC)_{1-x}(AlN)_x$. In this case the chemical contribution in substitution energy was significantly smaller due to transfer of electron from the nitrogen atom to aluminum one. Inhomogeneous regions in $(SiC)_{1-x}(AlN)_x$ system were evaluated.

Mon-1.92po

Exchange coupled pairs of dangling bond spins as a new type of paramagnetic defects in nanodiamonds

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Keywords: nanodiamonds, paramagnetic defects, exchange coupled spins, low temperatures, EPR

Electron paramagnetic resonance (EPR) is a powerful tool for probing magnetism (both intrinsic paramagnetic defects and transition metal ion impurities) in novel diamond material obtained by the explosive synthesis — detonation nanodiamonds (DND, particle size ∼ 5 nm). The intrinsic paramagnetic defects in DND particles originate from the presence of lone orbitals of the fracture of C - C sp^3 bonds in the crystal lattice, inside both the diamond core and the interface. The characteristics of the main carbon inherited EPR signal are as follows: line width $\Delta H_{pp} = 0.80–0.87$ mT, $g = 2.00282(3)$, spin concentration $N_s = 6–7 \times 10^{19}$ spin/g. This value of the spin concentration yields on average 13–15 spins per each DND particle. Temperature dependence of doubly integrated EPR signal intensity (DIN) for the main signal follows the Curie-Weiss law within $4 \leq T \leq 300$ K with the Weiss temperature $\Theta \approx -1$ K. All this implies the intrinsic defects in DND are localized and weakly antiferromagnetically coupled. Para- and ferromagnetic impurities (mostly iron) in primary DND sample provide relatively broad ($\Delta H_{pp} \sim 35$ mT) signal in the half-field region ($g \sim 4.3$). Additional chemical treatment of primary DND powder allows practically complete removal of trace amounts of transition metal impurities. Disappearance of the broad EPR signal with $g = 4.28$ and $\Delta H_{pp} \sim 30$ mT reliably evidences this removal. This deep purification reveals a new doublet signal consisting of two narrow lines ($\Delta H_{pp}^{(1)} \sim 2.9$ mT, $g_1 = 4.26$; $\Delta H_{pp}^{(2)} \sim 1.4$ mT, $g_1 = 4.00$ at $T = 4$ K) separated by a distance of 10.4 mT [1]. The DIN value for this doublet signal is $10^4–10^5$ times lower than that of the main carbon inherited EPR signal. The former signal has been observed in a wide variety of DND samples disregarding of the impurity level reached and thus may be attributed to some intrinsic defects in DND particles. Such half-field EPR signals perfectly correspond to so-called "forbidden" ($\Delta M = 2$) transitions between Zeeman-split states of the thermally populated triplet level with $S = 1$ that may be observed in polycrystalline samples containing exchange dimmers — antiferromagnetically coupled spin pairs. Estimates suggest that the concentration of such defects is about one dimer per 100–150 DND particles. Observation of the dimer signals at low temperatures (down to 4 K) votes for a quite small singlet-triplet energy gap in an exchange-coupled spin pair. Temperature dependence of the doublet EPR signal shows its DIN obeys closely the Curie-Weiss law and correlates with the DIN behavior for the main carbon-inherited EPR signal. This provides *additional evidence* that two types of the intrinsic signals observed — the half-field doublet EPR signal and the main signal from the localized intrinsic paramagnetic defects in DND — are of the *same nature*.

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Tue-1.1po

Diffusion Al from implanted SiC layer

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Keywords: ion implantation, annealing, diffusion, modelling

Diffusion Al from SiC layers implanted by ions Al^+ at a room temperature at energy 300 and 150 keV with dozes 5×10^{14} cm^{-2} and 5×10^{16} cm^{-2}, accordingly below and above a threshold amorphization doze ($Q_a \approx 8 \times 10^{14}$ cm^{-2}) was investigated. After implantation it was spent rapid thermal annealing (RTA) during time $t = 15$ or 50 seconds at temperature 1700°C in Ar atmosphere. After implantation profiles of Al are quite satisfactory (except for near surface region) described by Gauss function according to LSS theory. After annealing at low dozes of implantation, $Q < Q_a$, redistribution of impurity Al concerning a maximum of distribution has symmetric character and is described by one diffusion coefficient. The estimation of diffusion coefficient gives value $D = 5.8 \times 10^{-12}$ cm^{2}s^{-1} at $t = 15$ c, that more than on 3 orders more than the equilibrium value certain at diffusion Al from a vapor phase [1–3]. This known phenomenon of transient enhance diffusion (TED) is connected with introduction of radiating defects during implantation and their subsequent annealing.

At greater dozes of implantation, $Q > Q_a$, character of impurity redistribution sharply varies. At depths, smaller thickness of amorphous layer, $x < x_a \approx$ 250 nanometers, a plateau on Al profile are formed. The volume part of a profile at $x > x_a$ thus remains practically without change in this connection profiles get rectangular ("box-shaped") kind. For the description of the observable phenomenon the segregation-diffusion model is offered.

At annealing of SiC, implanted by a high doze, $Q > Q_a$, solid phase epitaxial (SPE) recrystallization of amorphous layer occurs, during which between an amorphous layer (α) and a monocrystal phase (c) segregation of impurity occurs. Redistribution of an impurity is described by model of segregation at the zone-directed crystallization [4]. At continuation of annealing after end of SPE crystallization, in crystallization layer and in remained initially monocrystal parts of the implanted layer there is a redistribution of an impurity according to the equation of diffusion with boundary condition of impurity evaporation from a surface. From comparison of decision profiles with experimental it is found diffusion coefficients: $D_1 = 1 \times 10^{-10}$ cm^2/c, at $x \leq x_a$ and $D_2 = 3 \times 10^{-14}$ cm^2/c at $x > x_a$, evaporation coefficient $k_v = 1.4 \times 10^{-6}$ cm/c at $t = 15$ c and $k_v = 0.8 \times 10^{-6}$ cm/c at $t = 50$ c. The big difference in diffusion coefficients D_1 and D_2 leads to formation rectangular "box-shape" profile. The segregation-diffusion model allows to explain the basic features of Al profiles in SiC at the dozes of implantation exceeding a amorphization threshold.

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Tue-1.2po

Local neutrality and electronic properties of irradiated semiconductors

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Keywords: semiconductors, radiation defects, local neutrality, branch point, Fermi-level pinning

High-energy irradiation radically influences on the semiconductors electron properties. As a final, it results the Fermi-level pinning in the so-called steady state (limiting) position $\mathrm{F_{lim}}$, which is the representative ("intrinsic") parameter of the semiconductor. To predict the $\mathrm{F_{lim}}$-value and the electronic properties of irradiated semiconductors the concept of the local neutrality used. The position of local neutrality level $\mathrm{F_{lnl}}$ determines by the electrons occupation of the radiation — induced gap states and so

F_{lnl}-level is authenticable to F_{lim} position in heavy irradiated semiconductor. Such definition of F_{lim} position calculated from first principles band structure as the generalization of the definition of the branch point in the complex band structure of the crystal using some heuristic models [1–3]. The numerical calculated F_{lnl}-values in the large group (more than 20) of semiconductors (group IV and III-V, some semiconductors of II-VI group, SiC) presented. The concept-based calculation reveal the satisfactory agreement with experimental F_{lim}-data and shown that F_{lnl}-level serves as fundamental crystal parameters for characterizing the electronic properties of the irradiated semiconductors with some accuracy. Under this, the "ultimate" electronic properties of irradiated semiconductors depend on the specific features of the energy spectra, i.e. the position of F_{lnl}-energy with respect to the edges of the minimum band gap of the crystal only and are independent of both the condition of irradiation and the history of the material. Thus, for example, InN, InAs and HgTe obtain n^+-type conductivity; InP — n-type; GaAs, AlAs, GaP, CdTe, GaN, AlN, BN, e.t.c. — i-type and InSb, GaSb, Ge — p-type conductivity upon hard irradiation. This underlines the unified behavior of so-called narrow gap and wide gap semiconductors upon hard irradiation. It shown, that F_{lnl}-level is a universal common reference level in all semiconductors with related types of the chemical bonding. For the group of the investigated materials the absolute mean F_{lnl}-energy (respective to the "vacuum level") corresponds to the same values at about 4.7 eV. This 4.7 eV-energy is the asymptotic level to which the Fermi-level converges upon exposure to hard irradiation in related semiconductors. It needs to be note, even though the presented models [1–3] are unambiguous to predict the experimental F_{lim}-data, they are attractive due to their common and universal character, because they depend on the ideal crystal band structure only. Precise examination of the irradiated semiconductors electron properties ought to be done based on microscopic description of the real defects only, but it is impossible to-day and probably in the future too to done in the most semiconductors.

A final comment, irrespective of the electronic properties of he heavily irradiated material, the response of the electron subsystem of a semiconductor to high-energy irradiation is the manifestation of Le Chatelier's compensation mechanism. This process defines the evolution of the semiconductor electronic properties upon irradiation due to shifting of Fermi-level up to its canonical position near F_{lnl} in the crystal.

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Tue-1.3po

Observation of vacancy in crystalline silicon by ultrasonic measurements with piezoelectric copolymer transducers

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Keywords: silicon vacancy, softening, ultrasound, piezoelectric transducer, ferroelectric copolymer

Recently, the elastic softening of crystalline silicon observed by low temperature ultrasonic measurements has been attracting much attention, since the magnitude of the elastic softening indicates the concentration of the vacancies, which plays an important role in controlling the oxygen precipitation in the device fabrication processes [1]. In the conventional ultrasonic measurements, the piezoelectric transducers fabricated with $LiNbO_3$ plates are often used. In the case of the ultrasonic measurements for the crystalline silicon, however, the so-called negative thermal expansion of crystalline silicon causes bond-break of the $LiNbO_3$transducers. Thus we have been using piezoelectric ZnO films in the measurements for silicon. In this case, however, it takes too long time to form ZnO films of considerable thickness, namely, 5–10 mm. This causes the crucial problem in measuring the distribution of vacancy concentration in silicon crystal ingots, where we have to take sufficiently many sampling points.

In this paper, to reduce the time of fabricatin, we demonstrate a method of adopting piezoelectric transducers formed by pasting the solution of ferroelectric copolymers of vinylidene fluoride and trifluoroethylene, P(VDF/TrFE). The elastic softening observed for the silicon crystals by this new method is well explained by the coupling of the elastic strain and the quadrupole of degenerate vacancy orbitals of T_d symmetry, as in the case of the softening observed by the method using the ZnO transducers [1].

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Tue-1.5po

Far-action radiation defects and gettering effects in 6H-SiC implanted with Bi ions

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Silicon carbide is one of the most radiation-resistant semiconductors and is attractive for the use in harsh environments, including strong radiation, high temperature and chemical activity. SiC finds application in space electronics, various nuclear-power plants, in control of fissionable materials, and as a diluent of nuclear fuel. The results of numerous experiments show that electron, proton, light ions and neutron irradiation lead to similar kind of radiation damage and change in the SiC structure. At the same time the study of the mechanism of defect formation in SiC subjected to irradiation by heavy ions (> 1 MeV/a.e.m.) is of great interest for modeling structural damage induced by fission fragments. Under the condition of high and superhigh amount of ionization loss and the high rate of generation of radiation defects, there is a possibility of formation of both point and extended radiation-induced defects, as well as of the occurrence of latent tracks [1]. The point of interest of this investigation is behavior of irradiated SiC in working temperature range 400–500°C.

6H-SiC Lely crystals with $N_d - N_a = 1 \times 10^{19}$ cm^{-3} was irradiated by Bi ions at 710 MeV implantation energy. Three samples with different fluences were produced, 5×10^{10} cm^{-2}, 1×10^{11} cm^{-2} and 1×10^{13} cm^{-2} correspondingly. The samples were studied by Local Cathodoluminescence (CL) technique. CL Pictures in natural colors as well as CL spectra were obtained for all samples at room and liquid nitrogen temperatures.

The sample modification varies with the implantation fluence. For low-fluence (5×10^{10} cm^{-2}) sample minor modification were observed within implantation layer (implanted layer thickness is about 28.8 mkm). Samples with higher fluences were significantly modified during irradiation. Implantation layer were readily distinguishable due to color contrast in CL image. The contrast is accounting for radiation defects formed by Bi ions penetration. Also an area containing radiation defects was found at depth (up to 400 mkm) one order of magnitude larger then Bi ion penetration depth (28.8 mkm). We assume that this area is a result of far–action radiation-accelerated diffusion of defects occurred during the implantation. There is an area lacking of radiation defects relatively to the Far-action area adjoined to implanted layer. As we believe, the radiation defects from this area are gettered to the implanted layer.

The samples were annealed at 500°C during 30 minutes. Far-action area totally disappeared after the annealing at medium-fluence (1×10^{11} cm^{-2}) sample. Sample annealing result in improvement of crystal quality. Similar effects were observed for 4H-SiC irradiated by Al ions [2]. Sample with high (1×10^{13} cm^{-2}) fluence was not changed significantly after annealing. Therefore this fluence exceed the critical value at which crystal can be recovered to initial state.

SiC irradiated by heavy ions and annealed at 500°C does not loose its crystal quality and can be used in aggressive environment.

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Tue-1.6po

Computer simulation of 90° edge dislocation in silicon with gold impurity

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Keywords: silicon, edge dislocation, gold impurity, molecular dynamics, electronic structure

In recent years some researchers take an interest to dislocated silicon doped with metals. In particular, gold impurities are considered [1]. In the present work the equilibrium space configurations of dislocation core with gold impurity were investigated by a method of the molecular dynamics. Were considered both substitutional impurity positions, and interstitial impurity positions. Clusters $Si_{540}H_{270}$ and $Si_{595}H_{318}$were used for simulation of 90° edge dislocation in silicon. Si-Si and Si-Au interactions were featured by means of the potential [2], allowing to obtain data about structural properties of Si-Au systems to the results of LDA calculations. For considering of Si-H interactions was used potential [3]. Au-H interactions it was completely neglected. The modification of the program written earlier for examination of polar systems [4] was used. Positions of the most probable arrangement of an impurity near of an edge dislocation core are discussed. Further the estimates of electronic structure of some clusters are made.

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Tue-1.7po

Computer simulation of some optical properties of one-dimensional photonic finite systems (Si/a–SiO$_2$)$_m$ with defects

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Keywords: Si, SiO$_2$, transmission spectra, photonic crystal, defect

Using transfer matrix method transmission spectra for the layered ordered structures of (Si/a-SiO$_2$)$_m$ with defect were investigated as in constant inductivity as with the account of dispersion of refraction index. It was found that the account of the refraction index in silicon has a relatively weak effect on position of the stop-bands in the considered photon-crystalline but considerably changes location and the value of peaks in the transmission spectrum connected with the presence of defect in the structure. A special emphasis was attended to the analysis of numerical stability in transfer matrix method by comparing the results of calculations made with a double and quadrupole accuracy. Transfer matrix method was found to lead in appearance of some non-physical peaks in the calculated transmission spectra for some values of the number of layers. An area of applicability of this method for the calculation of transmission spectra in photonic crystals is discussed. Our work is development of paper [1].

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Tue-1.8po

Photoluminescence excitation spectroscopy and time-resolved PL studies of erbium luminescence in epitaxial Si:Er/Si, SiGe:Er/Si and Si:Er/SOI structures

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Keywords: erbium, silicon, luminescence

Erbium-doped silicon is a subject of considerable interest due to the wavelength of the radiative transition $^4I_{13/2}$–$^4I_{15/2}$ in the 4f-shell of the Er^{3+} ion ($\lambda = 1.54$ μm) which lies in the spectral region of maximum transparency and minimum dispersion of quartz optical-fiber communication lines. In spite of much investigation, the details of the excitation mechanism of erbium ions in the silicon matrix remain poorly understood.

In our previous studies [1–3] we have demonstrated that considerable signal of erbium PL in the Si:Er structures can be obtained with excitation photon energies much lower than the band gap of Si ($h\nu < Eg$(Si)), which is at variance with the commonly accepted excitonic model of the erbium excitation in silicon. In this report we present the detailed studies of the photoluminescence excitation (PLE) spectra and time-resolved PL studies of the epitaxially grown Si:Er/Si, SiGe:Er/Si and Si:Er/SOI (silicon-on-insulator) structures.

The PLE spectra of erbium luminescence have been measured using Nd:YAG-pumped optical parametric oscillator in a wide spectral range (700–1600 nm). Besides the regimes of band-to-band and sub-band-gap excitation we have observed and studied erbium PL in conditions of direct excitation of erbium ions in silicon matrix in the range of excitation wavelengths 1460–1600 nm. The time-resolved spectroscopy of erbium PL has been performed with about 10 ns resolution by using InP/InGaAs-based Hamamatsu PMT detector (950–1700 nm). Based on the obtained results we discuss the mechanisms of excitation of erbium ions embedded into Si and SiGe matrix and the contribution of Auger-deexcitation in the temperature quenching of erbium luminescence.

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Tue-1.9po

Radiation defects as nanocrystals in bulk crystalline silicon

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Radiation defects in Silicon introduced under proton bombardement with simultaneous heating of sample (500°C) was carried out. As it was previously shown [1], under such treatment mostly the rod-like defects of $\{311\}$ type can be created in silicon. In our work it was established that such defects are as an origin of PL in 1.3–1.6 micron spectral interval. The spectrum of PL was investigated in 10–300 K temperature diapason. Such a PL observe only in p-type samples doped with Boron during the crystal grow process. On the same samples the $\{311\}$ type defects were observed with TEM method. On the n-type sample the discussing PL was not observed, the $\{311\}$ defects were absent as well. The intensity of PL decreases with temperature increasing but this Pl band exists even at room temperature.

In this spectral interval the form of spectral line can be changed if the procedure of irradiation will be repeated. In this case according to the TEM results of investigation the rod-like defect can be transformed into nano disperse interstitial clusters.

The analysis of this defects has shown that they can play role of quantum wires and quantum dots.

The possibility of realization of quantum size effects in observed rod-like defects and nano-disperse interstitial clusters for observed PL is discussed.

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Tue-1.10po

Self-interstitials and related defectsin irradiated silicon

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Keywords: self-interstitial, radiation defects, EPR, DLTS

Paper presents deep level transient spectroscopy (DLTS) and electron paramagnetic resonance (EPR) data on interactions of the primary and secondary defects in silicon irradiated by light ions (protons or a-particles) with emphasis on self-interstitial atom properties. Although Si_i is known unstable under electron irradiation and can migrate in p-type silicon even at temperatures $T = 4.2$ K, in case of irradiation of p-FZ-Si at 80 K by protons or a-particles the C_i and Al_i centers monitored by EPR and DLTS are introduced only in very low concentrations. Instead of these impurity defects a new defect giving a DLTS level at $E1 = E_c - 0.39$ eV and the EPR center Si-AA12 are detected in the as-irradiated Si.

The E1 state is observed in Schottky barrier diode irradiated with protons or a-particles at 77–270 K under zero-bias conditions as well as in n^+p junctions but in this case it disappears swiftly. E1 is not introduced at $T > 200$ K under reverse-bias conditions. 4 MeV electron irradiation also introduces the E1 defect but the E1 signal had an insignificant amplitude. The best conditions of E1 defect introduction are achieved at temperature 200–270 K when the E1 is predominant defect and concentration of impurity interstitials defects is very low. The E1 defect anneals thermally in a broad range from 280 K up to $\sim$ 330–350 K but disappears very fast under minority carrier injection at 77 K. As a result of E1 injection annealing, the impurity interstitials such as C_i in p-FZ-Si, C_i and $(Si\text{-}O)_i$ in p-Cz-Si as well as C_i and Al_i in p-ZF-Si(Al) samples emerge.

In n-type silicon irradiated by protons or a-particles the impurity interstitial centers (C_i) appear upon thermal annealing of the FZ-Si and Cz-Si samples at $\sim$ 140 K and $\sim$ 250 K, respectively, as in case of electron irradiation and the E1 center is not observed. The level would be too deep to observe with DLTS before the center anneals at $\sim$ 160 K.

Irradiation of FZ-Si samples with protons at 80 K introduces Si-AA12 isotropic ($g = 1.9998$) EPR spectrum with hyperfine structure due to a ^{29}Si at one equivalent site ($A \sim 45.5$ MHz) and 4–6 equivalent sites ($\sim$ 9.5 MHz). The hyperfine structure characteristic for vacancy-related dangling-bond type defects was not observed. The AA12 was not observed in Cz-Si immediately after irradiation and appeared only after the annealing of $(\text{Si-O})_i$ defect at $\sim$ 250 K.

Mon-2.1po

Short range ordering in dilute GaInAsN alloys

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Keywords: GaInAsN, ordering, band gap

In quaternary alloys the relative number of bonds cannot be uniquely determined from the atomic composition and depends on atomic arrangement. The statistics of bonds in equilibrium can be obtained by minimizing the free energy with respect of relative number of bonds. Since the relative numbers of bonds are not independent at a given atomic composition, they are conveniently expressed using the additional parameter ξ. The parameter describes the deviation of atomic distribution in the first shell from a random case and has the meaning of short-range order parameter (SRO): $\xi > 0$ — preferential formation of Ga–As and In-N bonds, $\xi < 0$ — preferential formation of Ga–N and In–As bonds, $\xi = 0$ — random alloy.

Correlations that occur in the second coordination sphere are responsible for microclustering. This type of short-range ordering is described by the second shell SRO parameter: $\gamma < 0$ — ordering, i.e. the second neighbors are unlike atoms, $\gamma > 0$ — microclustering, i.e. second neighbors are the similar atoms.

We considered a supercell $3a \times 3a \times 3a$ containing 7% In atoms and 2.3% of N atoms either in random manner or in special configurations. For each configuration, the relaxation of atoms was performed according to valence force field model. After determining the equilibrium positions of the atoms, we calculated the energy structure of the supercell in tide-binding approximation with sp^{3}s* basis set and interaction of second neighbors

Our calculation show that in correlated $\text{Ga}_{1-x}\text{In}_x\text{As}_{1-y}\text{N}_y$ alloys the number of In_2Ga_2 tetrahedrons, centered on N atoms, and As_2N_2 ones, centered on In atoms, is increased relative the random case. There are also specific atomic configurations — chains of nitrogen and indium atoms in [100] directions. N-centered tetrahedrons give rise to energy levels in conduction band, In-centered tetrahedrons and chains give rise to energy levels in band gap.

Any of these configurations changes localization of electron wave function, causing strong coupling of different conduction band states. Electron density is localized around N atoms, doping with In increases the localization. Conduction band minimum is strongly modified, since it is formed mainly from nitrogen states. Valence band maximum is determined by localization of hole wave function on In atoms and VBM shift is not large. The changes correspond to perturbation first order terms.

Correlation effects are evident in perturbation second order terms. For dilute $Ga_{1-x}In_xAs_{1-y}N_y$ alloys these corrections depend on the strength of Γ_{1c}-L_{1c} and Γ_{1c}-X_{1c} interaction and can lead both to increase and decrease of band gap relative random alloys. Γ_{1c}-L_{1c} and Γ_{1c}-X_{1c} interactions are determined by the type and localization of wave function: in the case of In_2Ga_2 tetrahedrons and zigzags the band gap increases, in the case of As_2N_2 tetrahedrons and [110] chains the band gap decreases.

Mon-2.2po

Photoluminescence characterisation of InAs:Cd films grown by MOCVD

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Keywords: InAs, MOCVD, photoluminescence, cadmium

Apart from the interest in InAs and related compounds for high speed electronic devices, this material forms an integral part of numerous nanostructures for opto-electronic applications, such as InAs/GaInSb strained layer superlattices and InAs nanorods. Very little effort has been expended, however, to understand the role of defects and impurities on the optical properties of this promising III–V semiconductor. Particularly, the residual doping level in thin films of this material is often too high to identify impurity-related levels from the emission detected in luminescence. Also, the true bulk electrical properties of p-doped thin films (deduced from Hall effect measurements) is often masked by an electron rich surface accumulation layer and the dominant contribution of electrons to the Hall coefficient (due to their high mobility). Often, the hole concentration of p-doped films are extrapolated from Hall measurements on highly doped (10^{18} cm^{-3}) films.

In this paper, the radiative processes in InAs:Cd films grown by MOCVD are investigated by Fourier Transform infrared photoluminescence spectroscopy. High quality epitaxial films grown on both InAs and GaAs substrate are investigated in order to establish the energy level associated with cadmium acceptors in this material. The band-to-band peak energy is correlated with the true bulk hole concentration in cadmium doped films. An empirical relationship between this transition and the true hole concentration extracted from temperature dependent Seebeck coefficient measurements is established, allowing an estimate of the hole concentration in p-type InAs films in the range 10^{17} cm^{-3} to mid-10^{18} cm^{-3}.

Mon-2.3po

Electroluminescence properties of 1.5 mm light-emitting devices with Er,O-codoped GaAs

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Keywords: erbium, codoping, GaAs, electroluminescence, laser diode

Rare-earth (RE) doped semiconductors have gained significant attention as a promising new class of materials that emit light from the RE 4f shell by means of electrical injection. In Er,O-codoped GaAs (GaAs: Er, O), one kind of Er center was formed selectively as an Er atom located at the Ga sublattice with two adjacent O atoms (hereafter referred as Er-2O) together with two As atoms, resulting in drastic enhancement in intensity of Er-related luminescence due to intra-4f shell transitions of Er^{3+} ions. We have fabricated GaInP/GaAs: Er, O/GaInP double-heterostructure (DH) light-emitting diodes (LEDs), aiming at realizing the stimulated emission at the Er center under current injection. Radiant Er-2O electroluminescence has been successfully observed at around 1.54 mm at room temperature under forward bias [1]. In this contribution, we report on electroluminescence properties of two types of 1.5 mm light-emitting devices with GaAs: Er, O grown by organometallic vapor phase epitaxy (OMVPE).

In a laser diode (LD) with a GaAs:Er,O active layer exhibiting a room-temperature lasing at the GaAs band-edge, the threshold current density (J_{th}) increased with the Er flow rate during the growth. The J_{th} dependence on the reciprocal cavity length indicated that the effective gain factor of the LDs is decreased by the codoping of Er and O, which is due to ultrafast capturing of injected carriers by an Er-related trap. The fast capturing process allowed us to observe both the spontaneous Er-2O emission at 1.54 μm and the stimulated emission at the GaAs band-edge in the Er-doped LDs. The Er intensity rose up steeply with the injected current density and then decreased gradually in the spontaneous emission region. The gradual decrease originates from an Auger process; excitation of injected carriers by excited Er ions. In the stimulated emission region, the intensity remained almost constant, reflecting an ultrafast energy transfer to Er ions [2]. In a LD exhibiting a room-temperature lasing from strained GaInAs quantum wells (QWs) embedded in GaAs: Er, O, on the other hands, the lasing wavelength was designed to tune to the energy separation between the second excited states ${}^4I_{11/2}$ and the ground state ${}^4I_{15/2}$ of Er^{3+} ions. The J_{th} for the lasing at room temperature was seven times larger than that of a GaInAs QW-LD with an undoped GaAs waveguide layer. The increase in the J_{th} also reflected the ultrafast carrier capture by the Er-related trap in GaAs: Er, O. In the region for spontaneous emission from the GaInAs QWs, the Er intensity revealed initially a steep increase with the injected current density, which was followed by a saturation. In the stimulated QW emission region, the intensity continued to increase with the current density, indicating a feasibility of resonant direct excitation of Er^{3+} ions.

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Mon-2.4po

Structural bistability and spin polarization of multivacancies in GaN identified by first-principles calculations

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Keywords: group-III nitrides, first-principles calculations, spin polarization, multivacancies

Group-III nitrides such as gallium nitride are of significant importance not only in optoelectronic devices but also in potential applications to spintronics. Indeed, room-temperature ferromagnetism has been reported for transition-metal- and rare-earth-metal-doped GaN [1]. Doping procedures of magnetic elements have been reported to introduce cation vacancies and their complexes [2]. Although intrinsic point defects including cation vacaincies have been intensively investigated by means of first-principles calculations [3, 4], multivacancies such as di- and tri-vacancies have hardly been studied so far. More importantly, the possibility of the spin polarization of vacancies has almost been overlooked.

In this study, we perform first-principles calculations that clarify the spin polarization and the lattice relaxation of multivacancies with various charge states in GaN. We show that the exchange splitting for the stabilization of electronic states competes with an electron transfer from gallium to nitrogen dangling bonds caused by cation breathing relaxation. As for the charge state of vacancies, the thermodynamic charge-state Fermi level of the vacancies does not correspond to the position of one-electron energy levels, because the fashion of the structure relaxation strongly depends on the charge state of the vacancies. Furthermore, the spin polarization of N dangling bonds results in ferromagnetic interaction among two Ga-vacant sites in trivacancies. We have also found that spins of cation monovacancies interact ferromagnetically in most cases [5].

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Mon-2.5po

Imaging charge transport and dislocation effects in ordered GaInP

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Keywords: transport, GaInP, dislocations, imaging, diffusion

An all-optical technique is used to measure transport properties in an ordered alloy of GaInP. Direct imaging of the minority-carrier diffusion distribution resulting from generation at a quasi-point source is obtained using an optical microscope coupled to a scanning electron microscope [1]. Minority-carrier diffusion lengths are measured by this technique in double heterostructures of AlGaInP/GaInP/AlGaInP on Ge substrates, providing a key parameter of interest to the performance of state-of-the-art triple junction solar cells [2]. Anisotropy associated with the ordering in the alloy is observed in the recombination distribution [3]. Because the technique offers high spatial resolution, it is possible to measure variations in minority carrier diffusion lengths associated with the dislocation bands produced due to lattice mismatch from the Ge substrate. New results will be presented where minority carrier diffusion measurements have been made across dislocation bands, using the electron beam to create a one-dimensional carrier generation source. Comparison of the intensity variations associated with these dislocation networks and the local minority carrier diffusion length demonstrate that diffusion lengths can actually increase near the dislocation, due to the combined effect of variations in non-radiative and radiative recombination rates.

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Mon-2.6po

Physical properties of copper oxide thin films prepared by dc reactive magnetron sputtering under different oxygen partial pressures

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Keywords: cuprous oxide, thin film, sputtering, oxygen partial pressure, XPS

Nano-structured copper oxide thin films were deposited on glass substrates by dc reactive magnetron sputtering. The structural, morphological, electrical and optical properties of the deposited copper oxide thin films were found to change with oxygen partial pressure. Changes in oxygen partial pressure during sputter deposition led to variations in Cu, Cu^{+} and Cu^{+2} concentrations, which resulted in corresponding changes in the electronic characteristics of sputtered semiconducting copper oxide films from initially n-type to p-type and then from p-type back to n-type. These phenomena demonstrate that p-type copper oxide thin films can only be deposited by dc reactive magnetron sputtering within a narrow oxygen partial pressure range.

Mon-2.7po

Thermal annealing behaviour of deep levels in as-grown p-type MOCVD GaAs

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Keywords: deep levels, annealing, group III–V, MOCVD, defects

Annealing behaviour of deep level defects in a semiconductor can help in shedding light on the nature of the defects. Under annealing, defects may become mobile and move around in the crystal, eventually either dissociating completely (if formed from a complex) or may combine with other constituents such as vacancies, interstitials etc. to form new types of defect. In either case, the annealing behaviour may help in identifying the constituents and thus the nature of the defect. The present study describes the effects of isochronal annealing on p-type GaAs grown by low-pressure metal organic-chemical vapor deposition (LP-MOCVD) over temperatures extending up to 670 K. Prior to annealing, deep level transient spectroscopy (DLTS) reveals the presence of two hole-emitting deep levels at $E_{\rm v} + 0.55$ eV and $E_{\rm v} + 0.96$ eV in the as-grown material in the majority-carrier deep level spectra, while the well-known electron-emitting native defect, EL2, at $E_{\rm v} + 0.79$, along with a broad band of deep

levels around ∼ 100 K, are observed in the minority-carrier injection DLTS spectra. Thermal annealing is found to introduce at least six new defects, four majority-carrier emitting deep levels, situated at, $E_V+0.11$, $E_V+0.27$, $E_V+0.44$ and $E_V+0.89$ eV in the bandgap, and two minority-carrier emitting defects, at $E_c-0.49$ eV and $E_c-0.99$ eV. The minority-carrier emitting band of deep levels around ∼ 100 K in the as-grown material has also been found to resolve into two distinct peaks corresponding to deep levels at $E_c-0.16$ eV and $E_c-0.21$ eV, upon isochronal annealing. Four of the annealed-in defects at $E_V+0.27$, $E_V+0.44$, $E_c-0.16$ eV and $E_c-0.49$ eV are identified with previously reported deep levels, while the other four defects cannot be identified with any of the deep levels reported in the literature. Detailed data on the annealing behavior and other characteristics of these annealed-in levels are presented. The thermal annealing behavior of the both inadvertent levels observed at $E_V+0.55$ eV and $E_V+0.96$ eV suggests that these levels are most likely related to arsenic antisite, As_{Ga}, defects.

Mon-2.8po

Radiation-induced deep levels in n-type GaAs grown by metal-organic chemical-vapor deposition

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Keywords: GaAs, deep levels, irradiation, DLTS, MOCVD

Extensive investigations have been performed on n-GaAs due to the technologically important native defect EL2 which can be easily observed electrically, as a majority-carrier (electron) emitting deep-level in this material, as compared to p-GaAs. Most of the earlier work, using deep-level transient spectroscopy (DLTS) technique, for instance, has been focused on Schottky-barrier diodes and, thus, deep levels observed only in majority-carrier (electron) emission spectra were investigated. Consequently, less attention has been paid to deep levels observable in minority-carrier injection DLTS spectra. We present a comprehensive study of both types of deep levels in alpha-irradiated n-type GaAs, grown by metal-organic vapor phase epitaxy (MOVPE), over a wide temperature scan range 12–470 K. An ^{241}Am radioactive source, emitting alpha particles of energy 5.48 MeV, has been used to irradiate the p^+nn^+ junction diodes at room temperature. Deep level transient spectroscopy (DLTS) reveals the presence of, at least, seven radiation-induced deep level defects at energy positions $E_c-0.05$ eV, $E_c-0.14$ eV, $E_c-0.19$ eV, $E_c-0.34$ eV, $E_c-0.38$ eV, $E_c-0.59$ eV and $E_c-0.69$ eV in the upper-half of the band gap, while two radiation-induced defects at energy positions $E_V+0.54$ eV and $E_V+0.77$ eV were observed in the lower-half band gap (minority-carrier injection spectra). The thermal emission rate signatures of the radiation-induced defects are compared with those of the previously reported defects introduced in alpha-irradiated, MOVPE grown, n-type Schottky-barrier diodes. It has been observed that while five of the majority-carrier emitting deep levels are similar to those found in alpha-irradiated Schottky-barrier n-GaAs, one majority carrier emitting level at $E_c - 0.69$ eV and two minority-carrier emitting deep levels, at $E_v + 0.54$ eV and $E_v + 0.77$ eV, observed in our junction diodes were not detected in Schottky-barrier diodes. Detailed data on the emission rates, capture cross-sections, and introduction rates of the radiation-induced defects are presented. The majority carrier emitting levels at $E_c - 0.05$ eV and $E_c - 0.14$ eV have been found to have electric-field dependent emission rate signatures as also indicated qualitatively by an earlier report [1]. Our detailed measurements and analysis of this field dependence lead to the assignment of square-well potential with well widths 2.8 nm and 3.6 nm to the two deep levels, respectively.

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Mon-2.9po

Surface and bulk passivation of A_3B_5 layers by isovalent diffusion from a localized source

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Keywords: phosphorous passivation

The isovalent dopant diffusion from localized source is applied to the surface passivation of $In_{0.53}Ga_{0.47}As$ and GaAs layers. The passivation effects are characterized by low-temperature (77 K) photoluminescence (PL) and the optical transmission spectroscopy measurements.

It is found that phosphorus doping from the gas phase effectively increases the PL intensity of InGaAs and GaAs layers. Investigation of the optical transmittance of p-InGaAs layers have shown that additional annealing in the P vapor results in more uniform distribution of Zn atoms, which is indicated by a steeper slope of the transmission spectrum curve.

The method of phosphorus diffusion was also applied to thin (100 nm) GaAs layers grown on Ge substrates. The PL spectrum of these layers consists normally of a broadband emission line at ~ 1.2 eV, associated with the donor-acceptor pair recombination. Both donors and acceptors in GaAs are usually assigned to Ge atoms diffused from the substrate occupying both Ga and As sites.

Drastic changes of the PL emission after the phosphorous diffusion have been observed: the intensity of the photoluminescence increases gradually and the blueshift observed with the pumping energy increase is more pronounced. These changes are explained by a decrease in the nonradiative recombination rate (e.g. at the heterointerface GaAs-Ge, antiphase boundaries, etc.) due to incorporation of phosphorus atoms into GaAs during diffusion.

The developed passivation method opens a promising way to improve the characteristics of multi-junction solar cells on Ge substrates.

Mon-2.10po

On the oxygen vacancy in Co-doped ZnO thin films

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Zinc oxide and related alloys are wide-band-gap semiconductors with numerous potential applications. However, such applications are currently hampered by the lack of control over electrical conductivity. ZnO is typically n-type, and high-resistivity material has been difficult to obtain; p-type doping has been reported but reliability and reproducibility are serious issues. The accepted idea is that the unintentional n-type conductivity is due to native point defects. Although oxygen vacancies have been widely discussed [1, 2] as possible origin for the residual conductivity there is still a lack of unambiguous experimental observations.

On the other hand, magnetic oxide semiconductors such zinc oxide doped with the 3d transition metals are promising for the emerging field of spintronics. However, in spite of extensive efforts in this area, there has been a great deal of controversy, especially on fundamental issues such as the origins and characteristics of the observed ferromagnetism. There is nevertheless some evidence to the effect that oxygen related defects play a significant role in stabilizing the magnetic properties of these materials [3, 4]. While, it is clear that the extrinsic as well as intrinsic defects are known to affect the carrier concentration and ferromagnetism, the exact nature and interdependence of these entities is far from understood.

In this work, we report the optical and transport properties of ZnO and Co-doped ZnO epilayers. Using photoluminescence measurements we identify a deep band centered at 2.4 eV for which we investigated the temperature dependance. We attribute this band to the oxygen vacancy. Using thermally stimulated current and deep level transient spectroscopy (DLTS) we identify several deep point defects in ZnO:Co. Among them a defect center O1 located at Ec — 0.5 eV is observed in all the studied materials. Annealing of our samples either in nitrogen ambient or in air revealed that the density of the center O1 increases when the annealing is made in nitrogen ambient. Performing the same DLTS measurements after subjecting the samples to a prior illumination with an UV light at low temperature causes the density of this defect to significantly decrease, thus showing the metastable nature of O1. We therefore attribute this center to the double-donor oxygen vacancy and propose a negative-U model for it. Furthermore, from what has been reported on the magnetic properties of ZnO:Co our results clearly suggest a correlation between the observed ferromagnetism in these materials and the oxygen vacancy.

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Mon-2.11po

An investigation of structural properties of GaN films grown on patterned sapphire substrates by MOVPE

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Keywords: GaN, nitrides, patterned sapphire, dislocations, MOVPE

In the recent years there has been an enormous demand for high quality epitaxial GaN films in the GaN-based electronic applications including high brightness LEDs, lasers etc. The high density of crystal defects such as threading dislocations (TDs) caused by the lattice mismatched substrates such as sapphire, SiC, and Si limits the internal efficiency of GaN-based devices [1]. Several approaches such as epitaxial lateral overgrowth (ELOG) [2], pendeo epitaxy (PE) [3], multistep method (MSM) [4], patterned sapphire substrates [5], and combinations of these methods [6] have been successfully proposed for reducing the TD density. A drawback of ELOG and PE methods is that one needs to perform epitaxial growth twice. In this sense the MSM and patterned sapphires have an advantage of a direct single epitaxial growth process.

There has been a lot of activity related to growth of GaN and the LED structure on patterned sapphire substrates. Many groups have reported improved GaN material quality and/or LED performance when the epitaxial structure has been grown on patterned sapphire substrate [6–10]. In principle the improved performance is claimed to be caused by two factors, enhanced light extraction by patterned substrate and improved internal efficiency due the decrease of TD density. However, there exists opposite opinions how important factor the reduced defect density is for the performance of GaN-devises grown on patterned substrates [6–10].

In this work we present an extensive study how the different substrate patterns affect the crystal quality of the MOVPE grown GaN films. The surface morphology and crystal structure were characterized by atomic force microscopy (AFM), etch pit density (EPD), high resolution X-ray diffraction (XRD), synchrotron radiation X-ray topography and scanning electron microscopy (SEM). The samples grown on patterned substrates offered reduced defect density compared to the reference sample. Changes in the other structural parameters were also observed and analysed.

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Mon-2.12po

Ab initio study of C-N centre in GaP

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Keywords: GaPN alloys

Uncontrolled defects in GaPN dilute nitrides are an important problem in developing devices based in these alloys. We investigate carbon-nitrogen complexes in GaP, using density functional-pseudopotential code and 64 atom supercell to simulate the bulk cubic GaP. We found a structure where carbon is triple bonded to a nitrogen atom and singly bonded to bulk phosphorus, being PCN atoms on $\langle 100 \rangle$ oriented line in a way similar to HCN molecule. This centre is only stable in the double positive charged state and is the lowest formation energy when compared with its positive, neutral and negatively charged CN interstitials for all values of the Fermi energy. The C_{2v} symmetry and the calculated stretch mode (1878 cm^{-1}) for the double positive PCN structure are in good agreement with the uniaxial vibrational experiments (2087.12 cm^{-1}) [1]. The downward 13C (15N) isotopic shift of the stretch mode are 45 cm^{-1} (24 cm^{-1}), in reasonable agreement with 56.5 cm^{-1} (38.7 cm^{-1}) experimental data. The anharmonicity of the stretch mode may account for a better agreement.

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Mon-2.13po

Deep level transient spectroscopy signatures of majority traps in GaN p-n diodes grown by metal–organic vapor epitaxy technique on GaN substrates

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Keywords: GaN, p-n GaN diodes, DLTS

Gallium nitride (GaN) and related III-nitride compounds are materials widely used for optoelectronic devices operating in the high energy range of the spectrum (from green to ultra violet) as well as for high energy, high temperature electronics. Light emitting diodes, laser diodes, detectors and field effect transistors represent variety of such devices. However the existence of defects responsible for the deep levels, which are located within the bad gap of the semiconductors, can seriously affect operation of devices made of the material possessing them. Therefore investigation of the defects, their origin and properties, plays a crucial role in improving the device performance and its quality.

In this study we present the results of investigation on p-n GaN diodes by means of deep level transient spectroscopy (DLTS) within the range of temperatures 77 K–350 K. GaN layers, Si-doped to nominal concentration of about $N_{\mathrm{Si}} = 5 \times 10^{18}$ cm^{-3} were grown by metalorganic vapor epitaxy technique (MOVPE) on Ga-polarity (0001) surface of GaN substrates. The thickness of Si-doped layers was set to 0.51 μm. Subsequently Mg-doped GaN layers of the thickness of 0.53 μm were grown. This latter layer had the nominal Mg concentration $N_{\mathrm{Mg}} = 5 \times 10^{19}$ cm^{-3}. The electron concentration in n-type material was found to be equal about 10^{18} cm^{-3} whereas the hole carrier concentration in the p-side — to 2×10^{17} cm^{-3}. The MOVPE grown layers were subsequently used for the deposition of Ni/Au contacts (25 nm/20 nm) to p-type material and Ti/Au contacts (30 nm/70 nm) to n-type material.

DLTS signal spectra disclosed the presence of two majority traps. Their activation energies obtained from Arrhenius plots are equal to $E_1 = 0.22$ eV and $E_2 = 0.65$ eV and respective apparent capture cross sections $\sigma_1 = 3 \times 10^{-17}$ cm^{-3} and $\sigma_2 = 1.5 \times 10^{-15}$ cm^{-3}. Trap concentrations are $N_{T1} = 5 \times 10^{16}$ cm^{-3} and $N_{T2} = 1 \times 10^{15}$ cm^{-3}. The location of the DLTS signal peaks is insensitive to the applied electric field and the duration of the filling pulses. The traps of similar signatures have been observed in n-type GaN and p-n GaN diodes grown by MOCVD technique [1, 2]. Electron trap of energy E_1 has been assigned either to the N vacancy [1] or dislocation line [2] whereas the E_2 electron trap to the N antisite, vacancy or complex [1, 2]. So far there was no report on barriers for capture for these defects. In present work we show that for both traps capture cross sections are thermally activated with energy barriers for capture equal to $E_{b1} = 0.09$ eV and $E_{b2} = 0.08$ eV. Based on obtained results it may be concluded that the traps have the point defect related origin.

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Mon-2.14po

Structural and optical properties of MOVPE-grown GaInSb/GaSb quantum well structures

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Keywords: GaInSb, type-I quantum well, photoluminescence

There has been major progress over the last two decades in the development of Sb-based heterostructures for photonic applications. More recently, superlattices based on the InAs/GaInSb system have revealed advantages over the more traditional HgCdTe, such as decreased Auger recombination at elevated operation temperatures and device design versatility. It is however clear that the Sb-based semiconductor technology has not been underpinned by a systematic effort to understand the fundamental material and device related issues [1].

In this work, the metalorganic vapour phase epitaxy of $Ga_{1-x}In_xSb$/GaSb quantum well (QW) structures, which is a precursor to the growth of InAs/GaInSb superlattices, is investigated. The main focus is to identify the interface defects influencing QW emission, as well as relate the indium incorporation efficiency into strain nanostructures to the growth rate, substrate temperature and annealing during interface formation. Multiple quantum well structures are considered, with $Ga_{1-x}In_xSb$ wells ranging in width from 2 nm to 10 nm, and an indium content up to $x = 0.20$. The impact of the interface structure on the QW bandstructure is deduced from photoluminescence spectroscopy and transmission electron microscopy.

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Tue-2.1po

The defect influence on transfer of charge and energy in layered semiconductors

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Keywords: anisotropy, conductivity, stacking faults, layered semiconductors

The anisotropy of bond forces in layered crystals causes not only peculiarities of their energy spectrums, but leads to specific defect distribution in layered crystals. The weak bond between layers causes to possibility of easy formation of character defects. The presence of multiple stacking faults of layers, dislocations lying between layers is the same inherent property of layered crystals as peculiarity of their energy spectrum.

Supposing the presence of extended plane defects, stacking faults of layers in layered semiconductors in particular in InSe, one can explain many peculiarities of their kinetic and galvanomagnetic properties. For example, the formation of two-dimensional gas of charger carriers revealing in specific "two-dimensional" oscillation behavior of Shubnikov-de Haas [1], Hall quantum effect [2] and etc.

The existence of great number of such defects for example in layered InSe, leads to different mechanisms of charge transfer in direction along layer plane and in direction perpendicular to layers. Break of wave functions takes place in direction perpendicular to layers and it leads to appearing of localized states in contrast to direction along layer plane. At low temperatures ($T < 150$ K) the conductivity of single crystals n-InSe in layer plane is caused by thermally activated impurity electrons on extended states, simultaneously the charge transfer perpendicular to layers takes place by means of electron jumps over localized states being in narrow energy bend near Fermi level (so called variable range hopping conductivity). As a result of this, the high anisotropy of electric conductivity $\rho_{\mathrm{per}}/\rho_{\mathrm{par}} \sim 10^2$–$10^3$ (ρ_{par} and ρ_{per} are resistivities in layer plane and direction perpendicular to the layers correspondingly) not corresponding to anisotropy of carrier effective masses is observed. The analogous one takes place in more typical layered crystal which is graphite. In graphite the anisotropies of carrier effective mass is $\sim 10^2$, whereas the anisotropy of resistivities varies in the limits $\sim 10^2$–10^5 in the dependence on sample quality.

The presence of extended plane defects, stacking faults of layers, different inter-layer dislocations in layered semiconductors is revealed not only on electron transport, but in heat transmission processes. In layered semiconductors GaS and GaSe the thermal conductivity anisotropy $\chi_{\mathrm{par}}/\chi_{\mathrm{par}} \sim 3$ (χ_{par} and χ_{par} are thermal conductivity coefficients in direction along layer plane and direction perpendicular to layers, correspondingly) doesn't correspond to anisotropy of phonon group velocity. In graphite single crystals the thermal conductivity anisotropy is $\chi_{\mathrm{par}}/\chi_{\mathrm{par}} \sim 600$ whereas the anisotropy of phonon group velocity is equal to 6 approximately.

Thus, the weak bond between layers leads to easy appearance of big number of plane defects, stacking faults of layers which essentially make difficult their transfer in the direction perpendicular to layers not influencing on charge transfer and energy in layer plane.

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Tue-2.2po

Defects in AlN: high-frequency EPR and ENDOR studies

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Keywords: AlN, EPR, ENDOR, donor, deep level defect

Unintentionally doped AlN crystals are highly resistive. The important reason for high resistance of AlN bulk crystals is compensation of shallow donors by deep level acceptors. Another important factor which may affect the doping is a transition of donors to a deep state. The latter deep state called a DX center arises from a lattice distortion at or near the donor site exhibiting a negative correlation energy U for electrons trapped at this site. The formation of DX centers leads to self-compensation of the shallow donor, according to the reaction: $2d^0 = 2d^+ + DX^- + U$. Here, d denotes a substitutional shallow donor impurity.

EPR is known to be the effective methods for identifying point defects in semiconductors. In this report the properties of deep-levels defects and of shallow donors in as-grown AlN single crystals have been investigated by high-frequency electron spin echo (ESE) and electron-nuclear double resonance (ENDOR) at 94.9 GHz.

AlN crystal growth of wurtzite polytype was accomplished by sublimation of an AlN charge. Two types of the AlN samples were studied: dark-amber color and yellow color.

A number of S=1/2 spectra were observed in as-grown single crystals of AlN. Deep-levels defect has been observed in yellow color and shallow donors in dark-amber color samples. In yellow color crystal the EPR spectra reveal the prominent unresolved central line with almost isotropic g factor of about 2.0. Another center (light induced) has additional structure that can be simulated as a six-line spectrum, as arising from hyperfine (HF) interaction with a single Al atom. The HF structure suggests that it arises from a displaced Al atom of some kind. It is suggested that this deep level defect is related to interstitial Al^{2+} atoms on the basis of the large mostly isotropic hyperfine interaction (about 10% of the free atom 4s value). The isotropic HF interaction constant $A(^{27}Al) = 406$ MHz, whereas for the free atom, $A = 3911$ MHz.

Two types of shallow, effective-mass-like donors have been observed in AlN crystals. The first type could be observed without illumination and is detected in a wide temperature range. The second type is only observed upon illumination with sub bandgap light at low temperatures and can be bleached after annealing at 200 K. The two types of shallow donors have similar EPR spectra and their shallow character is evident from the multitude of ^{27}Al ENDOR lines. The light-induced shallow donors correspond to coupled pairs with an exchange interaction of about 24 cm^{-1} and with a lowest triplet state. These pairs are believed to show a negative correlation energy U. Their Coulombic center is most probably located at the N position. For this reason oxygen is proposed to form the core of this donor.

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Tue-2.3po

Temperature and dose dependence of defect formation in ion implanted ZnO

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Keywords: magnetic effects, defects

Magnetic effects have been observed in both high dose ($> 10^{16}$ /cm^2) and low dose (10^{12} /cm^2) ZnO. The former has been attributed to clustering of implanted ferromagnetic ions, the latter to the formation of Fe_{Zn}-V_{Zn} defect complexes [1], the formation of which becomes more likely as the samples are irradiated and defects created. In this contribution we present results of our investigations on the dose dependence of the defect formation at different temperatures and discuss the results in comparison with models of Zn-vacancy diffusion in ZnO.

Radioactive 60 keV ^{57}Mn^{+} ($T_{1/5} = 1.5$ min) ions were implanted into single-crystal samples of ZnO at the ISOLDE-CERN facility at temperatures of 300–400 K to fluences up to 10^{12} ions/cm^2. Mössbauer spectra were measured with a resonance detector equipped with ^{57}Fe enriched stainless absorbers and mounted on a conventional drive system outside the implantation chamber. The samples were implanted for 114 seconds, and the spectrum recorded continuously up to $\sim$ 10 minutes, when only few percent of the implanted ^{57}Mn remain un-decayed in the sample. This process was repeated several times, until the spectrum had reached saturation. For the experimental data presented here, the fluence was estimated to be $\sim 6.2 \times 10^8$ ^{57}Mn/(cm^2 sec).

The Mössbauer spectra at low doses ($< 10^{11}$ ^{57}Mn^{+}/cm^2) are dominated by a single line due to the ^{57}Mn ions entering predominantly substitutional sites. Higher doses lead to increased level of defects, and sextet lines due to iron in Fe^{3+} state become more pronounced. The rate of Fe$_{\mathrm{Zn}}$–V$_{\mathrm{Zn}}$ defect complex formation is obtained from the spectral area of the sextet spectrum with dose, and modeling this in terms of an exponential dependence on dose, results in a parameter d_0 describing how rapidly the Fe$_{\mathrm{Zn}}$–V$_{\mathrm{Zn}}$ pair formation approaches saturation.

At elevated temperatures, the capture range of defects increases and therefore also Fe$_{\mathrm{Zn}}$–V$_{\mathrm{Zn}}$ pair formation becomes faster. The temperature dependence of the capture process suggests that mobile defects are indeed responsible for the temperature dependence and with comparison to data available from positron annihilation measurements [2], high temperature Mössbauer studies [3] and theoretical calculations [4] we argue that V$_{Zn}$ is mobile at room temperature in these experiments and can explain the experimental data.

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Tue-2.4po

Density-functional modelling of Li and its complexes in ZnO

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Keywords: ZnO, lithium, defects, interstitial

Zinc oxide (ZnO) is a multifunctional material combining exceptional piezoelectric, semiconducting, optical and optoelectronic properties. Its numerous applications range from the traditional uses such as piezoelectric transducer or transparent conducting electrodes to novel applications such as transparent field-effect transistors and nano-structure devices [1]. However, the engineering of advanced materials able to meet the new requirements relies on the ability to understand the behaviour of dopants and related defects which, despite major progress in the last few years, is still deficient.

In the present work we use atomistic modelling to predict the stability and electrical properties of isolated Li and its complexes with native vacancies and interstitials. Both a first-principles and a hybrid density functional scheme are employed.

We show that the bandgap correction preserves the picture of an acceptor substitutional (Li_Zn) center competing with a shallor donor interstitial (Li_i) center and affects little the calculated migration energy of Li_i.

Further, it is shown that Li_i forms complexes with interstitial oxygen (O_i) whereas Li_Zn binds both to oxygen vacancies (V_O) and O_i, and a model is proposed for the vacancy-related F_A center [2].

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Tue-2.5po

Intrinsic defects in CdTe and CdTe:Zn

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Keywords: CdTe, ZnTe, alloys, theory, anti-site, vacancy

Its large bandgap and high absorption coefficient have placed CdTe as one of the most promising materials for x- and gamma-ray detectors and high efficiency solar cells [1]. Doping with Zn opens yet another field of novel applications taking advantage of the unusual ferroelectric properties of the CdTeZn system [2]. However, a satisfatory description of the physical phenomena underlining ferroelectricity in this class of materials has not yet been proposed.

We have investigated the possibility that intrinsic point defects may play a significant role in the ferroelectric phenomena. The structural and electronic properties of the cadmium vacancy and tellurium antisite, the dominant defects in material grown in Te-rich conditions, are modelled using first-principles theory. It is shown that the Te anti-site defect has trigonal symmetry at low temperatures suggesting that it may be in the origin of the polarisation switching. The interaction of the intrinsic defects with Zn atoms are also considered in an attempt to clarify the role of the Zn doping.

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Tue-2.6po

Phase composition of microdefects in heavily doped n-GaAs

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Keywords: heavy doped n-GaAs, microdefects, X-ray diffractometry, phase composition, structural parameters

Although there are many reports [1] on observation of various microdefects in the GaAs crystals heavily doped by the VI-group impurities (Te, Se, S), a question on the nature of these microdefects still remains unsolved. With a use of electronic microscopy, it was shown that the heavily doped crystals involve the next basic types of microdefects: 1) single — and/or multilayer stacking faults 0.1–1.0 μm in size; 2) small (up to dozens of nanometers) prismatic dislocation loops, both full and partial; 3) small size particles of the extrinsic discharges g located within the square of a stacking fault or on a dislocation loop. There are various opinions concerning the nature of observed microdefects and about possible mechanisms of their formation. The majority of authors hold the opinion, that the interstitial layers and the particles of the extrinsic discharges consist of $Ga_2(Te, Se, S)_3$ phase. However there are no direct data on composition of the microdefects.

In the work direct observation of Ga_2Te_3 phase in Te-doped GaAs is presented. (100) plane oriented GaAs:Te single crystals grown by the Czochralski technique with a free carrier density $n_0 = 5 \times 10^{17}–5 \times 10^{18}$ cm^{-3} were investigated. The samples were characterized by X-ray diffractometry (XRD) with Shimadzu XRD-6000 diffractometer. On the XRD patterns 200 and 400 Ga_2Te_3 phase reflections were found.

The analysis of XRD patterns has given structural parametres of Ga_2Te_3 phase. On the basis of comparison of the reflection intensities from Ga_2Te_3 and GaAs phases, the estimation of Ga_2Te_3 relative volume fraction has been carried out. The volume fraction of Ga_2Te_3 phase has averaged 0.02% that corresponds volume fraction of Te atoms in the material under study.

The lattice constant of Ga_2Te_3 has averaged 5.892 Å. The analysis of factors of reflection lines broadening has shown that the broadening is caused basically by smallness of coherent scattering domain (CSD) size. On the basis of Scherrer equation, the estimation of the CSD size has been carried out. The CSD size has averaged 980 Å. This value twice exceeds the average size of particles of the extrinsic discharges, obtained by TEM [1]. The increased value of the CSD size is caused by small intensity and narrowness of XRD reflection of Ga_2Te_3.

Nonmonotonic dependences of the relative volume fraction and the CSD size of Ga_2Te_3 on Te doping level are obtained. On the basis of the comparative analysis of these dependences and dependence of microdefects density on doping level, the possible reasons of change of structural parameters with increase of doping level are discussed.

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Tue-2.7po

Structural, thermal and optical properties of ZnO nanopartciles, $SiO_2:Ce^{3+}$ and $ZnO:SiO_2:Ce^{3+}$ nanoparticles prepared by Sol-Gel process

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Keywords: ZnO, luminescence, nano particles, dopant

The rare earth metal ions and semiconducting materials are often used as activator and co-activator ions to improve the luminescence properties of silica for their special electronic structures. ZnO, SiO_2 and $ZnO:SiO_2:Ce^{3+}$ nanoparticles were successfully synthesized in an ethanolic solution by using a sol-gel method. Material property dependence on the PH of the precursor was investigated by varying the amount of NaOH during synthesis of ZnO. The corresponding influence of the ZnO on the SiO_2:Ce matrix was also monitored. The structural and optical properties were investigated by X-ray diffraction, transmission electron microscopy, Thermogravimetric analyses, Differential scanning calorimetry, UV absorption, and photoluminescence. The PH of the precursor was found to have influence on the size of the nano particles. The incorporation of ZnO nanoparticles enhanced significantly the photoluminescence intensity of the Ce ions in SiO_2 matrix.

Tue-2.8po

Self-assembling of isoelectronic impurity nanoclusters in III-V semiconductors

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Keywords: self-assembling, nanoclusters, isoelectronic impurities

Self-assembling (SA) of 1N4Al and 1As4Ga tetrahedral nanoclusters in GaAs:(Al, N) and zinc blende AlN:(Ga, As), respectively, was predicted in [1]. Later, SA in zinc blende AlN:(Ga, Sb) was studied [2]. The semiconductors with the zinc blende structure are considered in the dilute and ultradilute limits for the cationic and anionic isoelectronic impurities, respectively. Cationic and anionic co-doping transforms a binary compound into a quaternary submolecular alloy. The reasons of SA are a decrease of the contribution of the constituent compound free energies and decrease of the strain energy after formation of isoelectronic impurity clusters. SA conditions are represented by the phase diagrams describing three phase states. The first state is a state without self-assembled nanoclusters. The second one is a state in which

a fraction of the minority isoelectronic impurities are in nanoclusters. In the third state all minority isoelectronic impurities are in nanoclusters. In accordance with the developed model the occurrence and completion of SA should be results of the continuous phase transitions.

The last results on SA of 1B4Sb nanoclusters in GaAs:(B, Sb) are represented. BAs is fundamentally different from other binary semiconductor compounds. The electronegativities of boron and As are equal to each other and BAs is almost covalent compound having the anomaly small enthalpy of formation. Therefore, the GaAs and BSb bonding is significantly preferential over BAs and GaSb one from thermodynamic point of view. The tetrahedral covalent radii of boron and Sb are smaller and larger than those of Ga and As respectively. Accordingly, isolated boron and Sb atoms shrink and dilate a crystal lattice of GaAs. From the strain energy standpoint these impurities presence should lead to the complex formation. The distances between the nearest atoms in BSb and GaSb are larger and smaller, respectively, than such distances in GaAs and SA decreases the strain energy. Thus, there are two origins of self-assembling of 1B4Sb nanoclusters in GaAs-rich $B_xGa_{1-x}Sb_yAs_{1-y}$. All or almost all Sb atoms should be in nanoclusters in the alloys at temperatures up to 1000°C.

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Tue-2.9po

Deep electronic states associated with extended defects in GaN

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Keywords: GaN, MOVPE, dislocations, Laplace DLTS

Deep level transient spectroscopy (DLTS) and high resolution Laplace DLTS (LDLTS) have been applied to MOVPE-grown n-type GaN with varying dislocation densities, grown on c-plane sapphire. Samples were grown in a 6x2” Thomas Swan Close Coupled Showerhead reactor. Trimethyl gallium (TMG), silane (50 ppm SiH_4 in H_2) and ammonia (NH_3) were used as precursors and hydrogen as the carrier gas. The dislocation densities were varied by growing on different GaN templates, and ranged from 4×10^8 cm^{-2} to 4×10^9 cm^{-2}. The nominal carrier concentration of about 2.6×10^{18} cm^{-3} was confirmed by room temperature Hall effect measurements for all samples apart from the one with the lowest dislocation density which showed an upward deviation, presumably due to the presence of an unintentionally n-type doped region in the GaN-sapphire interface [1].

We have investigated the relationship between the time allowed for carrier capture (fill pulse duration) during the DLTS and LDLTS measurements, and the trap properties in the samples. Carrier capture into regions of local band bending caused by extended defects reduces subsequent carrier capture into that region, because of accumulated Coulombic repulsion. There is also an increase in the emission rate from deep levels associated with the dislocations due to this repulsive force. The latter can be directly observed by LDLTS measurements and can be a robust method for detecting defects at or near dislocations.

In the dislocated samples, multiple emission rates are observed in the LDLTS spectra, which suggests that the electrically active defects are close to dislocations, but often these rates do not change when the fill pulse duration is increased. Using the capture properties of the traps, the distinction is therefore drawn between point defects, point defects in the strain field of the dislocations, and band-like deep states at the dislocation cores, based upon the model of Schroter *et al.* [2]. By changing the LDLTS fill pulse duration, we show that a mixture of point defects and defects associated with dislocations are present, and their relationship to the dislocation density is established.

Finally, the results are compared with those from dislocated FZ Si which has been plastically deformed at 950°C, to illustrate the fact that the observed effects are common to all extended defects, both in unipolar and compound semiconductors.

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Tue-2.10po

Fano resonances in photocurrent spectra of p-GaAs and p-InGaAs/GaAsP quantum well heterostructure

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Investigation of phonon induced Fano resonances in photocurrent (PC) spectra of semiconductors doped with shallow impurities is attractive not only as theoretical knowledge but as practical way to determine phonon energy too. These features are more evident in PC spectra of polar material. But the shape of Fano resonance in polar semiconductors are strongly affected by dielectric permittivity behavior nearby phonon energies. This fact complicates identification of Fano resonance features in PC spectra of polar material. By now impurity PC spectra of p-GaAs are investigated thoroughly [1] excepting the restrahlen region between optical transversal (TO) and longitudinal (LO) phonon energies, where Fano resonance is expected to be.

Considering Fano resonances are induced by complicated resonance state "hole at acceptor ground state plus LO-phonon". These resonant states appear when wavefunctions of acceptor ground state and continuum states are mixed by means of hole-phonon interaction. In this case Fano resonances manifest themselves in the PC spectra as asymmetric features in the range of LO-photon energy. But excited state wavefunction can be mixed with continuum states wavefunctions too. In that case we will see features in the PC spectra at LO-phonon energy plus inter-level transition energy.

In this paper we report on Fano resonance detection and investigation in PC spectra on a series of p- GaAs samples (doped with C, Be, Zn), n-GaAs:Si and on quantum well (QW) heterostructure InGaAs/GaAsP delta-doped with C. PC spectra were measured using the BOMEM DA3.36 Fourier-transform spectrometer at 4.2 K.

In PC spectra of p-GaAs a broad peak (half-width is 12–15 cm^{-1}) is detected at LO-phonon energy, in contrast to n-type GaAs where half-width is 2.5 cm^{-1}. So smooth peak can suggest that there is no Fano resonance in p-GaAs. But for accurate consideration we took into account the sharp behavior of GaAs dielectric permittivity in restrahlen region. Therefore electric field strength has a dip at PO-phonon energy and sharp peak close to LO-phonon energy. Since PC signal is proportional to the electric field strength squared modulus $|E|^2$ we considered its dependence on energy. Besides, PC signal is proportional to dipole hole transitions probability and the probability spectrum shapes the Fano resonance in non-polar semiconductors indeed. In polar materials PC spectra does not reproduce dipole transitions probability. The probability characterizes resonant state, hole-phonon interaction and helps to determine phonon energy. Therefore we calculated dipole hole transitions probability for p- and n-GaAs using PC spectra. It was drawn that in dipole hole transition probability of p-type GaAs Fano resonances manifest themselves as narrow dips (~ 6 cm^{-1}), in contrast to n-type GaAs.

In conclusion note that Fano resonances in p-type GaAs and QW heterostructure were detected. The shape of the spectral feature was investigated and shown that in dipole hole transition probability of p-type GaAs Fano resonances manifest themselves as dips.

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Tue-2.11po

Annealing behaviour of Hf implanted $Al_xGa_{1-x}N$ $(0 \leq x \leq 1)$

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Keywords: AlGaN PAC

sThe annealing behaviour of 0.5 μm $Al_xGa_{1-x}N$ on sapphire substrate after implantation of ^{181}Hf was studied using the perturbed angular correlation (PAC) technique. $Al_xGa_{1-x}N$ samples with different molar fractions of AlN from the commercial supplier TDI Inc. were implanted with a fluence of 1×10^{13} at/cm^2 of the radioisotope ^{181}Hf with an energy of 160 keV at the Bonn Isotope Separator. Subsequently the samples were annealed in a rapid thermal annealing apparatus at temperatures up to 1373 K in nitrogen atmosphere. The strength of the electric field gradient, which is caused by the wurtzite structure of the host lattice at the probe site, varies almost linearly with the concentration x of aluminum in the ternary compound. The uniformity of this hyperfine interaction and thereby the homogeneity of the alloy has its minimum at $x \approx 0.5$. These results differ from PLE measurements [1] at similar samples, which report a maximum of alloy disorder for a molar fraction of $x \approx 0.7$.

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Tue-2.12po

New results on Cu diffusion in ZnO

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Keywords: ZnO, diffusion, copper

In recent years there has been much interest in the development of diluted magnetic semi-conductors based on transition-metal-doped ZnO. Recent theoretical and experimental studies found ferromagnetic behavior of ZnO:Cu at room temperature [1] although Cu and its oxides are non-ferromagnetic [2]. In addition, Cu is a deep acceptor in ZnO [3] and one of the causes of the green emission band [4].

We studied the Cu diffusion in bulk ZnO single crystals in the temperature range 1030 to 1180°C. The concentration profiles of substitutional Cu are determined via IR absorption at 5817 cm^{-1} [5]. We will discuss the possible diffusion mechanisms of the copper atoms to explain the profiles. Our findings reveal that the diffusion coefficient under oxygen-rich conditions is $7.6 \times 10^7 exp(-4.56\text{eV}/k_BT)$ cm^2 s^{-1}. This is about a factor of 25 faster than reported in the earlier studies [6]. The discrepancy is explained by the formation of Cu complexes, which occure at the higher copper concentrations in Ref 6.

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Tue-2.13po

Phase shift theory of dislocation scattering in ZnO

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Keywords: epitaxial films, threading dislocations, electron mobility

Zinc oxide (ZnO), a II–VI compound semiconductor, has a wide direct band gap of 3.37 eV at room temperature (RT), which underlies its use in short-wavelength optoelectronics and solar energy conversion technology. Transmission electron microscopy and x-ray diffraction studies demonstrate that the microstructure of heteroepitaxial ZnO thin films grown on lattice-mismatched (0001) sapphire substrates is dominated by a high density ($\sim 10^9 - 10^{11}$ cm^{-2}) of edge-type threading dislocations (TDs) [1–3]. Electron holography measurements [4] have yielded the result that the cores of TDs in n-type ZnO are electrically active and become highly negatively charged. Transport measurements [1, 2] show that the lateral mobility of conduction electrons in n-ZnO epifilms even at RT can be affected by the scattering caused by charged TDs. Motivated by experiments [1, 2], here we study the effects of carrier concentration and high temperature ($T \sim 300$ K) on the behavior of the TD-scattering limited mobility in n-type ZnO. Since highly charged [4] TDs induce very strong coulomb barriers for the motion of thermal electrons, we do not rely in our calculations on the small-angle Born approximation formalism [1, 2]. By utilizing the partial-wave decomposition method, we infer from the analysis of the scattering phase shifts that in the strong electron-defect interaction regime the quasiclassical transport across TDs is dominated by large-angle scattering events. The obtained non-perturbative picture demonstrates that the important impact parameters of electron-TD collisions are of the order of Read's screening radius, whereas the mobility of non-degenerate electrons falls off with decreasing the carrier concentration and/or increasing the temperature. We also show that below a certain critical doping concentration the network of highly charged TDs can induce at RT an electron localization transition.

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Tue-2.14po

Enhancing effect of hydrogen remote plasma treatment on luminescence of ZnO

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Keywords: ZnO, hydrogen, water vapor plasma, remote plasma treatment, photoluminescence

Zinc oxide (ZnO) has especially attracted much attention in wide band gap optoelectronics because of its wide band gap (3.4 eV) and large exciton binding energy (60 meV). The optical character should enable its potential application. In particular, ZnO is a most efficient candidate material for next-generation short-wavelength optoelectronic devices, such as both visible and ultraviolet light emitting diodes, laser, and solar cell at low cost. It is very important issue for the fabrications of such excellent optoelectronic devices to enhance luminescence of ZnO. The control of defect states is the most effective method for the improvement of luminescence properties of ZnO. In particular, passivation of radiative and non-radiative recombination centers by hydrogen should enhance ultraviolet emission and both ultraviolet and visible emissions, respectively. We report on the enhancement of luminescence of ZnO using remote plasma containing atomic hydrogen. We used hydrothermally grown ZnO single crystal and polycrystalline ZnO pellet prepared by sintering in this study. Microwave (2.45 GHz) plasma using two kinds of gas species (hydrogen, water vapor) was operated with a power of 50 W typically at approximate 100 Pa. Remote plasma treatment (RPT) was carried out in a horizontal quartz tube, where samples were heated at temperatures of 100–800°C for 30–120 min downstream approximate 15 cm apart from the plasma region. Some samples were annealed at 200–800°C for 30 min in Ar gas atmosphere without RPT. Photoluminescence (PL) was measured at 77 K and 300 K using a He-Cd laser (45 mW) emitting at 325 nm as the excitation source, a grating monochromator, and a lock-in amplifier. The enhancement of luminescence by RPT is observed in both ZnO single crystal and polycrystalline ZnO pellet. However, the enhancing effect of annealing on luminescence is a little in both single crystal and polycrystalline pellet. As a result of PL measurement at 77 K and 300 K, both ultraviolet and visible emissions are enhanced in ZnO single crystal. On the other hand, only ultraviolet emission is enhanced for PL at 300 K in polycrystalline ZnO pellet. The enhancement of both ultraviolet and visible emissions in polycrystalline pellet is observed for PL at 77 K. It is thought that passivation of non-radiative recombination center is dominant in polycrystalline ZnO pellet containing much defects. It is found that the enhancing effect of water vapor RPT on both ultraviolet and visible emissions is more effective than that of hydrogen RPT. Not only hydrogen but also oxygen in H_2O gas might have influence on radiative and non-radiative recombination centers in ZnO.

Tue-2.15po

Deposition of Al doped ZnO layers with various electrical types by atomic layer deposition

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Keywords: atomic layer deposition, transparent conductive oxide, Al doped ZnO

Recently, several research efforts on the development of transparent conductive oxide (TCO) layers have led to the improvement of devices such as displays (LCD and OLED), photovoltaics, light-emitting diodes (LED), and photodetectors. ITO, which is a representative TCO material, has been intensively investigated by industry demand but it has significant problems such as shortage and price advance of In metal. As an alternative TCO, metal (Al, In, Ga) doped ZnO films are promising candidates. These films can show the insulator, semiconductor, and conductor characteristics depending on dopant concentration at the same time.

Various deposition methods, such as sputtering, pulse laser deposition, chemical vapor deposition, atomic layer deposition (ALD), and sol-gel process, have been used to produce AZO films. Among them, the ALD process enables the growth of thin films with high-precision thickness control and excellent uniformity at a low temperature. [1] In addition, we can realize the growth of oxide films with all electrical types by the same facility. The ALD grown films are typically dense, pinhole-free, and extremely conformal to the underlying substrate.

In this work, the AZO layers were grown by ALD on a glass substrate with different pulse periods in order to control the electrical types. The electrical characteristics of the AZO films were investigated by Hall measurement system. As a result, the AZO film showed conductor property with a high carrier concentration ($> 10^{20}$ cm^{-3}) and low resistivity ($< 10^{-3}$ Ω cm) in less than 10% Al_2O_3 contents, while insulating property with a high resistivity ($> 10^5$ Ω cm) was observed in more than 20% Al_2O_3.

In addition, we obtained semiconducting property of $10^{-2} \sim 10^{2}\ \Omega\,\mathrm{cm}$ in the 12.5%∼ 16.7% Al_2O_3.

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Tue-2.16po

Oxide thin-film-transistors using ZnO channels grown at various gas atmospheres by sputtering

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Keywords: ZnO, TFTs, RF Magnetron sputtering

Zink Oxide (ZnO) has been extensively researched by many research groups, because it has many physical advantages and the controllability of electrical properties. In addition, ZnO thin-film-transistors (TFTs) have recently received much attention due to possible applications in active-matrix TFT displays such as AMLCDs and AMOLEDs [1]. The electrical resistivity of the ZnO films can be easily controlled in the wide range of $10^{-4} \sim 10^{10}\ \Omega\,\mathrm{cm}$, which includes insulator, semiconductor, and conductor, by varying growth parameters, dopant concentration, and post-annealing process. Among them, the electrical properties of the ZnO films are very susceptible to the variation in gas atmosphere, oxygen content, for the deposition.

Because the electrical property of the oxide channel in the TFTs is the most significant factor, the effect of gas atmosphere on the device performance of ZnO TFTs should be investigated in detail. The electrical resistivity of oxide channel is considerably changed by intrinsic defects such as oxygen vacancy or oxygen interstitial, which can be suppressed by appropriate gas ratio of argon/oxygen in the sputtering growth.

In this study, the ZnO channel layers with 50nm thickness were grown by RF magnetron sputtering on the SiO_2/Si substrate in Ar and O_2 mixed gas atmosphere at room temperature. A working pressure is 15 mTorr and a RF power is 150 W. The argon/oxygen ratios of 30/0, 28/2, 20/10, 15/15, 10/20, 0/30 were used. Source and drain electrodes were Ti/Au bilayers deposited by E-beam evaporation. The carrier density and resistivity of all oxide films are carried out by Hall effect measurement. The part of samples are thermal-treated by rapid thermal annealing (RTA) before the fabrication of TFT devices. In addition, microstructural analysis of the ZnO films will be performed by transmission electron microscopy and be correlated with device performance.

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Tue-2.17po

Observation of new donor system in ZnO following implantation of radioactive 73As and 72Zn

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Keywords: excitons, photoluminescence, radioactive isotopes

ZnO remains much in vogue due to the multitude of applications for which it may eventually be used [1, 2]. However, some apparently simple and straightforward questions such as the nature of impurities in the material remain unresolved, in particular those responsible for doping the material p-type. Part of the reason for this is that not all textbook approaches to doping in ZnO appear to hold true. Work by Wahl *et al.* [3] showed that As — a group V element — occupies the Zn position in the lattice, rather than the O- position one might presume, thereby becoming a donor rather than an acceptor.

To further examine the properties of ZnO:As we implanted radioactive 73As — which decays with a half-life of 80.3 days into stable Ge — into high quality ZnO single crystal material. Following implantation the samples were annealed at 850°C for 30 minutes in vacuum, and photoluminescence measurements charting the luminescence as a function of the radioactive decay were made.

In the present case, any luminescence due to 73As should change over time according to the 73As half-life. We do not observe any such luminescence, so, contrary to what is observed for other group V impurities in ZnO — such as N [4] — 73As does not produce acceptor-related bound exciton luminescence, nor is there any donor-acceptor-pair-related signal. We find no evidence that the 73As atoms exist as isolated impurities on the O site in ZnO, and we conclude that the implanted atoms occupy Zn sites, as reported by Wahl *et al.* [3].

However, we do observe a new luminescence signal for which the intensity grows as the 73As atoms decay to 73Ge with an unusual band shape which peaks at 3.322 eV. Further implantations using 72Zn — which decays into stable 72Ge — have also been carried out, and this band was observed in that case also. In the latter instance, the Ge atoms are expected to occupy Zn sites since they are produced via the decay of parent Zn atoms. The details of the luminescence bandshape associated with the Ge double donor are examined and the implications of our results for the production of p-type material via implantation methods are also discussed.

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Tue-2.18po

Native point defects in ZnS thin films

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Keywords: zinc sulfide, thin films, native defects, photoluminescence, quasi-chemical formalism

The native point defects ensemble in ZnS thin films obtained by the close-spaced vacuum sublimation technique (CSVS) [1] at different growth conditions has been studied. The energy levels in the band gap were studied by the photoluminescence spectroscopy. Luminescence spectrums were recorded using MPF-4 Hitachi electrical fluorometer in the range of wavelengths $\lambda = 360-710$ nm under liquid-helium temperature 4.7 K and 77 K. As excitation source we used the xenon lamp ($\lambda = 325$ nm). In the band gap of ZnS a range of localized states with different energy were revealed. The most typical energies of these centers: 1.8; 1.94; 2.06; 2.13; 2.59 and 3.13 eV.

The native point defects ensemble in the ZnS films was calculated using quasi-chemical formalism [2, 3]. According to the most general defect creation model, which takes into account the formation of neutral and electrically active defects in the anion and cation sublattices. As a result dependences of concentration of free carriers and native defects on technological growth conditions of ZnS thin films have been received.

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Tue-2.19po

Electronic structure of oxygen-vacancy in crystalline $InGaO_3(ZnO)_m$

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Keywords: IGZO, first-principles calculation, oxygen vacancy

Among the homologous oxides $RMO_3(ZnO)_m$ (R = Sc, In, Yb, Lu; M = Al, Ga, In, Fe; m – integer), $InGaO_3(ZnO)_m$ is of particular interest because this oxide material is used as a promising active channel in transparent thin-film transistors (TFTs) [1]. The crystalline phase of $InGaO_3(ZnO)_m$ is regarded as a natural superlattice which is composed of an alternating stack of an InO_2 layer and a (Ga/Zn)-O block. The distribution of the Ga and Zn atoms within the (Ga/Zn)-O block is still a subject to be resolved. Previous theoretical calculations showed that a Ga-modulated boundary model for the (Ga/Zn)-block is energetically more favorable than a flat boundary model [2]. Experimentally, it was reported that, similar to ZnO, undoped $InGaO_3(ZnO)_m$ exhibits n-type conductivity, with carrier concentrations ranged from 10^{14} to 10^{19} cm^{-3} [1, 3, 4]. However, the origin of the n-type conductivity observed in $InGaO_3(ZnO)_m$ is not clearly understood yet.

In this work, we investigate the defect properties of oxygen-vacancy (V_O) in crystalline $InGaO_3(ZnO)_m$ ($m = 3$) through first-principles calculations in the generalized gradient approximation (GGA) for the exchange-correlation potential as well as within the GGA+U approach, which are implemented in the VASP code. We choose the flat boundary model for the distribution of the Ga atoms, where the Ga and Zn atoms are located at the trigonal-bipyramidal and tetrahedral sites, respectively. Due to different environments around the O atoms, V_O has various configurations, which depend on the type of metal ions in the neighborhood. We find a tendency that the defect levels of V_O near the InO_2 layer and at the boundary consisting of the Ga and Zn atoms are slightly higher than those in the ZnO region, where V_O is surrounded by only the Zn atoms. All of these V_O defects have the defect levels deep in the band gap, similar to ZnO. Thus, our calculations lead to the conclusion that V_O is unlikely to be the origin of the n-type conductivity, although the Ga-modulated boundary model is not considered. Finally, we find that the formation energies of various O-vacancies are similar to within 0.1 eV, indicating that the site preference of the V_O defect does not appear in crystalline $InGaO_3(ZnO)_m$.

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Tue-2.21po

High temperature antistructure disorder in undoped ZnS

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Keywords: zinc sulphide, defect equilibrium, antistructure disorder

This report presents high temperature defect equilibrium (HTDE) model for undoped ZnS based on high temperature electrical conductivity (HTEC) measurements. HTEC data were obtained under defined conditions of component vapour pressure and in the large high temperature range. The result is surprisingly similar to HTDE models for undoped CdS [1] and for undoped CdTe [2]. Slopes of HTEC isotherms varied with component vapor pressure change and so we could not propose any simple HTDE model to make approximation for analysis. The method for solving the system of quasi-chemical reactions without approximation [3] was used. The appearance of different slopes on HTEC isotherms can be explained by a two-carrier conduction mechanism involving electrons and holes. All HTEC isotherms investigated can be divided into three regions. The high Zn vapor pressure region is characterized by positive HTEC isotherm slope and is caused by native donors. The slope of HTEC isotherm change into negative at low Zn vapor pressures. It is caused by increasing part of holes in bipolar conductivity. Analogous behavior of HTEC isotherms is observed also at sulphur vapor pressures: changes in the free carrier isotherm slope are observed at low sulphur vapor pressures. Our experimental data can be explained only by the inclusion of abnormal site occupation i.e. by antistructural disorder. This involves the occurance of sulfur at a zinc lattice, which must be expected to be a donor. The native defects for compensation may be onefold ionized and twofold ionized zinc vacancies. Antistructure disorder disappear with increasing of Zn vapor pressure. Preliminary HTDE isotherms and isobars containing antistructure disorder are proposed.

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Tue-2.22po

The influence of sapphire substrate orientation on crystalline perfection of GaN epitaxial layers grown by hydride vapor phase epitaxy

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Keywords: nitrid gallium, stacking faults, sapphire, orientation

GaN films were grown by hydride vapor phase epitaxy (HVPE) using N_2 as a carrier gas and NH3 and HCl flowing over Ga as respectively nitrogen and Ga precursors. Vertical reactor was used, the growth was performed on sapphire substrates with c(0001), a(11-20), m(10-10) and r(10-12) orientations. The crystalline perfection was studied using high resolution x-ray diffraction (HRXRD), optical microscopy and scanning electron microscopy (SEM), the latter with imaging of the surface in the secondary electrons and monochromatic microcathodoluminescence modes.

It was found that for c and a-oriented substrates the grown GaN films had the c(0001) orientation. For m-sapphire substrates the films had the semi-polar (10-13) orientation. Growth on r-sapphire resulted in non-polar a(11-20) GaN growth. HRXRD studies showed that for all orientations the width of the rocking curves monotonically decreased with increasing layer thickness which points to improved crystalline perfection. The best quality films were obtained for growth on c-sapphire (c-GaN) and r-sapphire (a-GaN). With the film thickness of 400 mm the full width at half maximum (FWHM) of the rocking curves was as low as 460 seconds for c-GaN and 600 seconds for a-GaN. In contrast to that the semi-polar films grown on m-sapphire still showed a high FWHM of 1300 seconds even for the film thickness of $\sim$300 mm.

The film morphology was strongly determined by the substrate orientation and consistently deteriorated in the row c-sapphire, a-sapphire, m-sapphire, r-sapphire. The dislocation density as measured by selective etching steadily decreased with increasing layer thickness (it was $\sim 8 \times 10^7$ cm^{-2} for the thickness of 30 mm and $\sim 10^7$ cm^{-2} for thickness of 400 mm). The GaN films deposited on m-sapphire and r-sapphire also had a high density of stacking faults (SFs) that increased the FWHM of the x-ray rocking curves. The high SFs density correlated with growth striations observed on the non-polar and semi-polar films surface. The SFs linear density was typically around 5×10^4 cm^{-1} for growth on m-sapphire and 5×10^3 cm^{-1} for a-GaN films prepared on r-sapphire.

Tue-2.23po

Ruthenium related deep-level defects in n-type GaAs

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Keywords: deep levels, group III–V, DLTS, MOCVD, defects

Transition-metal dopants have attracted interest as a special class of impurities in semiconductors. While their special electronic structure sheds light on the fundamental physics of impurity defects, the mid-gap deep levels frequently found to be introduced by these impurities make them of obvious technological interest. The semiconductor literature is replete with studies of 3*d* transition metal dopants in many materials. However, the studies of heavier transition metals from the 4*d* and 5*d* are generally scarce. In order to fill this gap in our knowledge and also because of the interest in the use of the heavier, thermally stable dopants to produce semiinsulating compound semiconductors, we have undertaken a systematic study of this, hitherto, obscure class of impurities in different host semiconductors. Deep levels introduced by the 4*d* transition-metal impurity, ruthenium (Ru), in n-type GaAs are the subject of the present study. Epilayers of n-type GaAs are grown by low-pressure metal-organic vapour phase epitaxy (LP-MOVPE) with *in situ* incorporation of Ru impurity through a specially synthesized precursor. The structures are completed with the growth of a thin p^+ top layer to yield p^+nn^+ junctions. Mesa devices provided with appropriate ohmic contacts, suitable for investigations by deep level transient spectroscopy (DLTS) are fabricated from these wafers. DLTS scans over a wide temperature range (12–470 K) reveal two prominent deep-level peaks associated with Ru, when compared with control samples with no deliberate Ru doping. The well-known mid-gap defect EL2 is also observed in these scans. The Ru-related deep levels, Ru1 and Ru2, correspond to energy positions $E_c - 0.46$ eV and $E_c - 0.57$ eV in the upper half-bandgap of GaAs. No prominent deep levels associated with Ru are observed in the lower half-bandgap in the injection DLTS spectra; only the three inadvertent levels already present in the as-grown, control material are observed in these spectra. Although a possible Ru-related peak may be present with a rather small concentration in these injection DLTS spectra, it is difficult to clearly identify this peak present in the control (as grown, without Ru) samples at a closely similar position. Interestingly, doping with Ru reveals an interesting significant suppression of the pre-existing deep levels, including EL2. Detailed emission rate signatures are presented for the Ru-related deep levels and analyzed to obtain the relevant deep-level characteristics. Both Ru1 and Ru2 are found to show strong dependence on electric field, as demonstrated by the shift in the corresponding DLTS peak positions with the applied reverse bias during electron emission. Detailed study of this field effect and other characteristics of the Ru-related deep levels is in progress.

Tue-2.24po

Thermal annealing behavior of deep levels in Rh-doped n-type MOVPE GaAs

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Keywords: GaAs, Rhodium, deep levels, annealing, MOCVD

Little work has been reported on heavy transition-metal (TM) impurities in GaAs. As part of our ongoing investigations of TM impurities from the $4d$ and $5d$ series, we have reported studies of the electrical characteristics of the deep levels associated with some of these impurities. The important information on the thermal stability of these defect states is, however, lacking in the literature. While this aspect of their properties is technologically important for the use of these impurities as thermally stable dopants, studies of thermal annealing behavior can also potentially shed light on the nature and microscopic structure of the associated defects, especially those relating to complexes of impurities with native defects. Results of isochronal annealing study of deep levels in Rh-doped n-type GaAs grown by metal-organic vapor phase epitaxy (MOVPE) are presented in this paper. Deep level transient spectroscopy (DLTS) technique has been employed to study the effects of annealing on deep levels in Rh-doped p^+nn^+ junction samples. A majority-carrier emitting band of deep levels along with a high temperature peak (Rh3), corresponding to deep level energy position $E_c - 0.92$ eV and a minority-carrier emitting band of deep levels are identified with Rh-impurity prior to thermal annealing of our samples. In addition to these Rh-related deep levels, the well-known native defect EL2 at $E_c - 0.79$ eV is observed in majority-carrier emission spectra and two inadvertent deep-level defects, H1 at $E_v + 0.09$ eV and H3 at $E_v + 0.93$ eV, usually observed in reference (without Rh) samples, are also detected in the minority-carrier emission spectra of Rh-doped samples. At least one level is found to be introduced at $E_c - 0.13$ eV in Rh-doped samples at about the same position as the level E(A)1, observed in reference samples, as a result of isochronal annealing, while the other two levels observed in reference samples could not be seen in annealed Rh-doped samples. Data on the annealing behavior and other characteristics of both Rh-related bands of deep levels observed in majority- and minority-carrier emission DLTS spectra, as well as for the high temperature Rh-related electron-emission peak, are presented. Possible interpretations of these results for the nature and structure of the different deep-level defects are discussed.

Tue-2.25po

Trends on electronic and chemical properties of rare-earth lanthanoids in gallium nitride

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Keywords: erbium, rare-earth, III-nitride semiconductors, GaN

Considerable effort has been focused on rare-earth (RE) doped materials for photonic applications over the last decade. In such context, RE doped III-V semiconductors emerged as leading candidates for light emission in the visible region. Erbium doped gallium nitride (GaN) has long been used as light emitting devices [1]. Recent advances have allowed to get laser activity in Eu doped GaN at room temperature [2], which suggests that other lanthanoids could provide equivalent properties, but in different frequency ranges. Such optical transitions are believed to be associated with intra-f spin transitions. Although other RE dopants, such as Pr, Tb, and Tm, have also been considered in GaN for photonic applications, no comparative study on the properties of those impurities in this material have been performed so far.

Here, we carried a theoretical investigation on the physical properties of isolated 4f RE impurities (from Pr to Yb) in the cation site of GaN. The calculations were performed using the all-electron spin-polarized full-potential linearized augmented plane wave (FP-LAPW) methodology [3]. The calculations were performed within the framework of the density functional theory and the generalized gradient approximation plus a U-Hubbard potential (DFT/GGA+U). Additionally, the 4f electrons were treated as valence electrons, and atomic positions were fully relaxed with no constraints. The results allowed to establish a clear trend on the electronic and chemical properties of these impurities. These results were compared with those obtained in recent theoretical investigations [4, 5].

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Tue-2.26po

Deep centers in bulk AlN and their relation to low-angle dislocation boundaries

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Keywords: III-Nitrides, deep traps, luminescence

In contrast to other group III nitrides bulk AlN crystals can be grown with reasonably high quality using a modification of physical vapor transport technique. Such crystals can serve as good substrates for epitaxial growth of InAlGaN films for which the problem of reducing extended defects density by growing on lattice matched substrates is acute. However, electrical properties, deep centers spectra and luminescence properties of such undoped bulk AlN crystals are yet not studied particularly well. In this paper we present the results of admittance spectroscopy, PICTS, TSC, low-frequency C-V, MCL spectra and MCL imaging studies, X-ray diffraction studies and selective etching measurements performed on such undoped crystals. HRXRD results and selective etching show that the studied crystals consist of large grains with characteristic dimensions in the 50–100 mm range separated from each other by low-angle dislocation boundaries. Admittance spectra are dominated by 270 meV and 630 meV electron traps with concentrations around 10^{14} cm^{-3} and 10^{16} cm^{-3}, respectively, as determined by low-frequency C-V profiling. The latter centers also dominate the PICTS spectra of the crystals. It is shown that the shallower traps are partly responsible for persistent photocapacitance and photoconductivity observed in our bulk AlN. MCL spectra show the presence of near-bandedge luminescence and two prominent defect bands near 3.3 eV and 4.2 eV. For the 3.3 eV band it was observed that its density is strongly enhanced near the low-angle dislocation boundaries which suggests that the band could be due to native defects decorating dislocations. Possible nature of the observed centers will be briefly discussed.

Tue-2.27po

Time-resolved photoluminescence properties of metastable shallow acceptors in Mg-doped GaN layers

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Keywords: GaN, Mg-doped, metastability, shallow acceptors

Despite many years of study, properties of p-type GaN are not completely understood. For example, there are at least two shallow acceptors in Mg-doped GaN which demonstrate a metastable behavior in photoluminescence (PL) or cathodoluminescence (CL) at some conditions. However, these two acceptors are often referred in literature to one Mg-related acceptor. Previous studies [1] have also shown the presence of the metastable defect-related UV emissions in CL which are not observed in PL. In this work we report metastable optical properties of two shallow acceptors A1 and A2 studied by PL and by time-resolved PL (TRPL) in high quality Mg-doped 1 μm-thick GaN layers grown by metal-organic vapor phase epitaxy. We have investigated samples as-grown and also after annealing during 10 min at 800°C in nitrogen atmosphere. The effect of metastability is reduced in annealed samples, but does not disappear completely. The main effect of annealing is activation of a lower energy acceptor A2. The following optical signatures are typical for the shallower acceptor A1: acceptor bound exciton at $\sim$ 3.462 eV (ABE1) and a donor-acceptor pair (DAP) recombination at $\sim$ 3.27 eV with its two LO phonon replicas. The deeper acceptor related to Mg is associated in PL with acceptor bound exciton at $\sim$ 3.453 eV (ABE2) and with a broad band at $\sim$ 3.1 eV. Thus, all p-type samples with the ABE1 line at 3.462 eV after annealing demonstrate instead another ABE2 at the lower energy 3.453 eV.

To confirm the presence of two acceptors we have done TRPL measurements. We have observed a fast initial transfer ($\sim$ a few ps) between the free exciton (FE) and ABE1 for as-grown samples. The shallow ABE1 dominates PL for as-grown samples; however, there is a transformation of the spectrum from ABE1 to ABE2 seen after few min of exposure to the laser light in p-type samples. In annealed samples we could clearly see both ABE1 and ABE2 within the first 300 ps after PL excitation by the laser pulse with a complete domination of ABE2 after 2 ns. We have also observed that a broad DAP spectrum at $\sim$ 3.1 eV appears and dominates PL after 0.5 μs. Thus, TRPL measurements directly confirm the presence of two different shallow acceptors in Mg-doped GaN.

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Tue-2.28po

Defect-related photoluminescence in undoped and Mg-doped GaN nanostructures

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Keywords: GaN, photoluminescence, nanostructures, Mg-doping

Discovery of p-type doping in GaN created technologies that have seen tremendous growth and economic impact around the world, with solid state lighting being the most prominent one. GaN:Mg has been well studied in the literature although open questions still exist. GaN based nanowire is finding applications that combine the superior properties of III-nitrides with those of nanostructures, such as high surface to volume ratio, and possibility of growing defect free structures. Many groups have reported on growth and characterization of n-type GaN nanostructures such as nanowires but no report has been given on electrical or optical properties of p-type GaN nanostructures. It is therefore paramount that an in depth research is conducted to study Mg doping in nanostructures for its incorporation efficiency, and its similarities and differences with Mg doped GaN thin films. Thin film of GaN:Mg, pyramidal GaN:Mg on GaN, sapphire and AlN substrates were grown in a MOCVD system under exactly same growth conditions and at the same time. In samples with Mg-doped GaN pyramids a strong ultraviolet (UVL) band with few phonon replicas dominated at low temperature and was attributed to transitions from shallow donors to shallow Mg acceptor. In some samples the UVL band appeared as a structureless band with the maximum at about 3.25 eV. There is a possibility that the structureless UVL band and the UVL band with phonon structure have different origin. In addition to the UVL band, the blue luminescence (BL) band peaking at 2.9 eV was observed in some samples at low temperatures. The BL band may be caused by transitions from deep donors to shallow acceptors in Mg-doped GaN [1]. However, in contrast to the Mg-related BL band, exhibiting giant shift with increasing excitation intensity [1], no shift was observed for the BL band in samples with Mg pyramids. It is possible that the BL band is caused by transitions from shallow donors to Zn acceptor in GaN:Si substrate. Currently we conduct additional studies to elucidate the identity of the PL bands in Mg-doped nanostructures.

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Tue-2.29po

Photosensitivity of ZnO/CuIn$_3$Se$_5$ heterostructures at γ-radiation

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Keywords: diamond-like semiconductors, photoconverters

The advantages gained by adding complexity of the atomic composition of diamond-like semiconductors were illustrated by the research concerned with the development of photoconverters based on the I–III–VI$_2$ ternary compounds and their quaternary solid solutions [1, 2]. The main result of the research was the discovery of extra ordinary radiation resistance of thin film photoconverters made of the Cu(In, Ga)Se$_2$ alloys with the calcopiryte structure. This study belongs to the topical line of semiconductor electronics and is concerned with gaining insight into the effect of penetrating γ-ray radiation on photoelectric parameters of ZnO/CuIn$_3$Se$_5$ heterostructures created on a new CuIn$_3$Se$_5$ ternary compounds formed as a result of the phase interaction at the pseudobinary Cu$_2$Se–In$_2$Se$_3$ section.

The CuIn$_3$Se$_5$ crystals were grown by directed crystallization and can be obtained only the p-type conductivity with resistivity $\rho = 10^6\ \Omega$ cm and free-hole concentration $p = 10^{10}$ cm^{-3} at room temperatures (RT). Electrical properties of the crystals were controlled by acceptor centres with an activation energy of $E \approx 0.5$ eV. The created ZnO/CuIn$_3$Se$_5$ heterostructures (HS) were irradiated with γ-ray photons in a normal air medium at RT. We used a continous ^{60}Co γ-ray source ($E = 1.25$ MeV with the intensity of $\approx 10^{13}$ photon/(cm^2 s). It is established that the photoconversion efficiency h is retained if the HS are irradiated with γ-ray fluxes $\Phi \leq 2 \times 10^{19}$ photon/cm^2. Dependences of the open-circuit photovoltage and the short-circuit current on the γ-photon flux are studied. It is shown that the photoelectric parameters of HS remain unchanged under irradiation with the fluxes $\Phi < 10^{17}$ photon/cm^2. In contrast, if the $\Phi > 10^{17}$ photon/cm^2 the photocurrent decreases monotonically, while the photovoltage exhibits a maximum, after which the photovoltage return to the initial value. The potential for using the create HS under the conductions of high background radiation is established.

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Tue-2.30po

Interaction of single Zn vacancy and single S atom doped in ZnO : A density functional theory study

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Keywords: defect, magnetism, density functional theory

The magnetic properties of a Zn vacancy and the effect of a single Sulfur (S) atom in wurtsite-ZnO has been studied. The calculations were performed with the scalar relativistic version of the full potential local orbital minimum basis (FPLO) code [1] in the framework of local spin density approximation of density functional theory. A neutral cation vacancy in ZnO favors a magnetic triplet state and yields a total spin magnetic moment of $M_S = 2$ Bohr magnetons in agreement with experiments and theoretical finding [2]. However, a single Zn vacancy in $Zn_7 O_7S$ yields a total magnetic moment in the range of $M_S = 1.56$–1.66 Bohr magnetons. The total energy calculations for different positions of vacancy and S in a suppercell (including the vacancy and S) have been performed. By means of total energy calculations and doing atom relaxation, we found that the configuration of nearest neighbor Zn vacancy and S atom has the lowest energy and being more favorable than the other configurations. The effect of doping S in presence of a Zn vacancy on the gap size of ZnO semiconductor has been studied.

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Tue-2.31po

Investigation of defects in nitrogen implanted n-type ZnO by capacitance spectroscopy and simultaneous optical excitation

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Keywords: ZnO, ion implantation, capacitance spectroscopy, DLTS

Nitrogen ions were implanted into a zinc oxide thin film on sapphire substrate, grown by pulsed laser deposition. Subsequent to the implantation, the sample was annealed at approx. 600°C for 30 minutes in a 700 mbar nitrogen atmosphere. Palladium Schottky contacts were deposited onto the sample. The sample as well as three reference specimen, an as-grown, an annealed but not implanted and an oxygen implanted and annealed sample, were investigated by capacitance - voltage spectroscopy (CV), deep level transient spectroscopy (DLTS), optical DLTS (ODLTS), photo-current (PC), and photo-capacitance (PCAP).

By CV measurements a net doping concentration of 4e16 cm^{-3} was determined. PCAP measurements proved that the total trap concentration is underestimated by this value due to high compensation with acceptors. The prominent defect E3 [1] was detected by DLTS in the nitrogen implanted sample as well as in all reference samples. A trap, in the following labeled TN1, with a binding energy of $\approx$ 580 meV was found only in the annealed and nitrogen implanted sample. We attribute TN1 to a nitrogen related defect which has to be distinguished from E4 [2] at similar energy but much larger electron capture cross-section. PC, PCAP and ODLTS measurements gave reason to assume the existence of (at least one) state close to the valence band which can be optically excited with light of energies $E > E_\text{g}(T) - 0.1$ eV.

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Tue-2.32po

ZnSe based films characterization by local cathodoluminescence

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Keywords: $A^{II}B^{VI}$, defect activation energy, cathodoluminescence

Investigation of the heterostructures based on wide band gap $A^{II}B^{VI}$ semiconductors attracts considerable attention as a result of wide applications in compact blue-green semiconductor lasers production. These lasers become essential in projection laser television systems, laser navigation and location, high quality color printing devices and other. From this point of view a solid solutions ZnCdSe, ZnSSe, ZnMgSSe are of particular interest since they are presently used in active, waveguide and emitter blue-green laser regions.The aim of the study was the research of the electron structure (the depth of trap levels and defects levels in band gap) of ZnSe, ZnSSe and ZnMgSSe films. These films with a different composition were grown by molecular beam epitaxy on GaAs substrate. The thickness of the films was about 1 μm.

The local cathodoluminescence is used as primary analyzing technique. The experimental results were obtained on X-ray microanalyzer Camebax Microbeam with the original cathodoluminescence system. The film composition was measured by electron probe microanalysis. The cathodoluminescence spectra of binary ZnSe, ternary ZnSSe and quaternary alloy ZnMgSSe were obtained. For these materials the cathodoluminescence intensity time variation were measured in dependence on the electron beam current density and sample temperature for interband electron transitions under electron beam irradiation. The intensity rise and then decay was observed and these processes are from 50 ms for rise to minutes for decay. The investigation was performed at different temperatures in the range from liquid nitrogen to room temperature and various electron beam current density.

The rise of emission intensity relates with the presence of electron traps in the films. If the depth of trap energy level is comparable with kT the trap deactivation process has high probability and radiative recombination occurs. The catch of electron by the trap and an electron transition from trap energy level to upper level leads to radiative recombination. The cathodoluminescence intensity rise time increases with lowering temperature and raising the electron beam current density. The intensity decay is caused by electron transition from conducting band to the defect energy level. This defect energy level considered to be the reason of nonradiative carrier recombination. The cathodoluminescence intensity decay time remains constant with the electron beam current increase so we assume that the intensity does not concerned with temperature decay due to electron beam irradiation.

The depth of the electron trap and defect energy levels in band gap was calculated. For different samples it varies from 0.02 to 0.06 eV below conducting band depending on its structural perfection. We attribute it to impurity or intrinsic defect levels.

The cathodoluminescence can be used in analysis of barrier layers inside the complex heterostructure with quantum wells. It allows studying the internal layers as well as the surface layers.

Tue-2.33po

One more unstable deep level related to the metastable hydrogen-related defects in n-GaAs epilayers

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Keywords: GaAs, deep levels, hydrogen, metastability

The hydrogen influence on the defect structure of compound semiconductors, such as GaAs, GaN etc., is the important point of interest in recent material science. Being included in the most of grown and processing techniques, hydrogen is known to interact with grown-in defects causing not only defect passivation but also giving raise to new defects. Since energies of interaction between hydrogen and other defects in a crystal, as a rule, are low enough, hydrogen-related complexes in many cases demonstrate unstable behaviour. So, studying of processes and of a mechanism of defect transformations for such complexes is quite important for understanding of hydrogen behaviour in the crystal.

The interesting example from this point of view is the system of metastable hydrogen-related defects M3/M4 in GaAs, which was rather extensively studied during last decades [1–4] but have not a complete model up to now. On the other hand, the significant number of unstable or metastable defects in n-GaAs was reported after various types of hydrogen treatment [5–7], but their structures were not also completely understood, and, in addition, most of them were not associated with M3/M4 defects.

In the present work, the set of n-GaAs samples grown by the chloride VPE technique and then subjected to atomic hydrogen treatment for the formation of M3/M4 defects is studied by the Deep Level Transient Spectroscopy (DLTS). It is shown that, in these samples, the trap with the energy level of $E_C - 0.45$ eV (similar to that observed previously [5, 6] and exhibited metastable behaviour) is included in metastable changes of M3/M4 defects. Particularly, it is found that, under the transition from the M4 to M3 state, the peaks M3 and $E_C - 0.45$ eV are appeared simultaneously after zero bias annealing (ZBA) in the temperature range of 310–360 K, and the sum of their amplitudes correlates well with the decrease of M4 peak.

Thus, the trap $E_C - 0.45$ eV in the DLTS spectra could be a revelation of the second metastable defect in M3/M4 defect system that was assumed [3] to overcome the discrepancy in M3 and M4 peak amplitudes and was not previously observed by DLTS.

It is important to note that in previously studied set of samples [4], the trap $E_C - 0.45$ eV was not appeared during metastable transition. This could be related to the parameters of sample preparation (e.g., type of shallow dopant) or to a sample history and gives interest opportunities for further investigations. The work is partially supported by the Erasmus Mundus External Co-operation Window Programme of the European Union.

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Tue-2.34po

Persistent photoconductivity of ZnO

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Keywords: ZnO, photoconductivity, magnetic resonance

Persistent photoconductivity is observed in ZnO single crystals and ceramics together with persistence of electron paramagnetic resonance (EPR) spectra of defects and impurity centers. It is shown that when the light is switched on and off the microwave conductivity detected from absorption of the microwave field is well correlated with the dc-conductivity measured with electrical contacts applied to the sample. The microwave photoconductiviy arises together with light-induced EPR spectra and persists after switching off the light. Coexistence of the conductivity and EPR spectra shows that the photoexcited electrons cannot return back to the paramagnetic centers. The persistent photoconductiviy in ZnO ceramics is large in comparison with the effect observed in powders prepared from the same material and in ZnO single crystals. This suggests that surface conductivity is the dominant mechanism of persistent photonductivity in ZnO.

The investigations of spectral and time dependences of the EPR signal intensity and microwave photoconductivity at different light quantum energies below the ZnO band gap showed that photoconductivity appears under excitation of electrons from impurity atoms (Li, Pb) or from oxygen vacancies. The well correlated spectral dependences of photoexcitation of the EPR spectra and the microwave photoconductivity show that after excitation from deep energy levels the electrons become captured at surface donor states.

Tue-2.35po

Thermoelectric evaluation of the acceptor concentration of p-type InAs and InAsSb

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Keywords: thermoelectric, Hall, InAs, doping

Hall effect measurements have been the preferred method for determining the conduction characteristics of semiconductor materials since its first conception. However, difficulties associated with more complex conduction systems, such as contributions from additional surface and/or interface conduction paths have necessitated more complex analysis to extract the basic doping and conduction properties. The additional variables associated with these degenerate conduction pathways also require more detailed Hall measurements, considering the dependence on temperature, layer thickness, magnetic field strength, etc. to separate the various contributions to the measured Hall voltage [1, 2]. The success of these methods is further hampered for materials with low mobilities and high intrinsic carrier densities. This has been apparent for studies of p-type InAs, where a surface accumulation layer [3] completely conceals the bulk characteristics. As a result, Hall effect measurements typically rely on measurements obtained for highly doped material in order to extrapolate the doping characteristics of lightly doped material [4].

The fundamental limitation of the Hall effect lies in the sensitivity to degenerate conduction pathways. We will demonstrate an alternative approach where the thermoelectric properties of small bandgap materials are related to the doping properties. As with the Hall voltage, the thermoelectric power and sign is related to the concentration and type of charge carrier [5]. The primary difference lies in the relatively small contribution to the measured thermoelectric voltage from degenerate layers. Contrary to the Hall voltage, the thermoelectric emf is more sensitive to the nondegenerate components of the thin film, with degenerate conduction layers decreasing the measured thermoelectric voltage. The thermoelectric sign reversal [5] from positive (extrinsic region of p-type material) to negative (intrinsic region) is consequently dictated by the bulk doping concentration and can therefore be directly related to the observed transition temperature. This new approach has been verified over a large doping range, and was used to demonstrate the linear incorporation efficiency of cadmium in InAs and InAsSb. The evaluation does not require any thickness information, is significantly less sensitive to the layer quality and aids the interpretation of Hall effect measurements.

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Tue-2.36po

Characterization of defects in undoped non c-plane and high resistance GaN layers dominated by stacking faults

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Keywords: GaN, deep defects, stacking faults, thermal emission

Recently, GaN-based materials are used in optoelectronic and microelectronic devices like LEDs, vertical cavity surface emitting laser or high electron mobility transistors. In some applications strong piezoelectric fields in c-plane GaN are undesired evoking for instance the quantum confined stark effect (QCSE). In this case the reduced polarization of non c-plane GaN layers is useful for better radiative efficiency.

Unfortunately, due to its anisotropic nature the growth of semipolar GaN produces much more stacking faults than in c-axis oriented GaN. The basal and prismatic plane stacking faults act as deep defects which are well known from photoluminescence measurements. However, little is known on their thermal emission and trapping behavior.

Therefore, we have characterized deep defects of a series of high resistance and undoped semipolar GaN samples grown by MOVPE on sapphire substrates by comparison of defect-related transitions in photoluminescence (PL), thermal dependent photocurrent spectroscopy (PC) and in thermally stimulated currents (TSC). We found correlations between the radiative emissions in PL and of absorption induced peaks in PC spectra at 365 nm and 375 nm which are caused by basal and prismatic plane stacking faults, respectively. The TSC spectra are dominated by traps with activation energies between 180 meV and 500 meV. Additionally, we investigated the semipolar GaN layers with scanning capacitance (SCM) and scanning surface potential microscopy (SSPM) in plan view and bevel configuration and found space charge regions correlating to stacking faults.

All results are compared to measurements on polar c-plane GaN samples and the correlation between the stacking faults and trapping behavior is discussed.

Tue-2.37po

Detailed electrical characterization of AlN/AlGaN multilayer structures on Si(111)

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Keywords: AlN/AlGaN-multi layers, defects, interface, conductivity

High-quality AlGaN layers open attractive applications in UV-optoelectronics due to the large direct energy gap variation between 3.4 eV (GaN) and 6.2 eV (AlN). Excellent material quality with respect to structural, optical and electrical properties is required for the use as basic material in UV light emitting or absorption devices.

Here, we investigate the impact of deep defects and different heterojunctions on the electrical conductivity of AlGaN layers with varying Al-content between 5% and 66% by Thermally Dependent Conductivity (TDC) and photocurrent spectroscopy (PC). Furthermore, the AlN seeding and superlattice buffer layers were characterized by PC and internal photovoltage spectroscopy (IPV) as well as with admittance spectroscopy (AS).

In AlN buffer layers the band gap signal at 6.2 eV as well as a sub-band gap signal at 5.5 eV followed by a wide Urbach tail was observed in PC. This sub-band signal is commonly associated with N-vacancies and induces persistent photocurrent behavior.

TDC measurements between 80 K and 500 K show different activation energies in coplanar and sandwich contact arrangement in dependence of the superlattice buffer layers.

Additionally, potential barriers caused by heterojunctions are investigated with capacitance-voltage-characteristics in Schottky contacts, with scanning capacitance (SCM) and scanning surface potential microscopy (SSPM) in plan view and bevel configuration.

The influences of interface defects as well as of defects within the AlGaN- layer and of space charge regions within the buffer layers are discussed in detail in regard to the DC resistivity and the AC impedance of the whole AlN-superlattice buffer/AlGaN layer arrangement on the high conductive Si- substrate.

Tue-2.38po

Defects in impurity implanted AlN single crystal

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Keywords: AlN, defects, implantation, impurities

Cathode luminescence (CL) has been used to study optical property and defects in bulk AlN single crystal implanted with Si, Zn and Mg. A strong CL peak at 350 nm (3.54 eV) and a weak peak at 450 nm (2.76 eV) are observed in all the implanted and annealed samples. In contrast, as-grown undoped AlN single crystal has a weak 319 nm and a strong 459 nm CL peaks [1–4]. The results suggest that the 350 nm CL peak is related with implantation induced defects in AlN single crystal. Compared to the as-grown undoped AlN sample [5–7], the observed strong 350 nm CL peak implies an increase of V_N vacancy caused by the implantation. The results also suggest that the 450 nm CL peak is most likely related with V_{Al} complex defect [8–10]. It is suppressed through the occupation of the Al site by the implanted impurity after annealing activation.

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Tue-2.39po

Intrinsic and defect-related luminescence of NiO

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Keywords: non-stoichiometric materials, photo-induced defect, exciton instability, antiferromagnetic semiconductor

Various NiO crystals (single crystals, the sintered powder compacts and nanocrystals) were prepared and the half of them were annealed at high temperature in a vacuum, to remove crystal defects. We have measured the optical absorption, reflection and photoluminescence spectra of the crystals at different temperatures between 10 and 300 K. Under 3.81 eV photoexcitation, two luminescence bands are observed around 3.0 and 2.3 eV, for the first time, while only 3.0 eV luminescence band is observed under 3.49 eV photoexcitation. The obtained results clarify the optical excitation and its relaxation in NiO, and they suggest the existence of the resonance between the inneratomic 3d state and the 4s conduction band state of NiO, like as a virtual bound state. Defect effect on the optical and electronic properties is discussed.

Ultraviolet-laser-light (photon energy $=$ 3.81 eV)-induced photoluminescence spectral change has been also observed at room temperature for the NiO specimens, for the first time. The observed change is explained as a photo-induced associative detachment of O_2 molecule on the specimen surface, while that observed in O_2 gas is explained as a photo-induced dissociative adsorption of O_2 molecule on the specimen surface, accompanied by nickel vacancy.

Thu-2.1po

The peculiarity of the thermal memory effect in layered crystals of $TlGaSe_2$ type

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Keywords: ferroelectric–semiconductor, incommensurate phase, thermal memory effect

Layered semiconductors $TlGaSe_2$ and $TlInS_2$ attract attention of numerous investigators. These crystals on subsequent cooling exhibit a sequence of structural phase transitions to an incommensurate (INC) and commensurate ferroelectric phases. As it is known, the presence of INC phase in crystal leads to occurrence of interesting effects one of which is thermal memory effect (TME) of INC phase.

TME of INC phase caused by interaction of the INC-modulation wave with defect density wave (DDW) which is appeared because of the spatial redistribution of mobile defects in the periodic field of INC wave after annealing of a sample at certain stabilized temperature T_0 inside the INC phase. DDW formation is accompanied by appearing metastable lattice deformation wave. If T_0 is again approached in a time shorter than the relaxation time of the induced metastable state, the DDW interacts with the INC-modulation wave, "captures" it, and, thus, realizes the memory effect.

It is well known that, as a rule, TME of INC phase exhibits in crystals after a long-term annealing ($\sim$ 100 hours) and takes place in narrow temperature vicinity T_0 (several degrees).

In recent paper TME of INC phase studied in layered ferroelectric–semiconductors $TlInS_2$ and $TlGaSe_2$ by investigating of temperature dependences of dielectric constant. It is shown that unlike other ferroelectrics with INC phase, TME in studied crystals exhibits practically in all temperature interval of existence INC phase in annealing with duration $\sim$ 3–5 hours. This peculiarity of TME exhibition is caused by the presence of high concentration of interlayer defects with high mobility in layered semiconductors of $TlGaSe_2$ type. It is revealed that peculiar TME of INC phase in crystals of $TlGaSe_2$ type are caused by pinning of soliton superstructure with DDW in the presence of internal thermoelectret field appeared during thermal annealing at T_0. It is shown that by influence of external influences (electric field and light radiation) during thermal annealing at T_0 one can strengthen or weaken internal thermoelectric field and control purposefully the response of nonequilibrium metastabile conditions of system related to DDW.

Thu-2.2po

Structural and luminescent characterization of defects in triple junction III–V solar cells

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Keywords: Mismatch, epitaxy, dislocations, III–V, solar cells

High-efficiency multijunction solar cells have greatly impacted the power capacities of satellites and future improvement in power-to-weight ratio is greatly anticipated. Further, the demand for high-efficiency solar cells for terrestrial concentrating solar systems is rapidly growing, with demonstration installations increasing and many new companies entering the market. The power delivered by these concentrating photovoltaic systems is directly related to the efficiency of the relatively small solar cells at the heart of the systems.

Currently, state-of-the-art high efficiency III–V solar cells utilize a three-junction design that includes a Ge bottom junction formed in the Ge substrate in conjunction with lattice-matched $Ga_{0.5}In_{0.5}P$ and Ga(In)As top junctions. However, the Ge junction absorbs about twice the low energy photons than are needed for current matching with the $Ga_{0.5}In_{0.5}P$ and GaAs junctions. Spectrolab has achieved a record 40.7% efficiency under 240X concentration by reducing the band gaps of the top GaInP and GaInAs junctions. While this reduction in band gap increases the theoretical efficiency, the alloy compositions of these top two junctions are no longer lattice-matched to the Ge substrate, but are lattice-matched to each other. The misfit and threading dislocations that reduce solar cell performance have been minimized in this device using a composition-graded buffer in a metamorphic structure.

Alternatively, $Ga_{0.5}In_{0.5}P$ and GaAs top junctions lattice-matched to GaAs in conjunction with a 1.0 eV bottom junction increases the theoretical efficiency of a triple junction solar cell even more. $In_{0.3}Ga_{0.7}As$ can be used as the 1.0 eV junction, but it has a larger lattice constant than GaAs by about 2%. The dislocations generated by this large lattice mismatch can be reduced through the use of compositionally graded buffer layers, but the remaining threading dislocations significantly degrade any subsequently grown junctions with higher band gaps. The results of our detailed TEM, EBIC and cathodoluminescence studies of these structures will be presented and discussed.

Thu-2.3po

Multifonon tunnel ionization of negative-U centers and S-shaped current-voltage characteristics in chalcogenide glassy semiconductors

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Keywords: negative-U centers, chalcogenide glassy semiconductors

Nonlinear response of negative-U centers at strong electric fields is studied.

Probability of multiphonon tunnel ionization of attractive center in the semi classical approximation has been obtained for a wide interval of electric fields.

This result may be applied to the interval of electric fields much more then earlier known results. Obtained results have been applied for calculation of nonlinear current-voltage characteristics for semiconductors with negative-U centers.

Obtained nonlinearity can be well approximated as exponential with electric field in the first degree.

Our result were used for calculation of S-shaped current-voltage characteristic in the electronic-thermal model frame.

Both mechanisms of nonlinearity of current-voltage characteristic: multiphonon tunnel ionization and joule heating — well explains the nonlinear current-voltage characteristic of chalcogenide glassy semiconductors, which are used today for nonvolatile memory cells.

Thu-2.4po

Calculation of the density of the charged defects $N(E)$ in glassy systems

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Keywords: density of defects, glassy systems

Study of many classes of materials (polymers, liquid insulators, chalcogenide glassy semiconductors (CGSs), etc.) indicates the existence of relaxation spectra with significant deviations from classical Debye dispersion. These deviations are interpreted in terms of the concepts about diffuse dielectric spectrum, which can be due both to the presence of relaxators with somewhat different (but similar) relaxation times τ_i and to the interaction between different relaxators. Such relaxators are generally atoms, molecules, groups of atoms, structural defects, etc.; they can form a continuous set (spectrum) of relaxation times. Concerning glassy systems, it is well known that D+ and D- centers with negative correlation energy can play the role of such defects, which exchange electrons during charge transport and accumulation [1].

In this work the relaxation-time distribution function, its main parameters, and energy distribution of the density of states of charged defects have been calculated for the first time on the basis of the experimental isothermal relaxation curves for dark current in thin films of glassy semiconductors As–S–Se and Ge–Pb–S systems.

The isothermal relaxation of dark current was measured on thin films with a thickness of $\sim 1.0\,\mu$m, prepared by thermal evaporation in vacuum. The samples were sandwiched with aluminum electrodes (contact area 14.0 mm^2). Isothermal relaxation curves were recorded with a B7-30 electrometer (range of measured currents from 10^{-15} to 10^{-7} A for both polarities) and a stabilized voltage source (measurements in fields E from 10^{-2} to 10^{-4} V/cm). During measurements, the temperature varied in the range 294–344 K [2].

On the basis of the obtained values of the function of the relaxation-time distribution, we calculated the energy distribution of charged defect states in the semiconductor system under study by method proposed in [3]. The results obtained confirm the existence of non-Debye dispersion in this system at infralow frequencies and can be used for further study of the electronic properties of disordered semiconductors.

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Thu-2.5po

Effect of illumination on dielectric properties of $As_{40}S_{30}Se_{30}$ glassy system

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Keywords: chalcogenide glasses, dielectric properties

Chalcogenide glasses have received a great deal of attention for the last two decades due to their technological applications, namely electronics, optoelectronic, optical and memory switching devices [1–3]. At the same time the influence of illumination on dielectric properties of these systems has not been adequately studied so far.

In this work the effect of prolonged exposures on dielectric properties of the SnO_2–$As_{40}S_{30}Se_{30}$–Al structures was studied. The samples had a sandwich configuration and were prepared by method of thermal evaporation in vacuum on transparent substrates. The films thickness d was $\sim 4.0\ \mu$m. To study the mechanism of photoinduced structural transformations, we measured the conductivity G and the capacitance C in a variable field by using a High-Resolution Dielectric Analyzer (Novocontrol Concept 41). The samples were irradiated by integral light with illuminance $J = 5 \times 10^4$ lx for 30 min.

The prolonged exposure of samples leads to the structural transformations. Measurements in the frequency range $f = 10^2 \ldots 10^5$ Hz demonstrated an increase in G and C after illumination. According to [4], this suggests an increase in the concentration of localized states responsible for the transfer of charge carriers and an increase in their contribution to the capacitance of the structured. Probably, these states are defect centers of the D^0 type.

An increase in the real component of the complex dielectric constant ε' and a variation in type of its dispersion are observed. For original $As_{40}S_{30}Se_{30}$, the dispersion of ε' is insignificant. After illumination, the character of dispersion is close to the Debye one with the characteristic relaxation time $\tau \sim 2 \times 10^{-4}$ s, which is likely to be caused by the appearance of a group of relaxing centers with close parameters.

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Thu-2.6po

Delta-doping of gallium arsenide by manganese

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Fabrication of materials, combined ferromagnetic and properties, is important for progress in spin electronics. For this purpose, common semiconductors are doped by magnetic impurity. Specifically, GaAs doped by Mn with concentrations about 5 at.% is typical magnetic semiconductor possessing Curie temperature up to 110 K. However, incorporation of relatively thick (≈ 0.1 μm) GaMnAs epilayers into device structures is faced with difficulties, related to high diffusion coefficient of Mn and its high activity as center of nonradiative recombination. In this connection it is of interest to study delta-doping of GaAs by Mn.

GaAs structures with delta-doped Mn layers were grown by technique combined MOCVD epitaxy with laser deposition. We used i-GaAs (001) substrates of two types: exactly oriented (singular) and vicinal (tilted by 3° in [001] direction). Firstly, buffer undoped GaAs layer was formed by the MOCVD on substrate, heated to 600–650°C. Then substrate temperature (T_g) was reduced to 350–450°C, and delta-doped layer was deposited by pulse laser sputtering of metallic Mn target in flow of arsine and hydrogen. Quantity of Mn in delta-layer (Q_{Mn}) can be controlled by time of deposition. A value of (Q_{Mn}) was measured in fraction of a monolayer (ML), and in our experiments was varied in the range from 0.09 ML to 1.4 ML. Finally, a top GaAs layer with thickness of about 25 nm was grown by the laser sputtering at the same lowered T_g. The technique of secondary ion mass-spectrometry (SIMS) was applied to study distribution of impurities with use of TOF.SIMS-5 set-up. Galvanomagnetic properties (Hall effect and magnetoresistance) were investigated at 10–300 K temperatures and ± 3000 Oe magnetic fields.

As shown SIMS results, at $Q_{Mn} \leq 0.12$ ML the depth distribution of Mn atoms is symmetric about position of delta-layer (x_{Mn}) in GaAs. Beginning on $Q_{Mn} = 0.18$ ML, Mn atoms collect on surface of the structure. For $Q_{Mn} \geq 0.30$ ML the concentration of Mn atoms at the x_{Mn} point remains practically fixed, and excess impurity was pushed into top-layer. This process can be associated with segregation of Mn atoms at movement of GaAs growth front. The SIMS data correlate well with results of Hall effect measurements. As Q_{Mn} increases from 0.09 ML to 0.3 ML, sheet hole concentration shows a rise from 3.7×10^{12} cm^{-2} to 5×10^{13} cm^{-2} at 300 K. In these conditions effective Hall mobility decreased from 80 to 20 cm^2/(V·s) at 300 K and from 1500 to 280 cm^2/(V·s) at 77 K. For $Q_{Mn} > 0.4$ ML the value of sheet hole concentration was essentially unchanged. This fact allows to suppose that Mn atoms, pushed into top-layer, are in an electrically inactive state.

The structures possessed ferromagnetic properties as revealed by nonlinear magnetic field dependences of Hall resistance with hysteresis loop (coercive field $\sim$ 80 Oe) and negative magnetoresistance (up to 4% at field of 3000 Oe) for temperatures below $\approx$ 30 K. The Mn delta-doped GaAs structures, grown on vicinal substrates, demonstrated anisotropic galvanomagnetic characteristics depending on disposition of current strip of the Hall bar in directions of [110] or $[1\bar{1}0]$. This anisotropy can be related with dominant arrangement of Mn atoms along growth steps in the delta-layer plane.

Thu-2.7po

Cation self-diffusion mechanisms in copper indium diselenide

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Keywords: CIS, diffusion, density functional theory

In search of new solar cell materials, the chalcopyrite-type CuInSe2 (CIS) has received much attention due to its high absorption coefficient and radiation hardness. In spite of extensive studies, the defect properties of CIS are far from being completely understood. Particularly, the data on its diffusion characteristics is rather scarce. In this work, we calculate the activation barriers for the self-diffusion of copper and indium with density functional theory based ab initio methods. We found that self-diffusion mechanism of copper and indium in CIS is a monovacancy mechanism having quite a low migration energy of 0.81 eV for both copper and indium vacancies migrating on their own sublattices. The corresponding energy of Cu self-diffusion is also sufficiently low, being equal to 1.29 eV, while that of In is 3.08 eV. This enables efficient copper self-diffusion already at rather low temperatures, while self-diffusion of In is practically suppressed. Moreover, we found that self-diffusion mechanisms which involve the creation of antisites are energetically unfavorable. The diffusion- driven defect redistribution and possibilities of kinetical defect complex formation are also considered and discussed.

Thu-2.8po

Features of mechanisms of generation of defects in the heavily doped p-TiCoSb and n-ZrNiSn intermetallic semiconductors

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Keywords: solid solution, electrical resistivity, seebeck coefficient, electronic structure calculation

The effect of the transition 4f- and 3d-metal impurities on structural, electrotransport and magnetic characteristics of the intermetallic p-TiCoSb and n-ZrNiSn semiconductors (so called half-Heusler phases) was investigated by magnetic and electrical measurements. Crystal refinements from X-ray patterns and electronic structure calculations were also performed. As effect, partially vacant crystallographic sites become possible and a disordered crystal structure with sites partially occupied is evidenced with MgAgAs structure type. Occupations on Ti, Zr, Co and Ni sites in p-TiCoSb and n-ZrNiSn are 93.3, 90.0, 95.8 and 91.6%, respectively.

Thu-2.9po

Photoluminescence measurements on Cu_2SnZnS_4

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Cu_2SnZnS_4 is a promising candidate for thin film solar cells with absorbers made of non toxic and abundant elements. Efficiencies up to 7% have been found so far [1]. But very little effort has been put up to now into understanding the basic material properties. Not even for such fundamental parameters like the band gap agreement has been reached: values between 1.4 eV [2] and 1.6 eV [3] have been reported. It is assumed that this is due to uncontrolled composition variations.

Cu_2SnZnS_4 is a material which is predominantly doped by intrinsic defects. To reveal the defect structure of Cu_2SnZnS_4 photoluminescence (PL) measurements have been carried out. So far only PL spectra with broad asymmetric peaks have been reported [4, 5], which are due to spatially fluctuating potentials. Spatially fluctuating electrostatic potentials are caused by compensation and induce a band bending, which allows a wide range of transition energies between the defects, and so leads to an asymmetric broadening of the peaks. Therefore PL measurements at highly compensated samples are not suitable to draw conclusions about the defect levels in the material.

Our samples were grown using the iodine vapour transport method and have near stoichiometric composition. These crystals have a much lower degree of compensation and allow for the first time the observation of narrow defect related emissions that enable us to do defect spectroscopy. We measured temperature and intensity dependent PL spectra and observed three narrow PL peaks, which are due to an excitonic transition and two defect correlated transitions. Initial results reveal defect energies of 30meV and 45meV. Extrapolating from the excitonic transition we observe a room temperature band gap energy of 1.50 eV.

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Thu-2.10po

Photoelectronic and electrical properties of $CdIn_2S_4$ single crystals

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Keywords: $CdIn_2S_4$, structural defects, photoconductivity, recombination and trapping

Cadmium indium sulfide ($CdIn_2S_4$) is a semiconducting ternary chalcogenide of $A^{II}B_2^{III}C_4^{VI}$ type. It has an indirect band gap energy E_g^i=2.28 eV at 300 K. $CdIn_2S_4$ is one of the photosensitive semiconductors with potential applications in optoelectronics.

$CdIn_2S_4$ has two kinds of atoms in cationic sublattice. It is possible formation of antistructural defects, due to substitution of cations (Cd_{In} and In_{Cd}), apart from cation and anion vacancies. As a result, in the forbidden band of $CdIn_2S_4$ presence a lot of local levels. However, the energy spectra of the local levels and nature of local centers in $CdIn_2S_4$ are investigated insufficiently.

The aim of this work is obtaining additional information about the localized levels and the nature of local centers in $CdIn_2S_4$ crystals. We have investigated a photocurrent infrared quenching (IRQ) as a function of the wave length by secondary light, kinetics of IRQ, temperature dependence photocurrent and dark electrical current, thermally stimulated current (TSC). Were studied stoichiometric (undoped), nonstoichiometric and copper-doped $CdIn_2S_4$ single crystals obtained by the freezing method.

In $CdIn_2S_4$ localized levels inducing high photosensitivity are investigated through photocurrent IRQ. IRQ takes place in energy range 0.73–2.0 eV at $T = 110$ K. By long-wave threshold IRQ are determined energy interval of photoconductivity sensitizing centers from edge of valence band. It was found that photoconductivity sensitizing level located 0.73 eV above valence band for undoped crystals. It was established that cadmium and indium deficiency does not change energy position sensitizing centers in band gap. But doping with impurity Cu leads to change energy position of sensitizing centers in band gap. In copper-doped samples sensitizing level is located 0.86 eV above valence band top.

Processes within short-wave threshold of the photocurrent IRQ have been studied. Spectral position short-wave threshold IRQ in $CdIn_2S_4$strongly depends on the filling-exhausting processes of centers. As a result short-wave threshold IRQ becomes sensible to external effects. It was shown that within short-wave region spectra IRQ have character competition photoexcitation and quenching of photocurrent in $CdIn_2S_4$. As a result, division photoexcitation and quenching, activation energy of local levels have been determined. It was 1.35 eV for undoped and cadmium deficiency samples, for indium deficiency samples 1.08 eV and for copper-doped samples 1.2 eV.

We presented investigation results of thermal quenching of photocurrent below the fundamental absorption edge at different illumination intensities, temperature dependence of dark electrical current and TSC in same crystals in temperature range 110–450 K. It was found the activation energies different levels located at 0.03, 0.15, 0.22, 0.5 and 1.0 eV below the conduction band bottom.

The obtained results allowed making some assumptions about on the nature of local centers in $CdIn_2S_4$ single crystals. The role of the cationic deficiency and impurity Cu on forming sensitizing and trapping centers in $CdIn_2S_4$has been discussed. We analyzed our results and data reported in literature have proposed model for the excitation and recombination processes and scheme of levels localized in gap of $CdIn_2S_4$.

Thu-2.11po

Conduction mechanisms in $TlSbSe_2$ crystals

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Keywords: crystal growth, semiconductors, electrical properties, Poole–Frenkel effect, activation energy

$TlSbSe_2$ sample used for electrical measurements were cleaved from larger crystals grown by using the Bridgman–Stockbarger method. Electrical properties of $TlSbSe_2$ have been carried out as a function of temperature (203–258 K) at different dc electric fields. The dcstudies revealed the non-ohmic type of conduction. The field lowering coefficient b is evaluated from log I versus $E1/2$ plot. It is found that the dominant conduction mechanism in these samples is Poole–Frenkel type. The activation energies are also calculated at different voltages. It is seen that the activation energy decreases with increase of applied voltage.

Thu-2.12po

Shallow traps and limitation of injection current by space charge in PbSnTe:In narrow gap ferroelectric

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Keywords: ferroelectric, narrow gap, shallow traps

In the context of a single model based on the limitation of injection current by space charge in the presence of traps and taking into consideration the ferroelectric properties of PbSnTe:In layers [1, 2] the following experimental results are discussed:

– behavior of the current-voltage characteristics at $T = 4.2$ K within the current range of 10^{-15}–10^{-1} A

– giant and anisotropic change of the current in the magnetic field: decrease by a factor of up to 10.000 and increase by a factor of up to 1.000 depending on the direction of magnetic field with the strength of up to 4 T [3];

– high photosensitivity within the fundamental spectral region (up to 20 mm) [4, 5];

– photosensitivity in the THz spectral region (up to 330 mm) [6, 7] including the negative photoconductivity.

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Thu-2.13po

Fabrication of low-resistive p-type AZO thin films by N_2 co-doping RF reactive magnetron sputtering

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Keywords: p-type, AZO, thin film, co-doped, reactive sputtering

P-type aluminum-nitrogen (Al-N) co-doped zinc oxide thin films were deposited on glass substrate at 300° by RF reactive magnetron sputtering using an aluminum-doped zinc oxide (AZO) (2.4 Wt% Al_2O_3) target and N_2 reactive gas. In addition, the effect of N_2 reactive gas on the electrical and structural properties of AZO thin films was also investigated. It was found that p-type AZO thin films could be obtained only when the volume ratio of N_2 in the N_2-containing Ar working gas exceeded 20%. P-type AZO thin films with a minimum resistivity of 0.141 Ω cm, a p-type carrier concentration of 5.84×10^{18} cm^{-3}, and a Hall mobility of 3.68 cm^2/V s were obtained in this study when the volume ratio of N_2 in the working gas was 30%.

Thu-2.14po

Charge carrier scattering on the short-range potential of the crystal lattice defects in ZnCdTe, ZnHgSe and ZnHgTe solid solutions

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Keywords: semiconductors, defects, carrier scattering

Usually the charge carrier scattering models in ZnCdTe, ZnHgSe and ZnHgTe are considered in relaxation time approximation. However, these models have essential shortcoming — they are long-range which contradict special relativity. From the other side in [1, 2] the short-range models of electron scattering were proposed for $Cd_xHg_{1-x}Te$ and $Cd_xHg_{1-x}Se$ in which the above mentioned shortcomings were absent. The purpose of the present work is to use this approach for description of the charge carrier scattering in ZnCdTe, ZnHgSe and ZnHgTe solid solutions.

For the charge carrier scattering on the nonpolar optical and acoustic phonons, neutral defects, disorder and static strain potential the interaction radius of the short-range potential is limited by one unit cell. For the charge carrier scattering on the ionized impurity, polar optical and piezoelectric (piezoacoustic and piezooptic) phonons the interaction radius of the short-range potential is founded in a form $R = \gamma a$ (a — lattice constant, γ — the respective adjusting parameters).

To calculate the conductivity tensor components the method of a precise solution of the stationary Boltzmann equation was used [3]. The temperature dependences of the charge carrier mobility in the range 4.2–370 K in $Zn_xCd_{1-x}Te$ ($0 \leq x \leq 1$), $Zn_xHg_{1-x}Se$ ($0.02 \leq x \leq 1$) and $Zn_xHg_{1-x}Te$ ($x = 0.15$) crystals are calculated. The influence of the different scattering mechanisms on the charge carrier mobility is considered. A good agreement between theory and experiment in all investigated temperature range is established. The scattering parameters γ for different scattering modes are determined.

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Thu-2.15po

Influence of defect structure of γ-$La_{2(1-x)}Nd_{2x}S_3$ crystals on their spectro-luminescent and kinetic properties

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Keywords: intrinsic luminescence of the non-activated

The chalcogenides of rare-earth (RE) elements, Ln2X3 (Ln — RE ion, X — chalcogen ion) crystallize into several structure types, denoted as α, β, γ, etc. [1]. One of these types is defect γ-phase with body-centered cubic lattice of Th3P4-type [2], and composition variable between terminate compounds Ln2X3 and Ln3X4. The crystal chemical formula is written as [3]. Here x varies from 0 to 1/3, V is a vacancy in cation sublattice, e- — conduction electron. If $x = 1/3$, there appears a Ln2X3 phase with terminate composition. In this phase, one third of the cation sites in the unit cell including four formula units are vacant and the resultant compound is an isolator. It was shown in the work [4] that cation vacancies in γ- Ln2X3 are distributed statistically over the crystal volume.

There have been established the following experimental facts.

Under $\lambda = 0.53$ micron excitation of the non-activated at room temperature, there is observed a broad-band emission with maximum at $\lambda = 0.775$ micron. This intrinsic luminescence of the non-activated is practically no longer excited under excitation wavelength $\lambda = 0.6$ micron. The luminescence band experiences a blue-shift upon decreasing temperature.

Under $\lambda = 0.53$ excitation of crystals with small activator concentrations, the onset section of the decay curve of the meta-stable level 4F3/2 appears to be non-exponential. Besides, the slowing down of the decay is observed at later stages of the process. The shape of the neodim 4F3/2 decay curve has not been changing with increasing excitation density. This witnesses that the above-described anomalous behavior of the decay curve has nothing in common with some kind of a cooperative phenomenon. Under excitation with a light wavelength of 0.6 micron, the exponential decay is observed.

The lines in the absorption and luminescence spectra of neodim ion in crystal at helium temperature turned out to be broadened.

Formation mechanism of the activator centers was studied using selective laser excitation. It was found that the shape and position of the luminescence line did not change upon varying excitation wavelength.

The results of the present work will be discussed in terms of the scheme [5] proposed for the trap energy positions in the forbidden gap of.

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Thu-2.16po

Evidence trapping levels and photoelectric properties of Cu_3BiS_3 thin films

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Keywords: defects, Cu_3BiS_3, thin films

Voltage and Cu/Bi ratio mass dependence of photocurrent was studied in Cu_3BiS_3thin films prepared by co-evaporation technique. The intensity dependence of steady state photocurrent (I_{ph}) follows a power law with intensity (F), $I_{ph} \quad \mu \quad F^g$ where the power g is in the range between 0.5 and 1.0, suggesting bimolecular recombination. Photocurrent signal was found to be decaying as a function of both applied voltage and intensity, initially decreasing very fast and later at slower rates, due to the continuos distribution of defect states; differencial life time constants were calculated. Measurements of temperature effect on conductivity (from 100 K to 450 K) were carried out. It was found that at temperatures greater than 350 K, the conductivity is predominantly affected by transport of free carriers in extended states of the conduction band, whereas in the range of temperatures below 250 K, the conductivity is dominated by the VRH (variable range Hopping) transport mechanism. The flow of charge carriers was also found to be limited by grain boundaries potencial barriers.

Thu-2.18po

Bipolaron formation and electron correlations

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Keywords: bipolaron, electron correlations, virial

It is studied the relation between the variational method and the virial theorem with regard to the problem of singlet bipolaron stability, analyze additional restrictions that optimize variational electronic wave functions of the bipolaron problem, and discuss the physical consequences of these restrictions. Studies of the dependence of the Hartree-Fock selfconsistent solution of the bipolaron on the distance R between the centers of gravity of the polarons have shown that the interpolaron potential has a maximum as $R = 0$ and, therefore, a one-center state of bipolaron is unstable. A minimum of the interpolaron potential appears only at intermediate equilibrium distances between the polarons. Therefore, it is important to study the role played by the electron-electron correlations in the stabilization of singlet bipolarons and elucidate whether the electron-electron correlations can indeed change the Hartree-Fock basic solution so strongly that the bipolaron passes from an axially symmetric two-center state to a spherically symmetric one-center state as claimed, for example, in [1].

It is shown, for solutions that take the electron-electron correlations into account, the virial theorem imposes an additional condition on a variational solution. In fact, the variational solution of the bipolaron problem is reduced not to finding the absolute (unconditional) minimum of total energy but rather to determining a conditional minimum of the energy functional in the presence of nonholonomic constraint, which should be taken into account consistently or by using the Lagrange multiplier method. "Floating" wave functions in this work for the account of electronic correlations are entered. It was shown in [2] that the Hellman-Feynman variational theorem for optimum wave function can be strictly satisfied only with such "floating" functions. It is obtained that total energy singlet bipolaron at $R = 0$ is lowered due to the inclusion of electron-electron correlations in the wave function, the bipolaron total energy reaches a maximum for $R = 0$, as is the case in the Hartree–Fock approximation; therefore, a one-center state remains unstable, in agreement with result obtained by Pekar.

When using the direct variational method, the applicability of the virial theorem for a bipolaron at $R = 0$ and the bipolaron stability with regard to electron-electron correlations cannot be ensure simultaneously without contradicting the basic principles of quantum mechanics. In general, minimization of the total energy functional using a direct variational method is inevitably reduced to analyzing the unconditional minimum of the system, which can be devoid of physical meaning. The bipolaron one-center model [2] is also in contradiction with the available experimental data for the optical absorption spectrum of a singlet bipolaron.

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Thu-2.19po

On the possibility of the existence of one-dimensional polaron structure

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Keywords: polarons, one-dimensional, periodical structure

It is studied the possibility of existence of one-dimensional periodical polaron structures in semiconductors. Earlier, it was established [1, 2] that the interpolaron potential for adiabatically and strongly coupled polarons offers attraction properties. Under certain conditions imposed on the dielectric parameters of the medium and the electron-phonon coupling constant, coupled two-particle objects of bipolaron character arise. At the same time, it is known that attraction between the particles may alter the collective properties of a many-particle system. Namely, the initially uniform distribution of the particles becomes unstable and may change to the nonuniform structured state under specific conditions imposed on the temperature of the medium, particle concentration, and parameters of the pair interpolaron potential.

To study the collective properties of an equilibrium polaron structure in one-dimensional filamentary systems, we will use an infinite set of coupled steady-state integro-differential Bogolyubov equations [3]. It is assumed the equilibrium polaron system is stable of the presence of neutralizing positive charges. The author determined the one-dimensional interpolaron pair potential by direct variational method in the framework of the adiabatic translation-invariant theory of bipolaron. The set of Bogolyubov's equations was reduced to the nonlinear integral equation of Hammerstein type. It is known, however, that Hammerstein nonlinear integral equations have many solutions. For certain values of the parameters involved in integral equation there appear bifurcational solutions of qualitatively different character, which are not spatially uniform function. For a given polaron concentration it is defined the critical temperature meets the existence conditions for the bifurcational solutions to initial integral equation, which differ from the spatially uniform distribution and reflect the irregular (spatial) arrangement of the polarons.

The possibility of existence of a periodic one-dimensional structure of small-amplitude polarons that is imposed on the polaron uniform distribution in semiconductors is estimated in terms of temperature and concentration criteria. A dispersion relation between the probability of existence of the one-dimensional polaron periodical structure and the translational velocity of the polarons is determined. As the translational velocity along the z axis increases, the temperature range where the periodic contribution to the polaron distribution exists shrinks and spontaneously disappears when critical velocity is reached. The periodic contribution in polaron distribution disappears virtually stepwise as the velocity approaches its critical values. It shown that this specific polaron-polaron interaction leads to results that are basically different from those observed for Coulomb interactions.

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Thu-2.20po

Long-term room-temperature relaxation of the defects induced in (Hg,Cd)Te by low-energy ions

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Keywords: HgCdTe, ion treatment, defect structure relaxation

It is known that (Hg,Cd)Te solid solutions have a low energy of defect formation due to a very weak Hg-Te bond. As a result, defects in these materials can be easily formed even with a low-energy treatment. The example is ion milling, where the energy of the ions affecting the surface does not exceed 1 keV. In (Hg,Cd)Te such ions easily release interstitial mercury atoms, which quickly propagate into the crystal and interact with its point and extended defects, thus strongly influencing the electrical and optical properties of the material [1].

One of the interesting features of the effect of ion milling on (Hg,Cd)Te is long-term relaxation of the electrical properties of the material after the milling. Carrier concentration gradually decreases at the room temperature for tens of thousands minutes after the treatment, and its total decrease can constitute up to three orders of magnitude. Though this effect was first observed back in 2001 [2], very little attention has been paid to it so far. At the same time, the relaxation data show that disintegration of the defects induced by low-energy ions in (Hg,Cd)Te proceeds in a complicated way, and its mechanisms may strongly differ from those of the formation of the defects [3]. Thus, by studying the relaxation, one can get a deep insight into the defect structure of these materials, which are so important for infra-red optoelectronics.

We report on the results of the extensive study of the relaxation in (Hg,Cd)Te. Low-energy ion treatment was applied to bulk crystals and epitaxial layers grown by liquid-, vapor- and molecular beam epitaxy. Formation and relaxation of defects in the un-doped, vacancy-doped and extrinsically (acceptor- and donor-doped) material has been studied. The relaxation was studied at the room temperature and under isochronous annealing. We consider the mechanisms of the formation and relaxation of defects in ion-milled (Hg,Cd)Te and their implications to the technology of this material.

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Thu-2.21po

Study of alloy disorder in (Hg, Cd)Te with the use of infrared photoluminescence

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Keywords: HgCdTe, alloy disorder, luminescence, red-shift

The intinsic luminescence of many disordered systems, including II-VI solid solutions, is believed to arise from recombination of excitons localized in the potential wells of a profile induced by the disorder. A common feature of such systems is a considerable red-shift of the luminescence with respect to the band-edge as defined from the absorption experiments. Among many II-VI compound semiconductors, this effect has been observed in (Hg, Cd)Te alloy, one of the most important materials for infrared optoelectronics. The components of this alloy have the same crystal structure and very similar lattice parameter, which makes it almost free of lattice-mismatch stresses and good for studying the nature and effects of alloy disorder.

We report on the results of the study of photoluminescence (PL) of (Hg, Cd)Te alloys with CdTe mole fraction varying from $x = 0.32$ to 0.64 (energy gap $E_\mathrm{g} = 0.33\ldots0.85$ eV at 300 K). The samples were grown by molecular beam epitaxy on GaAs substrates with ZnTe/CdTe buffer layers. The PL was studied in the temperature range 4.2–300 K under pulse excitation with InGaAs/GaAs and AlGaAs/GaAsP semiconductor lasers emitting at 0.98 and 0.84 μm, respectively. The PL spectra were recorded with a Ge photodiode and a cooled InSb photodiode. Studied were as-grown (Hg, Cd)Te structures and those annealed in a He atmosphere and saturated Hg vapors.

The main feature of the PL spectra recorded appeared to be a red-shift of the luminescence peak much stronger than that predicted by the commonly used theory of optical transitions related to recombination of excitons localized by single alloy composition fluctuations. To explain the experimental data obtained, we develop an approach, which considers for correlation of single fluctuations as well as for the presence, besides statistical alloy disorder, of macroscopic (technological) composition fluctuations. We also discuss the effect of the annealing on the observed disorder and the influence of the latter on the optical properties of (Hg, Cd)Te and prospective light-emitting structures based on this material.

Thu-2.22po

Evaluation of the crystalline quality of β-Ga_2O_3 films by optical absorption measurements

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Transparent electrode materials such as indium oxide (ITO) and zinc oxide (ZnO) are widely used but have some drawbacks related to toxicity and limited availability. Gallium oxide (β-Ga_2O_3) is a wide band gap semiconductor with a band gap of about 4.9 eV which can be useds both as a transparent electrode and as a gas sensor, due to the fact that the electrical conductivity of β-Ga_2O_3 increases by impurity doping. The aim of this work is to study the use of β-Ga_2O_3 as transparent electrode. In previous work, the impact of growth conditions such as sputtering gas and annealing temperature on the crystalline quality of the films was studied. Optimizing the growth conditions allowed to improve significantly the surface flatness and crystalline quality of the thin films. The resistivity of the films was however still high and of the order of a few kΩcm. The purpose of the research activities reported in the present paper was to decrease the resistivity of the film while keeping a good crystalline quality.

β-Ga_2O_3 thin films were evaporated on quartz substrates using RF magnetron sputtering with a sintered Ga_2O_3 target. After dipping in a 5%-HF solution and cleaning, the substrates were introduced into the sputtering chamber after which β-Ga_2O_3 was deposited. The thin films were sputtered in a mixed atmosphere of Ar and O_2 with the base pressure fixed at 2 Pa. In the present experiments, Ar:O_2 partial pressures of 10:0, 9:1, 8:2, and 6:4, were used.

Next, a Si layer was deposited on the β-Ga_2O_3 film by evaporation of Si for 30 minutes at room temperature. To crystallize the deposited film, a 600°C thermal anneal was performed for 10 minutes. After the growth, the optical characteristics of the thin film were measure.

The absorption coefficient for light with energy around the β-Ga_2O_3 band gap increases with decreasing Ar/O_2 ratio. The increase of the absorption coefficient may be caused by the formation of oxygen related defect levels under the absorption edge of β-Ga_2O_3. In contrast, the band gap is increased with increasing sputtered Si ratios. This result indicates that there is a possibility that a mixed layer of Si, Ga, and O is formed at the top of the deposited β-Ga_2O_3 layer.

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Thu-2.23po

The effect of anti-structure defects on properties of CdTe:Te crystals

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Keywords: CdTe, point defects, electric properties

Point defects determine a majority of electrical and optical properties of crystals. Two-temperature annealing of previously grown cadmium telluride crystals allows an effective handling of the structure of point defects, and it is a one of the ways for obtaining of cadmium telluride crystals with the set properties.

Many studies are devoted to the structure of point defects in cadmium telluride. Despite of this, the question regarding dominant types and parameters (energies of formation and ionization, changes in oscillation frequency of atoms surrounding a defect) of point defects have yet no answer.

Thu-2.24po

XAFS studies of defects in nickel doped lead telluride

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Keywords: lead telluride based semiconductors, XAFS

The problem of impurity and defect states in IV-VI narrow-gap semiconductors is of crucial importance from the point of view of their practical application. As far as lead telluride based semiconductors are concerned, employment of X-ray Absorption Fine Structure (XAFS) technique has already enabled us to address some of these key issues. In this paper we present studies of Ni doped single crystal PbTe by means of XAFS measurements performed at HASYLAB (DESY) on Te and Ni K- and Pb L_{III}-absorption edges on two different temperatures (20 K and RT). Combined analysis of near edge and extended XAFS regions provided information of the exact local environment around each atom and revealed displacement of impurity atoms from the regular lattice positions, their charge state and microstructural ordering as well as overall influence of doping on the host PbTe crystal lattice.

Thu-2.25po

Nanometric semiconducting superlattices containing positron: momentum distributions of emitted annihilation radiation and electron structure

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Keywords: nanostructures, semiconductors, superlattices, positron-electron annihilation, theory

The electron and positron states in the band structure of GaAs–AlAs superlattice have been analyzed on the basis of empirical pseudopotential method of calculations which have been performed for different number of the atomic planes of sublattices containing Al and Ga cations [1]. When possible, the validity of results obtained has been checked by comparing them with positron annihilation spectroscopy data relevant to the constituents of GaAs–AlAs heterostructure.

Depending on both the difference of power of pseudopotentials and the number of monolayers the positron is capable of a selective confining in the defect-free sublattice to be characterized by the comparatively low potential. In spite of appearing in upper zones the confined states of a positron remain both deeply thermalized and elementally specific ones.

This confinement influences the anisotropy of the electron-positron momentum distribution in the crystal lattice of the heterostructure under consideration. In the presence of defects of a vacancy-type the regime of confinement may be changed to the trapping of positron in which case characteristic peculiarities of the momentum distribution of the annihilation radiation are predicted to appear. Being a "fingerprint" of a certain type of defects these peculiarities make it possible the non-destructive characterization of the superlattices by means of the positron annihilation spectroscopy. As an example, the positron-sensitive as-grown defects in the bulk of GaAs (assumedly, EL2 centers) are shortly considered in the light of the calculated data obtained for GaAs-AlAs superlattice. The question of sensitivity of the positron particle microprobe for studying details of the elementally specific electron momentum density distributions in superlattices is discussed.

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Thu-2.26po

An origin of the electromotive force in SmS

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Keywords: electromotive, impurities, Coulumb, donor

The appearance of an electromotive force (EMF) on heating of a semiconductor material in the temperature range about 400–500 K without external tempetature gradients applied was discovered and studied in [1]. The experiments were performed on the both volume monocrystals of samarium sulfide (SmS) and polycrystals as well as on the thin films samples [2, 5]. The phenomenon of emergence of a voltage caused by gradients of impurities has been recently called as the thermovoltaic effect (TVE) [1, 2, 3].

We should to remark that on some samples the attainable emf voltage can be as high as 1 v. It would be naturally to relate the voltage on a sample obtained to the semiconductor-metal Mott-type phase transition. But in contrast to this obvious analogy, the strong difference is that the transition mentioned above actually takes place only in the system of defected ions of Sm. The concentration of the Sm ions is not uniform over the semiconductor, the collective effect does not occur simultaneously everythere in the sample. The qualitative reason of the appearance of emf is due to accumulation of the critical concentration of free electrons which results in screening of the Coulumb potential of imputity ions being responsible for donor levels in the band gap of SmS. Moreover it has been also proved that the emf phenomenon takes place at the point where both the Bohr's and Debye's radii equals to each other [2, 4].

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Thu-2.27po

Point defects in the low-temperature phase of strontium titanate

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Keywords: defect, semiconductor, ChemShell, QM/MM, DFT

Strontium titanate (SrTiO3) is a wide band gap semiconducting perovskite [1] with applications that include catalysis and as a substrate for growing thin films [2, 3]. The material is also antiferroelectric [1] with defects that are electrically conductive [1] making it interesting from an electronics perspective.

The material is known to exist in at least two phases. As the temperature decreases bellow 105 K, it undergoes a second order phase transition to change from a cubic to tetragonal structure [1, 4]. There is speculation and some experimental evidence to suggest that it also has an orthorhombic phase [4] at very low temperatures as other perovskites are known to have this property.

Computational studies have been conducted, focusing on defects and dopants, using the hybrid QM/MM embedded cluster technique within ChemShell [5] and making use of the GAMESS-UK and GULP codes. The calculations are based on the orthorhombic structure of strontium titanate as predicted from QM studies and are supported by the development of new MM pair potentials.

We will present results of investigations into atomic structure, energetics and electronic properties including defect energy levels within the band gap of bulk strontium titanate. With this technique, we predict the defect levels using the full Born-Haber thermodynamic cycle, which will be used to gain insight into the relative stability of defect states and their optical and electric spectroscopic features. The calculations focus on oxygen vacancies and electron defects (polarons) as well as impurities such as yttrium, iron, nitrogen and hydrogen. We will further discuss effects of temperature and pressure on the defect properties of this material.

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Thu-2.28po

Deep level defects in proton irradiated p-type $Al_{0.5}Ga_{0.5}As$

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Keywords: proton irradiation, AlGaAs, deep levels, DLTS

Ion implantation is an essential process for producing the modern III-V semiconductor devices and has been proved to be a successful method of converting a conductive layer into the highly resistive one. In particular it has been shown that proton irradiation can be used to create the insulating sheet in GaAs and related AlGaAs compounds due to carrier trapping at defects introduced by the irradiation [1, 2, 3]. Thus, the understanding of the electrical properties of these defects is of great importance for achieving better device performance. The influence of proton bombardment has been extensively studied in n-type material but the data on the p-type material is rather poor [2–4]. In the present work, the electrical properties of defects introduced in MBE p-type $Al_{0.5}Ga_{0.5}As$ during the proton bombardment were investigated. The irradiation experiments were performed at room temperature with 300 keV protons of fluence on the order of 10^{11} cm^2. Electrical properties of the generated traps were determined by means of deep level transient spectroscopy (DLTS). The DLTS signatures of the radiation-induced defects are compared with the previously reported [5] defects in non-irradiated p- type $Al_{0.5}Ga_{0.5}As$. DLTS revealed five hole traps. Two of the traps located at 0.12 eV and 0.59 eV above valence badn edge were also detected for the non-irradiated samples. Thus it may be assumed that proton irradiation generates hole traps of thermal activation energy equal to 0.25 eV, 0.32 eV and 0.40 eV.

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Thu-2.29po

Structural properties and photoluminescence of the $ZnGa_2Se_4$ compound

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Keywords: photoluminescent, radiation, compound, rare-earth metals

Here are presented results of structural and photoluminescent researches of the $ZnGa_2Se_4$ and $ZnGa_2S_4$:Eu compounds. The synthesized samples $ZnGa_2Se_4$ and $ZnGa_2S_4$ + 3% Eu have undergone to the radiographic analysis. X-ray researches were on X-ray diffractometer type DRON-3M, at a mode 30 eV, 20 mA, 05<20<70 CuK_2 radiation. X-ray diffractions from both structures have been received. The analysis hkl indexes from 19 reflections has shown, that the most probable group of symmetry is $D^2_{2d} - P\overline{4}2C$ with or $P\overline{4}2M$. It is known, that investigated samples crystallize in tetragonal structure with the periods of a lattice $a = 5.497$ Å, $c = 10.993$ Å.

Unlike binary compounds in threefold compounds $A^2B^3_2C^4_6$ in view of presence of two grades of atoms in cation sublattice besides cation and anionic vacancies formation of the antistructural defects focused on interchanging cations are possible. These factors lead to presence of a rich spectrum of local conditions and variety of features of nonequilibrium processes. It is obviously vivid that, finding-out the localization of atom of activators Eu in a lattice is necessary. As is known, for rare-earth metals (REM) formation of coordination from six up to nine atoms chalcogenides in a aspects of octahedrons, trigonal and tetragonal prisms is characteristic. In other way vacant tetraedrikal positions in this case are not comprehensible to localization of atoms Eu. However, in a lattice of structures of type chalcopyrite is available octahedral and other type of futility. It is possible to assume, that activators (Eu) in the given lattice can freely be localized in octahedral or other kind of polyhedral formed free anion. In this case, the crystal structure of compounds of type $A^2B^3_2C^4_6$ is expedient for comparing with structural analogues of type $CuFeS_2$. In the interval of temperatures 77–230 K spectrum PL as, pure, and activated is investigated by europium $ZnGa_2Se_4$. In spectrum PL $ZnGa_2Se_4$ the maximum is found out at 591 nm, and in spectrum $ZnGa_2Se_4$: Eu below 100 K. Maximums were found out at 566, 591 and 646 nm. Analysis of obtained data shows that maxima at 566 nm in PL spectrum of $ZnGa_2Se_4$: Eu is caused by transition $4f^65d \rightarrow 4f^7 (^8S_{7/2})$ of Eu^{2+} ion, but maxima at 591 nm and 646 nm are related to donor-acceptor pairs.

The analysis of temperature dependences for half width at maximum PL in $ZnGa_2Se_4$ and $ZnGa_2Se_4$:Eu^{2+} shows that introduction of europium ions in compound $ZnGa_2Se_4$ reduces their structural defects.

Thu-2.30po

Atomic structure of threading dislocations in AlN thin films

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Keywords: dislocation, AlN, HRTEM, STEM

Group III nitrides have attracted much attention because of their potential applications for novel, high performance electronic and optoelectronic devices. It is well known that the group III nitride films grown on sapphire (α-Al_2O_3) substrates contain a high density of threading dislocations due to the peculiar growth mode, which is called mosaic growth [1, 2]. The dislocation in AlN films is supposed to lead electronic states in the gap, depending on the core structure [3]. Therefore, in order to know how the dislocations affect on the optical or electrical properties, it is important to study the atomic structure of the dislocation core. In this study, we investigated the core structure of threading dislocations in AlN films by high resolution Z-contrast imaging in scanning transmission electron microscope (STEM).

AlN films were grown on (0001) sapphire by MOVPE (DOWA Electronics Materials Co., Ltd.). Plan-view specimens for TEM observations were prepared by conventional methods including mechanical polishing and argon-ion-beam thinning processes. Conventional TEM observation was carried out using JEM-2010HC microscope (JEOL Co., Ltd.), and STEM observation was carried out using JEM- 2100F microscope (JEOL Co., Ltd.) equipped with an aberration corrector (CEOS Co.).

Based on the diffraction pattern obtained from the interface between AlN film and sapphire substrate, the orientation relationship for the interface was confirmed to be (0001)AlN//(0001)sapphire and [-1100]AlN//[11–20] sapphire. As a result of conventional TEM observations, the density of the threading dislocations was estimated to be about 4×10^{10} cm^{-2}. It was found that the threading dislocations formed in the films were mainly the perfect edge dislocations with the Burgers vector of **b**=1/3<11–20>. Z-contrast images of the edge dislocations showed the eight-fold ring structure in projection. If we assume that the unintentional dopant density is $\sim 10^{16}$ cm^{-3}, with the dislocation density as high as $\sim 4 \times 10^{10}$ cm^{-2}, the dislocations are thought to be charge-neutral. Then, the eight-fold ring structure without aluminum vacancy nor nitrogen vacancy is the most stable structure as predicted by Wright *et al.* This result indicates that the edge dislocation is expected to be electrically inactive.

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Thu-2.31po

On the stretched-exponential decay kinetics of the ionized DX centers in gallium doped $Cd_{1-x}Mn_xTe$

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Keywords: photoconductivity decay, DX centers, stretched-exponential relaxation

In semiconducting compounds possessing metastable defects, DX centers, persistent photoconductivity (PPC) effect is observed. At low temperatures a barrier for capture prevents recapture of electrons by photoionized centers and conductivity relaxes to its dark value for a long time after termination of illumination. The photoconductivity decay transients are non-exponential. Usually, they are fitted by means of the Kohlrausch-Williams-Watts (KWW) function $\Phi_{\mathrm{KWW}}(t) = \exp(-t/\tau)^{\alpha}$, where $0 < \alpha < 1$ is the stretching exponent and τ is a characteristic time constant of the transient. Performing the measurements of the photoconductivity decay kinetics at different temperatures the decay time constant as a function of temperature may be obtained and the capture barrier can be determined. Such approach allows to calculate solely the macroscopic parameter — the capture barrier. Within this model not only are the microscopic properties of the relaxing defects neglected but also the physical significance of the stretching exponent a is not explained. This deterministic interpretation is based on the assumption that properties of the whole investigated physical system can be represented by a single randomly chosen microscopic relaxation contribution (here — the DX center). However in the case of a complex system stochastic approach seems to be more relevant. The stochastic approach allows one to construct an “averaged” object representing the entire system. The statistical properties of individual relaxing entities (DX centers) determine the properties of the average representative of the system and the measured effective response of the studied material. In particular the stochastic analysis may bring information concerning correlations among the relaxing entities and their relaxation rates distribution. Moreover, the stochastic model clarifies the signification of the stretching exponent.

In present paper persistent photoconductivity decays due to gallium-related DX centers in $Cd_{0.99}Mn_{0.01}Te$ mixed crystals have been studied within the temperature range of 77 K–100 K. It was observed that the decay of PPC follows the stretched-exponential relaxation pattern and exhibits the short-time power-law. Based on these observations the electron capture barrier equal to 0.23 eV was determined. In order to investigate the statistical properties of metastable defects in $Cd_{1-x}Mn_xTe$:Ga the probabilistic approach to the time-domain relaxation processes has been applied.

It has been shown that the observed stretched-exponential relaxation response is a consequence of a heavy-tailed distribution of the DX centers relaxation times and has its origin in the local randomness of the relaxing defects. In particular, this model was for the first time implemented to discuss the photoionization kinetics of Ga related DX centers at different temperatures. It was found that the characteristic decay exponent α increases with increasing temperature in the range of 0.80–0.98. The physical interpretation of the temperature dependence of α and its relation to the defects relaxation times distribution was proposed.

Thu-2.32po

Relaxation spectrum of the $TlSbSe_2$ thin films

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Keywords:

Dielectric constant and the dielectric loss of $TlSbSe_2$ thin films, obtained via thermal evaporation of $TlSbSe_2$ crystals grown by Stockber–Bridgman technique, have been measured using ohmic Al electrodes in the frequency range 0.2–100 KHz and within the temperature interval 293–353 K. Dielectric constant is found to decrease with increasing frequency and increase with increasing temperature. The activation energy values were evaluated and there is a good agreement between the activation energy values obtained from capacitance and dielectric loss factor measurements. The variation of the relaxation time with frequency has also been determined.

Thu-2.33po

Dielectric polarization in anodic Al_2O_3 thin films

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We investigated the frequency and temperature dependence of the ac conductivity and dielectric constant of anodized Al_2O_3 thin films in the frequency range 0.1–100 kHz and 100–400 K temperature range. The ac conductivity $s(w)$ is found to be proportional to w^s where $s < 1$. The temperature dependence of both ac conductivity the parameter s is reasonably well interpreted by the correlated barrier (CBH) model.

Thu-2.35po

Qantum-limit anisotropic magnetoresistance of semiconducting n-Bi-Sb alloys

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Keywords: Bi-Sb, magnetoresistivity, quantum oscillations, quantum limit, anisotropy

The magnetic-field dependence of resistivities and Hall coefficients of single crystals $Bi_{0.93}Sb_{0.07}$ alloys were investigated at low temperatures. For $H||C_3$ and $j||C_1$ orientation the cyclotron frequencies of all three ellipsoids are equal and the electron concentration raises with the magnetic field in quantum limit. For $H||C_2$ and $j||C_1$ the quantum oscillations of resistivity were observed connected with the electrons of two ellipsoids, at higher fields the transition to the quantum limit takes place. The magnetic field increase in the quantum limit leads to the increase of electron energy from secondary ellipsoids and to their migration to the main ellipsoid. For $H||C_1||j$ orientation the quantum oscillations of resistivity were connected with all three ellipsoids. The electron energy for main ellipsoid raises in quantum limit with magnetic field, leading to the migration of carriers from main ellipsoid to the secondary ellipsoids. This work was supported by grant “Leading scientific schools” N 2184.2008.2.

Thu-2.36po

Diverse grain boundary behaviors in polycrystalline photovoltaic materials

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Keywords: photovoltaic materials, grain boundaries, DFT, passivation

Si, CdTe, and $CuInSe_2$ are currently the most promising polycrystalline photovoltaic materials. Structurally, these materials are very similar — they all have diamond-like structural feature. However, our density-functional theory total energy calculations reveal that a similar grain boundary behaves very differently in these materials. For example, the double-positioning boundaries undergo a reconstruction to eliminate dangling bonds in Si, but no such reconstruction is seen in CdTe and $CuInSe_2$. The boundaries exhibit large expansion in the boundary region in $CuInSe_2$, but such large expansion is not found in Si and CdTe. We also find that these structural differences lead to diverse electronic properties: the grain boundaries create deep levels in Si and CdTe but not in $CuInSe_2$. The passivation effects are also found to be different for the grain boundaries in Si and CdTe. The grain boundaries can be passivated completely by H in Si but not in CdTe. The high defect density in the Te-core boundary in CdTe can only be passivated through copassivation of Cu and Cl. Our study suggests that the different ionicity for these compounds are likely to be the main cause for these diverse grain boundary behaviors in these polycrystalline photovoltaic materials.

Thu-2.37po

Electron structure of extended defects in polar semiconductor nanosystems

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Keywords: nanosystems, silver chlorine, edge dislocations, charged defects

This work is a short review of our publications which are devoted to theoretical investigations of electron structure of the silver chlorine nanosystems with edge dislocations, and charged defects [1–7]. In addition the new results are presented for charged surface defects. Adsorption of silver ion was considered as on the atomically-rough surface (near the step and step fracture) as on the smooth surface. The electron structure of AgCl nanocrystals with the adsorbed silver ion were calculated by semi-empirical tight-binding method relying on a self-consistent approach for the effective charges and dipole moments of the ions and in frame of DFT method B3LYP/HW. The quantum transitions were investigated in semi-empirical approach. Visualization of the wave functions was performed for the localized states. Basing on the obtained data a conclusion is specifically made that one can expect an enhancement of photoelectron localization with a decrease of the anions number in the substrate nearest to the adsorbed ion. It means that the most efficient trapping of photoelectron should occur under adsorption on a smooth surface rather than near the steps and their fractures as it was assumed previously. Also probabilities of quantum transitions for different variants of adsorption were been discussed.

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Thu-3.1po

Electronic structure of diluted magnetic semiconductors $Pb_{1-x-y}Sn_xCr_yTe$

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Keywords: magnetic impurities, IV-VI semiconductors, deep impurity level, electronic structure

Doping with chromium induces an appearance of deep impurity states in the electronic structure of PbTe-based alloys. Magnetic properties of these materials are strongly dependent on the charge state of the chromium ions in the host crystal lattice, determined by the mutual arrangement of the deep impurity level, band edges and Fermi level. In particular, $Pb_{1-x}Sn_xTe$ ($x \leq 0.2$) alloys were Curie paramagnets due to the presence of magnetically active Cr^{3+} ions, whereas SnTe with Cr^{2+} ions demonstrated the weak Van Vleck paramagnetism only. One can suppose that in the first case partially filled impurity level situates in the conduction band, whereas in the second it lies in the valence band deep under the Fermi level and completely filled with electrons. In order to obtain the diagram of electronic structure for the chromium-doped $Pb_{1-x}Sn_xTe$ in the present work the galvanomagnetic effects ($T = 4.2-300$ K, $B \leq 0.08$ T) in $Pb_{1-x-y}Sn_xCr_yTe$ alloys under variation of the alloy composition were investigated. Single crystal $Pb_{1-x-y}Sn_xCr_yTe$ ingots with nominal concentrations $x = 0.08, 0.15$ and $y = 0.01$ were grown by the Bridgman technique. Chemical composition was determined on the basis of results of the X-ray fluorescence analysis, taking into account exponential distribution of Sn and Cr along the axis of the ingot. In two investigated ingots tin and chromium content gradually increase from the beginning to the end of the ingot, covering the composition ranges $x = 0.06-0.12$, $y = 0.002-0.033$ and $x = 0.12-0.22$, $y = 0.002-0.035$ accordingly.

It was found that in all samples temperature dependencies of resistivity $\rho(T)$ and Hall coefficient $R_H(T)$ demonstrated a metal-like behavior. Samples with low impurity concentration ($y < 0.003$) had the p-type conductivity. An increase of the impurity content lead to the sharp increase of the Hall coefficient at helium temperature, corresponded to the decrease in the free hole concentration, and p-n-conversion of conductivity type. The free electron concentration rises, tends to saturation and then ($y > 0.01$) slowly decreases with increasing chromium content. The absolute value of R_H in the latter samples increases more than two times with increasing temperature and passes through the maximum near the room temperature. Such behavior was observed previously in PbTe, doped with In and Cr, and are typical for IV-VI semiconductors with resonant impurity level, stabilizing the Fermi level in the conduction band.

Obtained experimental results were used to determine the position of the chromium resonant level relative to the bottom of conduction band and to construct the diagram of electronic structure reconstruction in the investigated alloys. Using the values of R_H at $T = 4.2$ K, the concentration of free electrons in the samples with stabilizing Fermi level were determined. Then in terms of the Kane dispersion law dependencies of Fermi level, stabilized by the resonant chromium level, on the tin concentration in the alloys were calculated. It was shown that in PbTe, in accordance with the previously known data, chromium impurity level lies about 100 meV higher the bottom of the conduction band. With increasing of the tin content it moves linearly down to the conduction band bottom with the rate approximately −2.5 meV/mol.%. Thus, in $\mathrm{Pb}_{1-x}\mathrm{Sn}_x\mathrm{Te}$ alloys with inverse band structure ($x > 0.35$) chromium impurity level should consecutively intersects the edges of the gap and enter the valence band.

Thu-3.2po

Properties of ZnO thin films doped with ferromagnetic impurities

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Keywords: zinc and cobalt oxides, ferromagnetic resonance, multilayer thin films

Wide-band-gap semiconductor ZnO doped with 3*d* transition metals is one of the promising materials which due to magnetic, optical and mechanical properties will have far-reaching impact on the emerging field of spintronics.

In this work, we present the results on magnetic and photoluminescence properties of Zn–Co–O “sandwich” thin film structures synthesized on glass or silicon substrates.

The sol-gel technique with using various solutions was applied to deposit by layer-by-layer method the transparent Zn–Co–O “sandwich” thin film structures. The average thickness of the sandwich films was 80–100 nm. X-ray diffraction analysis indicates a polycrystalline structure of the Zn–Co–O thin films.

Isotropic ferromagnetic resonance (FMR) absorption lines were observed by microwave absorption measurements on the Zn–Co–O multilayer films carried out at X- and Q-bands. The ferromagnetic behavior of Zn–Co–O films can be caused either substitution by Co atoms in the ZnO or due to clustering of Co atoms in secondary phases that are ferromagnetic. The resonance field is close to that expected for Co microparticles. An intensity of the FMR absorption depends on conditions of sol-gel process and subsequent treatment.

Furthermore, the Zn–Co–O “sandwich” structures show more intensive ultra-violet PL peak in comparison with PL spectrum of the ZnO films. It can take place due to increase in concentration of oxygen vacancies, formation of shallow donors and growth of concentration of free charge carriers. Good correlation between magnetic properties and PL is revealed.

Thu-3.3po

Characterization of II-VI:3d crystals with the help of ultrasonic technique

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Keywords: impurity, semiconductor, ultrasound, characterization

Ultrasonic investigation of a number of II-VI crystals doped with $3d$ ions have revealed a peak of attenuation at low temperatures (see [1] and references therein). This anomaly proved to be due to relaxation in the Jahn-Teller system. Attenuation $\alpha(T)$ is proportional to the concentration of the dopand n, therefore, ultrasonic technique can be used for non-destructive measuring of the impurity concentration. We may introduce a parameter characterizing the sensitivity of the method $\alpha_n = [(\alpha)_{\max} - \alpha_0]/n$, i.e., peak attenuation per the impurity ion obtained at fixed frequency (α_0 is $\alpha(T)$ extrapolated to $T = 0$). The following values of α_n were determined at $\approx$ 54 MHz with the use of shear ultrasonic waves propagated along the $\langle 110 \rangle$ axis: 1.9×10^{-18} dB·cm^2 (ZnSe:V^{2+}), 1.6×10^{-18} dB·cm^2 (ZnTe:Ni^{2+}), 0.06×10^{-18} dB·cm^2 (ZnSe:Ni^{2+}), and 0.008×10^{-18} dB·cm^2 (ZnSe:Fe^{2+}). Anomalously large value $\alpha_n = 23 \times 10^{-18}$ dB·cm^2 was found in ZnSe:Cr^{2+} that corresponds to the peak attenuation of about 90 dB/cm at $n = 3.8 \times 10^{18}$ cm^{-3}. Our set-up makes it possible to measure variation of $\alpha(T)$ with the accuracy of 0.02 dB. It means that this technique can be used for measuring of the concentration of the Cr^{2+} ions in ZnSe as low as 10^{16} cm^{-3}. The data on $\alpha(T)$ were used for reconstruction of relaxation time $\tau(T)$ with the help of the method described in [1]. Simulation made it possible to discuss the mechanisms of relaxation and to determine a number of the parameters of the Jahn-Teller cluster. This work was done within RAS Program (project No. 01.2.006 13395).

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Thu-3.4po

The impurities of iron and cobalt in mercury selenide: localization effects of hybridized electronic states in the temperature dependences of thermoelectric power

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Keywords: thermoelectric power, magnetic impurities, resonance scattering, hybridization

The features of electronic structure and spin polarization of transition element impurity atoms in semiconductors have an essential effect on the thermoelectric power coefficient value. The study of this parameter in mercury selenide crystals is of special interest, as far as in these systems the hybridization effects of impurity electron states of iron atoms and other transition elements are manifested [1]. The resonance scattering and partial localization of conducting electrons, due to the hybridization, lead to the anomalies of the conductivity and are also reflected in thermoelectric power. We have studied the temperature and concentration dependences of thermoelectric power coefficient in mercury selenide with iron and cobalt impurities in the temperature range from 2 to 200 K. One revealed and studied the impurity anomalies of the temperature dependences, due to hybridization of electronic states in conduction band and the interaction of electrons with localized magnetic moments. In crystals with iron impurities a peak and anomalously sharp drop of thermoelectric power was observed at the iron concentrations close to those, which conform to the concentration maximum of electron mobility below 25 K. These effects are explained by the manifestation of resonance scattering of electrons in hybridized states by donor iron impurities [2]. In crystal with cobalt impurities at low temperatures the anomalies, due to hybridization of electron states, are weaker exhibited and at the cobalt concentration above 1 at. % there is a rapid linear growth of exchange thermoelectric power with increasing the temperature. Above 50 K the temperature dependences of thermoelectric power for both crystals are similar and include the contribution of exchange interaction. We have quantitatively interpreted the observed special behaviors and obtained the data, characterizing hybridized states.

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Thu-3.5po

Magnetic impurity behavior in the type II broken-gap p-GaInAsSb/p-InAs:Mn heterostructures with 2D-semimetal channel at the interface

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Keywords: manganese, impurity, InAs, heterostructure, magnetotransport

We report study of Mn impurity behavior in type II broke-gap single heterostructures with 2D-semimetal channel at the interface grown by LPE. Low-field ($B < 1$ T) Hall resistance and magnetoresistance have been investigated in the bulk p-InAs:Mn substrate with concentration of $p = 7 \times 10^{18}$ cm^{-3} and the p-GaInAsSb/p-InAs:Mn heterostructures obtained on the same substrates. In p-InAs manganese can form a shallow acceptor level with the activation energy $E_\mathrm{A} = (0.028 - aN^{1/3})$ eV, where $a = 1.31 \times 10^{-8}$ eV·cm. Overlap of electron shells of closely located Mn atoms occurs at the hole concentration $p = 4 \times 10^{18}{-}1 \times 10^{19}$ cm^{-3} and the impurity levels reach the valence band. Anomalous Hall effect (AHE) and negative magnetoresistance (NMR) were observed in the heterostructures with 2D-electron channel at the interface at higher temperatures (77–300 K) in contrast to the case of the bulk InAs highly doped with Mn where such effects were found at lower temperatures (4.2–50 K) [1]. AHE was observed in a ferromagnetics and its value is proportional to magnetization of the sample. That is determined by additional s-d exchange between Mn^{3+}(d^4) ions in InAs substrate and coupling with s-electrons in the 2D-channel at the interface. High value of effective magnetic moment M described by Curie law was found from NMR study, $M = 200\mu_\mathrm{B}$, where μ_B is Bohr magneton, that is in 3 order of magnitude higher than for the bulk InAs with the same Mn doping (7×10^{18} cm^{-3}). High value of Curie temperature $T_\mathrm{C} = 200$ K was evaluated from the experimental dependence $R_\mathrm{AHE} \times \chi$ on temperature in the range 77–200 K, where χ is magnetic susceptibility. Relative NMR ($\Delta\rho_\wedge/\rho_0$) in the heterostructure under study as high as 30% was found at $T = 77{-}200$ K and its dependence on magnetic field was quadratic according to theoretical calculation for the classical NMR [2]. In addition, a role of Mn δ-doping of the GaInAsSb layer in quantum magnetotransport has been studied at high magnetic fields ($B > 8$ T) and low temperatures (1.5–4.2 K). The presence of 0.5 nm δ-layer of Mn deposited on the 0.5 μm thick p-GaInAsSb epilayer results in the spin-oriented tunneling of electrons across the p-InAs/p-GaInAsSb heteroboundary and appearance of steps in current–voltage characteristics due to increasing contribution of s-d interaction of 2D-electrons from the channel with spins of Mn ions [3]. Spin state of Mn near the interface owing to band bending exhibits spin configuration of 3d^5(Mn^{2+}) unlike to 3d^5+hole for the bulk p-InAs substrate. It leads to indirect double interaction between the magnetic ions with different charge states.

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Thu-3.6po

Ab initio study of Cr, Mn and Fe in germanium

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Keywords: Mn in Ge

We study chromium, manganese and iron impurities in germanium, using a density functional-pseudopotential method. Large $Ge_{148}H_{99}$ clusters simulate the bulk germanium, which avoids the gap problem presented in the supercell approach. We found that the substitutional site is more stable than the tetrahedral and hexagonal interstitial sites for Cr, Mn and Fe transition metal impurities.

Thu-3.7po

Optical and magneto-optical properties of thin $Zn_{1-x}Mn_xO$ films doped by nitrogen

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Keywords: ZnMnO, diluted magnetic semiconductor, MCD

Oxide-diluted magnetic semiconductors (O-DMS) have attracted a great deal of interest in recent years due to the possibility of inducing room temperature ferromagnetism. These materials are of particular interest for spintronic devices such as spin valves. ZnO is a wide-band-gap of 3.37 eV semiconductors and has recently received particular attention because of its promising applications for blue light emitting devices and as a candidate for the fabrication of diluted magnetic semiconductors (DMS) with a Curie temperature above room temperature. The possibility to create spin-optoelectronics devices based on $Zn_{1-x}Mn_xO$ films has stimulated interest in studding the effect of optical and magnetic properties these structures. In this work we report the results of the investigation photoluminescence, optical absorption and MCD measurements of the $Zn_{1-x}Mn_xO$ thin films in the temperature range 77–300 K. The nitrogen doped ZnO films were deposited on quartz substrates by ultrasonic spray pyrolysis method at ambient atmosphere. Aqueous solutions of zinc acetate -0.5 mol/l, manganese acetate -0.5 mol/l, and ammonium acetate -2.5 mol/l were used as sources of Zn, Mn, and N, respectively. The atomic ratio of Zn/N was 1:3 in the precursor solution. The substrate temperature was set at 300–500°C and the thickness of $Zn_{1-x}Mn_xO$ films was about 200 nm and 300 nm. The optical absorption spectra were measured by using a xenon lamp as an excitation source and the MCD spectra have been measured in Faraday configuration using a photoelastic modulator for thin films $Zn_{1-x}Mn_xO$ with $x = 0$, 0.01 and 0.05 and in addition alloyed by nitrogen. Measurements were carried out at temperatures 78 and 293 K near the absorption edge in an interval 3.27–3.55 eV. The exciton lines are dominant in the PL and absorption spectra of these samples, which indicate a high crystal quality of the films. A significant MCD signal near the band edge of $Zn_{0.99}Mn_{0.01}O$ at room temperature has been observed. The analysis shows that this MCD signal is due to the Zeeman splitting of the A and B excitons, which is enhanced by the sp-d exchange interaction in the Mn-doped ZnO.

Thu-3.8po

Vanadium-induced deep impurity level in $Pb_{1-x}Sn_xTe$

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Keywords: magnetic impurities, galvanomagnetic effects, deep level, persistent photoconductivity

Recently a new diluted magnetic semiconductors – lead telluride-based alloys, doped with vanadium, were revealed. In these materials vanadium acts as a donor. In PbTe it induces appearance of a deep impurity level, stabilizing the Fermi level under the bottom of conduction band ($\Delta E_V = E_c - E_V \approx 20$ meV). In $Pb_{1-x}Mn_xTe$ ($x \approx 0.05$) alloys an activation energy of vanadium level ΔE_V slightly exceeds 100 meV and there is no distinct dependence of its value on the alloy composition. In order to obtain the dependence of vanadium level position on the alloy composition and to study the photoconductivity induced by infrared (IR) illumination at low temperatures in the present work the galvanomagnetic properties ($T = 4.2-300$ K, $B \leq 0.08$ T) of $Pb_{1-x}Sn_xTe$ alloys, doped with vanadium, both in the chamber shielded from the background illumination and under the continuous IR illumination from the heat source were studied.

The monocrystalline $Pb_{1-x-y}Sn_xV_yTe$ was grown using the Bridgman method. The chemical composition was determined using the X-ray fluorescence analysis, taking into account an exponential distribution of tin and vanadium along the ingot, typical of the IV–VI semiconductors. In two investigated sets of the samples concentrations of components monotonously rise along the ingots: $x = 0.06-0.13$, $y = 0.002-0.045$ and $x = 0.13-0.26$, $y = 0.003-0.065$ accordingly.

In the heavily doped samples of the first group there are three distinct activation intervals on the temperature dependencies of resistivity ρ and Hall coefficient R_{H}: intrinsic conduction, impurity conduction and hopping conduction via impurity states at low temperatures. In the vicinity of transition to hopping conduction the Hall coefficient and magnetoresistivity coefficient pass through the maximum, indicating the sharp decrease of electron mobility at low temperatures. At helium temperatures an effect of persistent photoconductivity was observed. In the alloy with maximal tin content the resistivity falls more than an order of magnitude under the IR illumination. The alloys possess a high photosensitivity to IR excitation at temperatures up to $T_{\mathrm{c}} \approx 40$ K. From the slope of the activation range on the $\rho(1/T)$ dependencies we have determined an activation energy of the vanadium level ΔE_{V}, that decreases almost linearly from 48 to 12 meV with the decrease of the tin content. However, further decrease of the tin content leads to the n–p-conversion of the conductivity type. All samples of second group are p-type and demonstrate metallic behavior of $\rho(T)$ and $R_{\mathrm{H}}(T)$ dependencies. Upon an increase of the tin content Fermi level, determined from R_{H} values at $T = 4.2$ K in the frame of the Kane dispersion relation, passes through the maximum at $x \approx 0.2$ and then decreases, moving down linearly relative to the valence band top.

Obtained experimental results were discussed assuming the pinning of the Fermi level by the vanadium deep level in the heavily doped alloys. It was shown that as the tin content increases vanadium impurity level E_{V} falls almost linearly relative to the bottom of the conduction band, intersects valence band top at $x \approx 0.2$ and enters the valence band. The n-p-conversion of the conductivity type in the lightly doped alloys may be a result of interplay between concentration of vanadium impurity ions (donor centers) and concentration of the native intrinsic defects (metal vacancies), responsible for the p-type conductivity. High IR photosensitivity at temperatures below critical value T_{c} may be attributed to the Jahn-Teller instability of the impurity centers in the alloys.

Thu-4.1po

Electronic structure of a perylene tetracarboxylic acid dianhydride film upon surface doping by a conjugated organic overlayer

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Keywords: surface electronic phenomena, conjugated organic molecules, organic film, organic film interface

Surface doping of a conjugated organic film surface by another organic molecular material can be used to achieve optimal parameters of organic electronics devices, such as, rectifiers, photovoltaic cells and organic light emitting diodes. The electronic structure at the Pyronine B interface with the PTCDA surface is particularly interesting because Pyronine B was suggested as an organic dopant serving for improvement of electron transport properties of PTCDA layers [1].

Ultrathin conjugated layers of Pyronine B were thermally deposited in UHV on the surface of perylene tetracarboxylic acid dianhydride (PTCDA) film. The structure of unoccupied electron states located 5–20 eV above the Fermi level (EF) and the surface potential were monitored during the Pyronine B overlayer deposition, using an incident beam of low-energy electrons according to the total current electron spectroscopy (TCS) method [2]. Electronic work function of the PTCDA surface changed from 4.9 ± 0.1 eV, during the Pyronine B deposition due to the change of the contents of the surface layer, until it reached a stable value 4.6 ± 0.1 eV at the Pyronine B film thickness 8–10 nm. The interface dipole corresponds to electron transfer from the Pyronine B overlayer to the PTCDA surface and the polarization in the Pyronine B overlayer was found confined within approximately 1 nm near the interfaces. The edges of major bands of density of unoccupied electronic states (DOUS) of PTCDA substrate and of the Pyronine B overlayer were unaffected by the process of the interface formation. The major TCS spectral features of the Pyronine B film corresponding to the DOUS band edges were identified and the assignment of the p*, s*(C-C) and s*(C=C) character was suggested.

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Thu-5.1po

Electron microscopy of novel transrotational microstructure formed after amorphous-crystalline transformations in thin films

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Keywords: electron microscopy, novel transrotational microstructure, amorphous-crystalline transformations

Novel structures with unexpected, dislocation independent, regular internal bending of the crystal lattice planes formed after phase transformations in amorphous films are characterized on the scale micro–nano. Such "single crystals" with perfect though curved lattice (built up by simultaneous translation and small regular rotation of the unit cell) demonstrate the new "transrotational" [1] type of atom order for solid state. Thin (10–100 nm) crystallized areas with transrotation vary from fine crystals (0.01–100 microns), ribbons, whiskers or spherulites to large-scaled polycrystalline areas with a complex texture. They can be grown with the help of heat treatment or local annealing (by focused electron or laser beam) in free-standing amorphous films (different chalcogenide-based films, e.g. Se, Se–Te, Sb–Te, Sb_2Se_3, Sb_2S_3, $Ge–Sb_2Se_3$, Ge–Te, Tl–Se, Cd–Te, Cu–Te/Se, also some oxides, alloys). The films are prepared by thermal/laser/e-beam evaporation, solid state amorphization, pyrolysis and studied primarily by means of transmission electron microscopy TEM (bend-contour technique [2], high resolution HR TEM). *In situ* TEM studies (supported by video) and atomic force microscopy are also presented.

Two main factors are important for transrotation: initial amorphous state and thin film/layer. Transrotation can be revealed for a growth of dislocation-free single crystal (Se, $Cu_{2-x}Te$, CuSe). Transrotation is realized preferably around axes lying in the film plane with the maximal values observed $\sim 360°$ for crystal length 2–3 mm. It corresponds to 2–4% of elastic deformations accomplished in the surface layers (large but possible values for thin perfect crystals).

The geometry and the magnitude of transrotation depend upon the substance, film preparation and crystallization conditions, orientation of the crystal nucleus, the presence of the sublayers and the film thickness. Maximum-containing function of transrotation against the growth rate V_g (in the range 10^{-2}–10^3 micron/s) is studied. It disappears for low V_g ($V_g < 0.01$ micron/s for Se). V_g may be constant or may vary rhythmically depending on crystal anisotropy. Dynamic changes of diffraction contrast for large V_g (revealed by analysis of TEM video) fit our earlier proposed mechanism for transrotation formation based on the surface nucleation. Reversible local transformations "amorphous-transrotational crystalline" is studied for Se–Te.

Microstructure with transrotation can be considered as an intermediate between amorphous and crystalline (similarly to structure of liquid crystals intermediate between crystalline and liquid). Transrotation was recently observed in PCM (phase-change materials) [3] and we suppose it is one of the reasons of easy switching in chalcogenide-based memory.

The new transrotational model of amorphous state is also proposed.

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Thu-5.2po

Spatial distribution of crystalline phases in Sm-doped ZrO_2

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Keywords: zirconia, phase stabilization, micro-Raman, confocal microscopy

Investigation of zirconia is highly interesting because of its high potential in practical applications like dielectric layer in semiconductor industry or as a surface coating due to it's high mechanical strength. Doping with lanthanides is widely used for stabilizing zirconia in tetragonal and cubic phases and improving it's ionic conductivity [1]. Additionally doped zirconia has many other applications like light emitting devices, laser cavities and gas sensors [2]. Different type and shape of zirconia samples can be prepared by using increasing number of preparation methods ranging from high quality crystalline solid state reactions to various amorphous sol-gel methods. The diversity of the methods means that the morphology and phase structure of such zirconia is often unknown or characterized only by averaged characterisation method like x-ray scattering which does not reveal the microscopic structure of the material.

The aim of current paper is to address the issue by describing a optical characterization method for mapping the spatial phase distribution of zirconia on microscopic scale by using micro-Raman scattering of zirconia and photoluminescence of the dopant ion.

The bulk zirconia samples doped with different concentrations of samarium are prepared by directional solidification of melt technique (a skull melting technique). Applied technique allows to obtain the melt at very high temperature to keep it in a stable state and crystallize it under controlled conditions. During the RF heating prepared samples reached up to 3000°C.

Characterization of the phase structure of the samples was performed on a Renishaw micro-Raman microscope in Raman scattering and in photoluminescence gathering mode.

By lateral confocal scanning of the samples a microscopic segregation of tetragonal and monoclinig phases of zirconia is revealed both via Raman scattering of the zirconia and photoluminescence spectra of the samarium ions [3, 4]. The phase stabilization is shown to be related to samarium ion concentration leading to the formation of tetragonal phase at higher dopant levels compared to the monoclinic.

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Thu-5.3po

NMR study of isolated nitrogen impurity in rutile TiO_2

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Keywords: shallow acceptor, beta-NMR, photocatalysis, TiO_2

Nitrogen impurities are expected to be one of the key dopants in TiO_2 to facilitate its use as a visible light responsive photocatalyst, since the photocatalitic activity in nitrogen-doped TiO_2 has been shown under visible light irradiation [1, 2]. Substitutional nitrogen doping for oxygen in TiO_2 is thought to cause the band-gap narrowing, and to shift the optical response from ultraviolet to visible light range [2]. So far, there have not been sufficient experimental studies of the electronic structure of the nitrogen doped TiO_2. In this situation, techniques of nuclear magnetic resonance using radioactive probes (beta-NMR) are quite useful, which achieve extremely high sensitivity to the NMR so that microscopic properties of an isolated impurity atom are studied through the hyperfine interactions of an impurity nucleus with surrounding electrons.

In the previous report [3], the beta-NMR study of radioisotope ^{12}N in rutile TiO_2 suggested the formation of shallow acceptor levels. NMR spectra indicate that small internal magnetic fields emerge at low temperatures other than the diamagnetic center peak. This is due to the existence of an unpaired electron localized at the nitrogen site and the Bohr radius of the electron is estimated to be much larger than that for vacuum hydrogen. We have continued further studies such as dependence on the crystalline orientation relative to the exernal field for deterimnation of anisotropic hyperfine structure and/or precise temperature depencende of the NMR spectra for ionization energy of acceptor levels. Our preliminary result suggests large anisotropy in the hyperfine constant expected from anisotropic dielectric constant. We will introduce the beta-NMR technique and present the recent progress in this conference.

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Thu-5.4po

In-situ analysis of optical properties of dislocations in ZnO by opto-TEM

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Keywords: dislocations, ZnO, opto-TEM

Dislocations are of considerable importance in semiconductor electronics, since they are frequently introduced during crystal growth and device fabrication, and they affect the electronic properties of semiconductor devices. Recently, ZnO is expected for UV light-emitting devices and is supposed that dislocations are more easily introduced than GaN and SiC. However, the nature of the electronic properties of dislocations in ZnO has not been fully elucidated. In this paper, optical measurements in a transmission electron microscope (opto-TEM) and photoluminescence (PL) spectroscopy have revealed the optical properties of the dislocations induced freshly in ZnO by plastic deformation at elevated temperatures, which are comparable to the ZnO-based device fabrication temperatures.

Wurtzite ZnO bulk single-crystals were compressively deformed at elevated temperatures 923–1123 K to introduce an arbitrary number (typically 10^9–10^{10} cm^{-2}) of fresh dislocations with the Burgers vector of $a/3\ \langle 1120\rangle$. Deformed specimens showed excitonic PL light emission with photon energies of 3.100 and 3.345 eV, as well as their LO phonon replicas at 11 K, and the light intensities increased with increasing dislocation density [1]. The activation energy for a thermal quenching of the 3.100 or 3.345 eV emission band, which corresponds to the depth of the localized energy level associated with the emission band, was estimated to be 0.3 or 0.05 eV, respectively [2]. The origin of the energy levels was proposed as point defect complexes involving mixed dislocations. The introduction of the dislocations at the elevated temperatures above 923 K did not influence the intensities of the emission bands except the dislocation-related emission bands.

TEM under light illumination and CL spectroscopy combined with light illumination revealed that screw dislocations, presumably acting as non-radiative recombination center, glide under the illumination of a light with photon energy above 2.4–2.5 eV, at temperature of 110 K [3]. The glide would take place due to an electron-hole recombination at a defect level of 0.9–1.0 eV depth, since the threshold energy was lower than the band gap energy (about 3.4 eV at 110 K). When the screw dislocations glided, the intensity of the green and yellow emission, which is associated with vacancies, increased. Since the introduction of vacancies by the irradiation of 80-keV electrons for TEM could be negligible, the recombination activity around the screw dislocations would be modified by the dislocation glide. It was explained that, the screw dislocations convert into mixed dislocations acting as radiative recombination center, or that acting as non-radiative recombination center with low recombination activity in comparison with the screw dislocations.

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Thu-5.5po

Pulsed and CW electron paramagnetic resonance of boron in isotopically purified ^{28}Si silicon at ultra low temperature

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Keywords: silicon, shallow acceptors, electron paramagnetic resonance

Pulsed electron paramagnetic resonance (pEPR) is a powerful technique allowing direct measurements of spin relaxation times of donor-bound electrons and acceptor-bound holes in semiconductors. A number of spin relaxation studies using pEPR have been reported for a wide variety of paramagnetic impurities in silicon. However, measuring spin relaxation times for shallow acceptors is known to be specially challenging. The main difficulty arises from the fact that boron has a fourfold degenerate ground state. This degeneracy is easily lifted by any symmetry breaking perturbations, such as random local strains or isotopic disorder, resulting in too broad an EPR linewidth to be detectable. Moreover, pEPR experiments are complicated by extremely short spin relaxation times due to strong spin-orbit interactions [1]. Consequently, all known relaxation studies up to date have been performed by applying a large external stress which removes the fourfold degeneracy and compensates for small inhomogeneous random strain, thus producing a narrower linewidth and longer relaxation times [2].

We have overcome those difficulties, by investigating an isotopically highly purified ^{28}Si sample with a low defect concentration using an ultra low temperature (0.35 K) pEPR system. In particular, we have succeeded in direct measurements of relaxation times of shallow acceptor-bounded holes in *unstressed* silicon. At 0.35 K, longitudinal relaxation times (T_1) are in the range 5–50 microseconds, and transverse relaxation times (T_2) are 0.5–3 microseconds depending on which transition in the spin 3/2 four level system is measured. The echo-detected field sweep spectra, measured using pEPR, show substantially broader linewidths compared to the CW-EPR spectra, suggesting that only a selected population of boron spins with long relaxation times is detected in pEPR spectra, and yet there is still a substantial population of fast relaxing spins which is not detected. We propose a model based on a statistical distribution of internal strains which explains this observation qualitatively.

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Thu-5.7po

Electrically detected magnetic resonance of phosphorous due to spin dependent recombination with triplet centers in irradiated silicon

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Keywords: EDMR, phosphorous, SL1 centers, silicon

Electrically detected magnetic resonance (EDMR) of phosphorous in Silicon has been attributed to the spin dependent recombination between neutral donor and paramagnetic states at the Si/SiO$_2$ interface [1]. Here, we report the effect of additional recombination centre created in the bulk by γ irradiation on the EDMR signal. All the measurements have been made under band gap illumination at weak magnetic field below 50 mT.

One of the most abundant defects produced in Si by γ irradiation is A-center. Under illumination with light these neutral A-center is excited to triplet state know as SL1 center [2, 3]. The EDMR signal of phosphorous in irradiated Silicon shows significant enhancement when compared with the signals from samples without γ irradiation.

This enhancement can be explained due to the spin dependent recombination between neutral phosphorous and the excess paramagnetic centers (SL1) created in the silicon. We also observed EDMR signals of SL1 center at (a)27.45 G (b)149.62 G, (c)280.34 G, (d)349.73 G and (e)417.66 G when the radio frequency used was 200 MHz. Signals at 27.45 G and at 349.73 G always appeared at the same position irrespective of the radio frequency used and could be attributed to the level crossing point of the triplet centers. We also observed that EDMR lines at 149.62 G and 417.66 G, move towards the higher magnetic field with the increasing radio-wave frequency while the signal at 280.34 G shifted towards low magnetic field with increasing radio-wave frequency.

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Thu-5.8po

EBIC investigations of defect distribution in ELOG GaN films

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Keywords: GaN, ELOG, EBIC, donor concentration

Epitaxial lateral overgrowth (ELOG) technique is one of approaches allowing a dislocation density reduction. In this method a GaN template is grown by standard metallorganic chemical vapor deposition (MOCVD). Then a mask of SiO_2 stripes is prepared by photolithography and finally a thick GaN layer is grown by MOCVD over the masked surface. The material above the mask grows predominantly in the lateral direction and has the dislocation density from two to three orders of magnitude lower than that in the material grown in the windows of SiO_2 mask, for which the dislocation density is the same as for standard MOCVD layers. A density of extended and point defects is very different in these two regions therefore the lateral inhomogeneity in their electrical properties is expected. These regions have width in the mm range, therefore some special microscopic techniques should be used for characterization of such structures. The similar problems could also arise in other fields.

An application of scanning electron microscopy in Electron Beam Induced Current (EBIC) modes for characterization of such structures are discussed. The examples, demonstrating possibilities of this method are presented. It is shown that in the ELOG films studied the EBIC allows not only to reconstruct the diffusion length distribution, i.e. the distribution of recombination centers but also the donor distribution. The accuracy of such estimations was checked by a comparison of EBIC results obtained on homogeneous GaN films with those obtained on the same films by the C-V method.

About three times difference between the donor concentrations in the laterally grown and window regions are revealed on the ELOG films. This difference conserved for the films with different average donor concentration that allows to propose the possible explanation of this effect. Investigations of neutron irradiated films showed that this method allows also to reveal and to study inhomogeneous radiation defect accumulation.

Thu-5.9po

STM and RHEED investigations of the $c(8 \times n)$ defect structure on Si(001)

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Keywords: silicon surface, defect structure, high-order reconstruction, STM, RHEED

Reduction of the process temperature is an important restriction imposed on the prospective epitaxial Ge/Si technology of the Si-based electronics by the requirement of CMOS compatibility. Deoxidization of the Si(001) surface for further growth of the Ge/Si heterostructure is one of the key high temperature treatments and its temperature is desirable to be lowered. In the UHV MBE chambers, this process is usually carried out at the temperature lower than 950°C in conditions significantly different from those of the clean Si surface preparation for studies in specially refined laboratory vessels. The differences are conditioned by the sizes of Si wafers used in the industry, method and temperature cycle of wafer annealing, possible presence of contaminants from different sources including materials of wafer heaters or evaporators of elements as well as foreign substances used for epitaxy and doping, etc. The results of studies of the Si(001) pure surface prepared by short annealing at the temperature of $\sim$ 925°C in the Riber EVA32 MBE chamber [1] are reported in this presentation. The investigations were carried out by two techniques — by means of

RHEED directly in the UHV MBE chamber during sample annealing and at room temperature immediately after sample cooling by UHV STM coupled with the MBE chamber through a UHV transfer line. The dependence of the Si(001) surface structure on the annealing duration and the sample cooling rate was investigated. It was found by means of RHEED that (2 × 1) and (4 × 4) structures arose on the Si(001) surface. The $c(8 \times n)$ reconstruction [1] was revealed by means of STM. A fraction of the surface area covered by the $c(8 \times n)$ defect structure was decreased as the rate of sample cooling was reduced. The (2 × 1) structure was observed on the surface free of the $c(8 \times n)$ one. The $c(8 \times n)$ structure revealed by STM was evidenced to be manifested as the (4 × 4) one in the RHEED patterns. The investigation of the reconstruction type dependence on the sample temperature carried out by RHEED showed the (4 × 4) reconstruction to arise at $\sim$ 600°C in the process of sample cooling down. The reconstruction was observed to be reversible. The (4 × 4) structure turned into the (2 × 1) one at the temperature of $\sim$ 600°C in the process of the repeated sample heating, the (4 × 4) structure appeared on the surface again at the same temperature at recurring cooling. A model of the $c(8 \times n)$ defect structure built on the basis of the STM data is presented in the repot. Origins of formation of the high-order structure on the Si(001) surface are discussed.

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Thu-5.10po

Local cathodoluminescence study of defects in semiconductors and multilayer structures

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Keywords: local cathodoluminescence, multilayer structures, epi-layers

Local cathodoluminescence (CL) is a very effective method for studying the defects in semiconductors, epi-layers and multilayer structures. As a photoluminescent method cathodoluminescence is very sensible to point defects, admixtures and structural modifications in semiconductors and insulators. But this method gives a lot of new possibilities comparing with photoluminescence.

One of the most important possibilities of the cathodoluminescent method is that of depth examination of the emission properties of semiconductors structures. Changing electron energy from 0.5 to 30 keV one varies electron beam penetration from 10 nm up to several microns. This permits one to study the luminescent properties in depth. This method has been used for the luminescent properties investigation of both multilayer structures and non homogenous epi-layers. Using this method we studied the distribution of In in $In_xGa_{(1-x)}N$ epi-layers, and Al in SiC epi-layers, as well as in $A^{II}B^{V}$, $A^{II}B^{VI}$ and SiO_2/Si multilayer heterostructures. This method allows characterizing charge carriers transport properties in the multilayer structures. The rate of emission associated with quantum dots or quantum well layers in the structures with high charge carriers transport properties induces, as a rule, an intensive luminescence related to this layer but weakly depends on the electron beam energy. This is why the ratio of CL intensity of bands associated with quantum well layer to that of bottom or top layers could characterize the charge carriers transport of such a multilayer structure. We use this method for the study of the laser heterostructures (ZnMgSSe-CdSe) and a structure for HEMT transistors based on GaAs–$Al_xGa_{(1-x)}As$–$In_xGa_{(1-x)}As$.

The next very important capability of the cathodoluminescent method is its ability to study electron trapping defect levels. The long-lasting increase of the cathodoluminescence intensity, for seconds and minutes, as a result of the electron irradiation gives information about the presence and the activation energy of the electron traps occurrence. The prolonged decrease of the cathodoluminescent intensity is a result of defect levels in a band-gap. The temperature dependences of the decay times of the CL intensity permit one to evaluate the energy of the defect levels. This method is very helpful for the study of the structures based on $A^{II}B^{VI}$ characterised by high defect content, SiO_2/Si system, $In_xGa_{(1-x)}N$–GaN, laser and light emitting structures based on $A^{III}B^{V}$.

Moreover high energy and power density of the electron beam lead to the excitation of high energy levels. One's attempt to excite these levels by an optical (photoluminescence) method should need vacuum ultraviolet radiation. This advantage is very useful for the study of high gap semiconductors ($Al_xGa_{(1-x)}N$–AlN) and dielectric materials. We have, for example, a good experience exploring SiO_2 point defects in a SiO_2/Si system. Excitation of several defects is produced by an energy much that 5 eV. On the other hand, such excitation leads to emission from the higher exited energy levels (the emission with 2.0–2.3 eV for GaAs, 2.8 eV for Ge and etc.). These emission bands provide information about the electron structure of semiconductors.

Thu-6.1po

Muonium as a probe of electron spin polarisation in CdTe

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Keywords: muonium, spin polarisation, shalow donor,magnetic impurities

Muonium, consisting of a positive muon and an electron, is a pseudo-isotope of hydrogen. Muonium formation involves a capture of an excess electron generated at the end of the track during muon implantation. Muon spin rotation (muSR) experiments with CdTe commercial single crystals, nominally undoped, were performed at Paul Scherrer Institut, in Switzerland, at 20 mK and under an external magnetic field up to 2 T, perpendicularly to the muon spin initial polarization. A weakly bound muonium state is formed in CdTe with a very small hyperfine interaction (260 KHz) [1, 2]. The frequency spectra show two symmetrically placed muonium satellite lines, on either side of a central diamagnetic line. The satellite lines correspond to different electron spin states (up and down), which have different energies in the presence of a magnetic field. The normalised intensity difference of muonium lines is therefore a measure of the polarisation of the electrons captured by the muon at the end of the implantation process. Measurements at 20 mK and at fields ranging from 0.1 T to 2 T indicate an electron polarisation increasing from zero up to 40%. Later similar measurements of the same sample demonstrate a clear inversion of the sign of the electron polarisation: the higher frequency line was the more intense one in the original measurements, but now the intensity of the lower frequency line becomes larger. The field dependence of the electron polarisation is also changed. The experiment demonstrates the muon can be used as a local probe for electron spin polarisation in the material and to study the electron polarisation mechanism.

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Thu-6.2po

Evidence for a shallow muonium acceptor state in Ge-rich Cz-$Si_{1-x}Ge_x$ alloys

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Keywords: muonium, hydrogen, silicon germanium alloys, shallow acceptor

We have observed a Muon Spin Rotation (μSR) signal that is consistent with a shallow Muonium acceptor state for several Ge-rich Silicon Germanium alloy compositions. Comparison of prior results in SiGe alloys indicate the Mu_T[0/-] defect level crosses into the valance band at a Ge content of roughly 92%, indicating that a shallow acceptor state should be formed for muons that stop in the acceptor related T-site. Low-temperature transverse-field (TF)-μSR measurements in $Si_{0.16}Ge_{0.84}$ indicate delayed formation of a paramagnetic state with a very small hyperfine constant typical of the anticipated shallow acceptor, most likely arising from a neutral precursor having a much larger hyperfine interaction. A similar feature was considerably weaker (if actually present) in the time-dependent spin precession measurements on $Si_{0.09}Ge_{0.91}$. However, for this sample, the difference between the diamagnetic amplitudes from RF-driven resonance measurements compared to TF-μSR, which requires spin-precession phase coherence, indicates a slowly formed state at temperatures below 50 K, consistent with a valence-band resonant Mu^- that would form the core of a shallow Mu acceptor. Efforts to understand the dynamics of Mu^- formation and the specific origins of the shallow acceptor states are obfuscated by the presence of two distinct neutral Mu_T hyperfine signals with slightly different temperature dependences, and the existence of shallow states outside of the alloy range where a band-resonant Mu^- is anticipated. An accurate determination of the deep (localized, impurity-like) Mu_T[0/-] acceptor level requires the separation of competing ionization processes and Mu^0 site changes, both of which are observed in temperature dependent Mu dynamics. We report a summary of hyperfine characterization and ionization energies of the various Muonium states found in these Ge-rich alloys and discuss options for the conditions under which shallow acceptor states may be formed.

Thu-6.3po

Muonium in 4H Silicon Carbide

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Keywords: silicon carbide, hydrogen, negative-U

Muon Spin Research has become a major technique to research isolated hydrogen behavior in semiconducting media. We have been investigating muonium transitions in several poly-types of SiC in an attempt to characterize hydrogen behavior in this wide band gap semiconductor. Previously we have claimed the existence of two diamagnetic centers, Mu^+ and Mu^-, created from their promptly formed long lived neutral precursors. These ionic centers undergo complicated dynamics in all of the electrical types of 4H-SiC as evidenced primarily by the diamagnetic amplitude steps as a function of temperature. One important feature is that in all types of the samples the diamagnetic (Mu^+ or Mu^-) amplitudes have shown a steep increase around 900 K, indicating the onset of site change, charge transfer, or booth. Further transverse field muon spin rotation experiments have shown that the signal growing above 900 K saturates at higher temperatures for p-type sample and inclined to saturate for the other types. This behavior suggests that the centers associated with these signals might be the appropriate ground states for the respected types of the SiC samples. This observation is in agreement with the theoretical prediction that in a negative-U defect system the neutral centers never dominate under equilibrium conditions. In an analysis where only single component was assumed to fit the data for high resistivity and n-type samples required also an increase in the signal's relaxation rates, suggesting strongly a site change in addition to ionization. For the p-type sample where a similar amplitude increase is observed, there is no increase on the associated relaxation rates. Estimated energy values from the amplitude steps appear to correlate with acceptor and donor ionization in at least one of samples. In this contribution we present these new data and discuss muonium charge and site transitions in 4H-SiC observed to date in our experiments for a wide temperature range, 10–1400 K. We will further present the sites assigned for the observed muonium centers and discuss the similarities and disparities of the observed muonium species and their assigned sites in 4H samples with those observed in 6H structure.

Thu-6.4po

Theoretical calculations of positron states and annihilation parameters in group-III nitride semiconductors

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Keywords: group-III nitride semiconductors, defects, positron annihilation, theoretical calculation, Doppler-broadening spectra

Positron annihilation is a powerful technique to investigate vacancy-type defects in solids. By measuring Doppler-broadening spectra for annihilation radiations, we can obtain one-dimensional projections of electron momentum distributions sampled by positrons. The spectrum shape is specific for the defect type. In a practical application of positron annihilation, such as the detection of process-induced defects in semiconductors, there might be several candidates as a predominant defect. But one can identify defect species using the results obtained by the theoretical calculations.

In this study, we made theoretical calculations of positron states and annihilation parameters for possible defects in group-III nitride semiconductors, which are thought to be promising materials for a broad range of applications. All the calculations have been performed with our in-house computational code QMAS (Quantum Materials Simulator) [1] based on the projector augmented-wave (PAW) method [2], which is suitable for the present purpose [3]. Calculated Doppler-broadening spectra have compared with experimental results directly or via S and W parameters, which are the weights of the center and wing parts of the spectrum, respectively. For the S-W map, systematic variations were confirmed by increasing the number of vacancies and/or by attaching impurity atoms. Successful examples [4–8] as well as new results will be presented.

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Thu-6.5po

Hyperfine spectroscopy and characterization of muonium in $ZnGeP_2$

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Keywords: muonium, hydrogen, diffusion, ionization energy

The chalcopyrite structured II–IV–V_2 compounds are well developed and optimized for their primary application as infrared active non-linear optical materials. Several members of this class of compounds have shown room-temperature ferromagnetism when doped with Mn. We have recently initiated a study of the defect states formed when positive muons are implanted into this class of compounds, mostly to extend our investigations of muonium defect centers as an experimentally accessible analog of isolated hydrogen impurities in semiconductors. An additional interest is to understand the probe dynamics associated with using positive muons to characterize the atomic-scale magnetism in Mn-doped II-IV-V_2 compounds. In this contribution, we report the initial observation of a neutral muonium defect center in $ZnGeP_2$. We have obtained the hyperfine spectroscopy from muon spin rotation (MuSR) results using a high frequency spectrometer operating in the M15 beamline at TRIUMF, Vancouver, Canada. The spin precession frequencies in a field of 4.0 Tesla applied perpendicular to the initial muon spin polarization direction yield a zero-temperature hyperfine constant of $\sim$ 1966 MHz for the observed Mu^0 state, approximately 44% of the value for a free Mu atom. The relaxation rates associated with the hyperfine spectral lines suggest rapid diffusion of this Mu^0 center, most likely via quantum tunneling below 100 K and by thermally activated hops above that temperature. A rapid increase in relaxation rate above 200 K implies a transition out of the observed Mu^0 state, presumably due to thermal ionization. In an attempt to further define the motion related dynamics, we subsequently performed T_1^{-1} depolarization measurements in low magnetic fields applied parallel to the initial polarization using the EMU spectrometer at the STFC ISIS Facility in the UK. Both of these measurements yield an ionization energy of roughly 200 meV. We present our preliminary evaluation of the motion or site transition dynamics as extracted from the longitudinal depolarization measurements in addition to reporting on the spectroscopic hyperfine characterization of the neutral muonium center observed in $ZnGeP_2$.

Thu-7.1po

MOS-structures with plasma deposited layered dielectrics Si(5 nm)/SiO$_2$(15 nm) and their properties

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Keywords: silicon, superlattice, nanocrystals, optic crystals

Silicon based superlattices attract scientists due to combination of well known good properties of Si/SiO$_2$ interface and possibility for realization of quantum properties at room temperatures due to large difference in forbidden zone values. This paper is devoted to structures with several nanometers thicknesses for Si and SiO$_2$ layers obtained within plasma-chemical technology.

Ways were elaborated for deposition of silicon dioxide films using hexamethyldisilozan and hexamethyldisiloxan, as well as amorphous silicon films from mixture of monosilane and argon. Analysis of capacitance characteristics reveals good electronic properties of the interface, so quite low fixed charge was detected (about 4×10^9 cm^{-2}) and interface density of states (from 5×10^{11} cm^{-2} eV^{-1} in the middle of forbidden zone up to 5×10^{12} cm^{-2} eV^{-1} near the edge of one). Achieved growth rates for deposition was allowed to deposit Si, SiO$_2$ films with thickness above 20 nm. Mode for manufacturing of SiO$_2$ films with thickness above 2 nm was found owing to oxidation of amorphous and crystalline silicon in plasma of pure oxygen. Multilayered structures were manufactured with interlaced layers of amorphous silicon and its oxide with correspondent thickness 5.15 nm. Ellipsometry data confirm homogeneity of the films within 1–3% both on thickness and optical constants on whole substrate with diameter 150 mm. Oxidation technique was realized both for crystalline and amorphous silicon. To crystallize embedded a-Si layers thermal treatment at 1100°C during 30 min was applied. Thermal treatment leaded to modification of Raman spectra according to phase transformation. Spectra for substrate, as grown and annealed superlattices are shown in comparison. After annealing the increasing of Raman signal was discovered both at 520 cm^{-1} and at 480 cm^{-1} possibly due to resonant effect. Increasing of the intensity near 520 cm^{-1} interpreted as transformation of amorphous silicon into crystalline form. As for as grown superlattice (Si-5nm/SiO$_2$-15nm)x6, as for thermal treated sample significant photoluminescence signal was detected. Difference is observed in shifting PL peak into infrared region after the thermal annealing. Electrical measurements reveal significant peculiarities connected with charge transport through prepared superlattices. Frequency dependence is significant compared with usual MOS-structure. At positive voltages and low frequency sharp increasing of capacitance was detected in correlation with conductivity behavior. Possibly this effect is connected with alternative current originating from charge exchanging between substrate and silicon dioxide layer. The exchanging may be the sequence of recharging of small silicon clusters or crystallites formed in dielectric layer.

Thu-7.2po

Dislocation defect influence on the current flow mechanism in contacts metal–wide bandgap semiconductors

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Keywords: dislocation defect, alloyed ohmic contact, current flow mechanisms, wide bandgap semiconductors

The creation of ohmic contacts to wide bandgap semiconductors are the actual problem because of the density of surface states in these materials is not high, and the position of the Fermi level on the surface may vary widely, dependent on the electron work function of the contacting metal. So the ohmic contact of these semiconductors must be formed if the electron work function of the metal is less than the electron affinity of the semiconductor (it's difficult to realise). We present a method for ohmic contact fabrication, which use dislocation defects for the ohmic current flow.

The current flow mechanisms in alloyed contacts to low-doped wide bandgap semiconductors (GaP, GaN, AlN, 4H-SiC) has been investigated. The temperature dependence of the specific contact resistance has been studied over the interval 77–450 K.

It was determined that the current flow mechanism depends on density of dislocations or other defects in semiconductors. At high dislocation density (for instance, $\sim 10^8$ cm^{-2} for In–GaN structures) the new mechanism of current flow is exhibit. This is not characteristic of Schottky diode: the current flow across metallic shunts shorting out the space-change layer. The shunts appear in a result on deposition in In atoms on the dislocations or other imperfections. In this case, the specific contact resistance decreases with the temperature.

Thu-7.3po

Structural distortions induced during stress relaxation affecting electrical transport of the nanometer thick $La_{0.67}(Ba,Ca)_{0.33}MnO_3$ films

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Keywords: interface, heterostructure, mechanical stress, distortion of stoichiometry

X-ray diffraction (XRD) and Medium Energy Ion Scattering (MEIS) were used to clarify distortions induced during mechanical stress relaxation of nanometer thick epitaxial $La_{0.67}Ba_{0.33}MnO_3$ (LBMO) and $La_{0.67}Ca_{0.33}MnO_3$ (LCMO) films fabricated by pulsed laser deposition. XRD and MEIS indicate that LBMO grew heavily strained but coherently on an almost lattice matched LSATO substrate. LBMO film deposited on mismatched $LaAlO_3$ was partly relaxed in the main part of the film, leaving an about 4 nm un-relaxed and distorted portion close to the interface. Due to better matching in lattice parameters, critical thickness of the LCMO films grown on $LaAlO_3$ substrate was several (5–7) times larger than that of the LBMO. Because of the distortion of stoichiometry, biaxial mechanical stresses and phase separation, electro- and magnetotransport parameters of the nanometer thick manganite films grown on mismatched substrates differed markedly from those of the LBMO and LCMO layers nucleated and grown on well matched ones. The charge transport of strained LCMO films was non-ohmic at low ($T < 130$ K) temperatures. A magnetic field linearized the current-voltage characteristics. The resistivity r of manganite films grown coherently at the substrate with small mismatch obeyed $r = r_1 + r_2(H)T^{4.5}$ at temperatures well below Curie point, where parameter r_1 was temperature T and magnetic field H independent while r_2 was temperature independent but decreased linearly with increasing H. The absolute value of r_2 of the partly relaxed LBMO film was roughly one order of magnitude higher as compared with that of a coherent film. A likely reason of the observed difference in the $r_2$coefficients of the non-relaxed and partly relaxed $La_{0.67}Ba_{0.33}MnO_3$ films is a larger excitation of the electron spin system in the latter because of an inhomogeneous distortion of the Mn–O distances and Mn–O–Mn angles during stress relaxation in manganite films.

Thu-7.4po

Interfacial electron doping

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Keywords: interface, doping, mobility, magnetic, transparent

Chemical impurity doping and gate voltages are the two main methods used to introduce carriers in semiconductors. However, doping increases crystalline disorder and decreases carrier mobility, and typical gate voltages are capable of providing only relatively small carrier densities. We therefore explore chemical potential driven carrier transfer at high electron surface densities into an insulator through an interface, while preserving order in the underlying conduction channel [1,2]. We demonstrate this method by transforming a widely used insulator model system, $SrTiO_3$, into a transparent conductor, using low energy Ion Beam Preferential Etching (IBPE).We report low temperature electron mobility up to 3000 $cm^2/(Vs)$. We also show a strong, for nonmagnetic metals, magnetoresistance and plateau-like Hall magneto-dependence, possibly caused by electron cyclotron effects in a strongly correlated quasi-2D Fermi gas. This phenomenon provides a strategy for device fabrication without disorder in the conduction channel.

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Thu-7.5po

Silicon nanopowder incrusted in dielectric layer of MOS structures for memory applications

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Keywords: silicon, nanopowder, nanoballs, memory

Separate nanoballs attract science attention due to unique properties of silicon with size about several nanometers. A both electrical and optical property is important, as well as promises for device application. For incrustation of nanoballs into silicon dioxide layers with thickness about several nanometers a method was chosen to prepare a suspension using silicon organic materials (hexametyldisilozan and hexametyldisiloxan). Preliminary the task for preparation of very thin oxide layers was solved owing oxidation of silicon surface in pure oxygen plasma. Series of nanopowder were manufactured using beam of relativistic electrons for evaporation of pure FZ-silicon in a result of silicon coagulation in gas flow of argon. 1.6 MeV electron beam accelerator was used for evaporation. Size selection was as in stage of manufacturing by means of filtering, as in stage of preparation of a suspension for nanopowder. The suspension was prepared due to placement of nanopowder into hexamethyldisiloxan representing liquid precursor for plasma-chemical formation of silicon dioxide films. The suspension was bring onto preoxidized silicon wafers using standard microelectronic method and then was oxidized in plasma of pure oxygen. Sublayer, separating nanoballs from substrate, have a characteristic thickness about 5nm. Time of oxidation was varied within the range (45 c, 120 c, 420 c). Ellipsometry data demonstrated that hexametyldisiloxan layer was fully oxidized during approximately 90c. Depending on time strong difference in electrical properties both for MOS- and MOS:NC-structures was revealed.

Electrophysical properties for manufactured MOS- and MOS:NC-structures were investigated. There was discovered frequency dependent increasing of both differential capacity and conductivity in depletion, inversion regimes, what was explained as exchange of charge between substrate and nanoballs. Calculations of single-electron IV were made taking into account diode characteristic for substrate and presence of parallel conductivity chains in dielectric layer. Instability of impedance observed for MOS:NC-structures at voltage above 7 V been explained as possible variation of nanoballs electronic spectrum due to influence of multi-electron effects. Increasing of frequency leads to approaching of characteristics to standard form for MOS-structures, what corresponds to retarding of charge exchange with substrate due to shortening period of voltage applied. Capacitance dependence well correlates with conductivity. Similar behavior was discovered earlier for 5 nm nanocrystals inside of thermal oxide. In that case results look more appropriate for industry applications, especially for memory cells and single electronics. Static volt-ampere characteristics were also analyzed as well as results for other samples. Thus, method was realized for creation of MOS:NC-structures with nanoballs in dielectric layer and researching of its electronic properties was provided.

Thu-7.6po

Structural and electronic properties of carbon-doped c-BN(110) surface

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Keywords: BN crystal, density functional theory, formation energies

Structural and electronic properties of substitutional C atom in neutral charge state on both the B and N site of c-BN(110) surface have been investigated from a theoretical point of view, through density functional theory calculations. The impurity formation energies [unrelaxed (E_f^0) and relaxed (E_f)] are reported for the first time for c-BN(110) surface.

Thu-7.7po

Strain relaxation mechanism in the Si-SiO$_2$ system and its influence on the interface properties

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Keywords: EPR, Si-SiO$_2$, strain

It is well known that internal mechanical stresses (IMS) due to the differences in the thermal expansion coefficient between films and substrates and lattices mismatch appear in the Si-SiO$_2$ system and that point defects (PD) generation and redistribution reduce partially the surface strain. However, no investigation of this process on the atomic scale has been carried out so far. The purpose of the present work is to investigate the stress relaxation mechanism in the Si-SiO$_2$ system by means of EPR, scanning electron microscopy (SEM) and samples bending measurements. PD density and stresses in the SiO$_2$-Si system were varied by oxidation condition (temperature, time, cooling rate, ambient) and by Si$_3$N$_4$ deposition on SiO$_2$. Different sign of the thermal expansion coefficient of the SiO$_2$ and Si$_3$N$_4$ on Si allow to modifay the IMS at the interface. It has been found that samples deflection decreases or increases saimultaneously with EPR signal intensity depending on the oxidation condition (temperature). At lower temperature (1100°C) the deflection of the samples decreases with an increase of the EPR signal intensity (E'centres in SiO$_2$ and vacancy complexes in Si) while at a higher oxidation temperature (1200°C) the deflection increase simultaneosly that allow to suggest that the relaxation mechanism of the stresses is different. After the laser irradiation the EPR signal with g-factor 2,006

connected with E'centers decrease. A possible reason for that can be the change of the IMS ander laser irradiation and compressive stresses appear in SiO_2 instead the tensil stresses. This assumption is confirmed by the change of the samples bending after laser irradiation.

Thu-7.8po

Influence ion bombardment on Si and GaAs defect structure

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The upper layers of target undergo in ion flow the essential changes in element consistency and structure. This feature is based the known technological ways of surface property change of the materials. The uncontrollable ion implantation occurs also during the secondary mass-spectrometry and the other diagnostic by ion beams.

Formed an implantation defects, the certain profile of an impurity atom distribution, and a lattice deformation on depth are caused by redistribution radiating defects.

X-ray diffraction methods allow receiving the information on disturbed at implantation of the surface layers, to register the quantitative characteristics of structure upper atom layers, the average change of the interplane distance $\Delta d/d$ and the effective disturb thickness L_{eff}. It doesn't demand the concrete model of deformation. The space resolution of this method equals to the changing 10^{-3}–10^{-4} nm for Δd are 0.1 microns for the sensitivity on depth.

In work the surface Si and GaAs data at various modes implantation and the subsequent anneal are submitted. Silicon doped by phosphorus was irradiated with He, B, N, P and Ar ions at room temperature.

In particular at silicon irradiated with Ar ions on the diffraction reflection curve the oscillation are observed both in the range more and less of Bragg angels.

Implantation reduces the intensity, gives the reflection curve broadening and increases the extent of the diffraction region. The designed parameters of the layers of crystals of silicon L_{eff} and $\Delta d/d$ after implantation and annealing are given. The comparisons of integrated characteristic dependences from ion weight both for calculated and experimental data reveals the interaction type.

The GaAs crystal lattice defects after implantation with H^+, B^+ and O^+ ions are investigated too.

Thu-7.9po

Point defects of F-type as centers of self-sensitization of ZnO in visible region

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Keywords: zinc oxide, photocatalyst, point defects, self-sensitization, visible region

Intrinsic defects of F- and F^+-type (an oxygen vacancy which captures one or two electrons) of ZnO might be used for its self-sensitization (i.e. without any change in the elemental composition of the photocatalyst) in the photoelectric and photocatalytic conversion of the visible light energy. Such defects play the role of absorption centers in the visible region as well as the adsorption sites for reactants or final products. The aim of the present work is to study the key parameters of F- and F^+-type surface defects.

The samples of ZnO powders with controllable and variable concentration of intrinsic defects were investigated using complementary experimental methods: a) diffuse reflectance optical spectroscopy (DRS) of the initial and photoactivated surfaces; b) ultraviolet (8.34 eV) photoelectron spectroscopy (UPES) for in situ monitoring of the evolution of the spectrum of occupied electronic states $N(E)$ and of the electrophysical parameters of the ZnO; c) mass-spectrometry of gaseous and adsorbed phases.

A dispersed powder of ZnO of special purity (OSCh, A2-14) with the mean size of particles $\sim 1\,\mu$m was purified in situ so that the coating with H_2O, CO, CO_2 and N_xO_y molecules did not exceed $10^{-4}-10^{-5}$ monolayer and then was oxidized by a heating in oxygen.

According to UPES data the Fermi level exceeds the top of the valence band by 1.75 ± 0.05 eV. For energies $E_{Fi} < 1.75$ eV a single peak $E_{Ci} = 3.0$ eV below the bottom of the conduction band is observed. It is assigned to dangling bonds of p-type on (1010) plane.Heating of the sample in ultra high vacuum (UHV) induces the peaks $E_{Ci} = 3.2$; 2.8; 2.3 eV in UPES and the absorption bands at 3.1, 2.9; 2.4 eV. The peaks 3.2 and 2.3 eV and the absorption bands 3.1 and 2.4 eV are assigned to the surface F and F^+ centers. Their surface concentration is in the range of $(1–3)\times 10^{-4}$ of a monolayer. The peak 2.8 eV and the absorption band 2.9 eV are assigned to interstitial ions Zn_i^+. The oxygen adsorption on photoactivated F and F^+ centers was studied in a flow-through reactor. Two maxima of photoadsorption efficiency of gaseous oxygen on ZnO are well pronounced just at 2.4 and 3.1 eV.

The cross-sections for the capture of an oxygen molecule by the F-type center was found to be equal to $(2-3) \times 10^{-18}$ cm^{-2}, the extreme coating is equal to the surface concentration of F-type centers. The spectral-selective photodesorption of molecular oxygen under illumination in the absorption bands of F and F^+ centers is revealed in UHV. Using O^{18} the dynamic nature of the photo(adsorption-desorption) processes is proved.

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Thu-7.10po

The role of intrinsic point defects in sensitization of titanium dioxide in the visible spectral range

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Keywords: titanium dioxide, photocatalyst, point defects, self-sensitization, visible region

Titanium dioxide (TiO_2) is widely used for photoelectric and photocatalytic conversion of energy radiation in the UV spectral region. However, only 3% of the solar energy belongs to UV region ($\lambda < 380$ nm, $h\nu > 3.2$ eV), while the visible light contains more than 40% of the solar radiation. In order to sensitize TiO_2 in the visible region, TiO_2 is usually doped with transition metals, sulfur, nitrogen, and other elements.

In order to obtain a self-sensitization of practically used meso- and nanostructures of TiO_2 we propose an original technique of low-temperature photoreduction of the surface from TiO_2 to TiO_{2-x} Such treatment of the sample surface results in the creation of local defects being colored in the visible region with no change both in the elemental composition of the photocatalyst and in the stoichiometry of the bulk. In the present work we study the key parameters of such surface defects.

The samples of Degussa P-25 TiO_2 powders with controllable and variable surface concentration of intrinsic defects were investigated with the aid of complementary experimental methods: a) diffuse reflectance optical spectroscopy (DRS) of the initial and photoactivated surfaces; b) ultraviolet (8.34 eV) photoelectron spectroscopy (UPES) for in situ monitoring the evolution of the spectrum of occupied electronic states $N(E)$ and the electrophysical parameters of the TiO_{2-x}–TiO_2 structure; c) mass-spectrometry of gaseous and adsorbed phases.

The characterization of the photoreduced samples revealed the presence of the heterostructure composed of the bulk (TiO_2) phase and the submonolayer surface (TiO_{2-x}) phase with the bandgaps of 3.2 and 2.7 eV respectively, as well as the local centers Ti^{3+} having the absorption band at 2.00 eV, and the oxygen vacancies (F^+ and F centers) having the absorption bands at 1.17, 2.81, and 2.55 eV.

The adsorption complexes formed during the interaction of O_2, CO, CO_2, NO and N_2O with defects were analyzed by a temperature-programmed desorption. The following environmentally important reaction of the photoreduction of nitrogen oxide with carbon monoxide was examined:

$$NO + CO + h\nu \rightarrow CO_2 + 1/2N_2.$$

It has been found that the proposed self-sensititization procedure actually sensitizes TiO_2 in the visible region and increases for several times the effectiveness of the initial TiO_2 sample.

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Thu-7.11po

Photo-induced spectral change in CeO_2 and CeO_2-based solid solution at room temperature

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Keywords: oxygen defects, photoluminescence, nanocrystals

Various CeO_2 specimens (bulk single crystal, film and nanocrystals) were prepared. We have found several photo-induced phenomena in the CeO_2 specimens at photoexcitation energies lower than the band gap energy (5.5 eV). The photo-induced photoluminescence spectral change of CeO_2 is observed at room temperature for the first time, as follows. When CeO_2 is irradiated with a continuous wave 325 nm laser light in vacuum, a broad visible luminescence increases considerably in intensity. After removing the laser light, the enhanced photoluminescence state is stored for a long time at room temperature under room light, in spite of any changes of atmosphere. By irradiating with the same laser light at room temperature in O_2 gas, the original photoluminescence state re-appears. The phenomenon observed in vacuum is a photo-induced associative detachment of O_2 near the specimen surface, while that observed in O_2 gas is a photo-induced dissociative adsorption of O_2 near the specimen surface. The photoreduction is accompanied both by a valence number change of cerium ions (Ce^{4+} to Ce^{3+}) and by oxygen defects. Such reversible photo-induced phenomena of CeO_2 can be applied to the optical control of the oxygen storage and oxygen release. The mechanism and dynamics of the observed photo-induced spectral changes are discussed, comparing with the results obtaind for other metal oxides [1–5], in the light of the exciton theory.

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Thu-7.12po

The electronic properties of the interface between ZnO and amorphous HfO_2

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Keywords: ZnO, high-k HfO2, interface, oxygen vacancy

Recently, Zn-based oxide semiconductors have attracted much attention because of promising active channel materials for flexible transparent thin-film transistors (TFTs) [1–4]. In a device where an amorphous HfO_x is used for the gate dielectric on crystalline $InGaO_3(ZnO)_5$ film, the field-effect mobility was reported as high as 80 cm^2/Vs [3], while it was shown to be smaller by an order of magnitude in TFTs with an aluminum oxide for the gate insulator. Improvement in device performance was attributed to the improvement of the interface between the gate dielectric and the active channel. As device performance is very sensitive to the interface structure and the existence of defects, it is important to understand the structural and electronic properties of the interface region.

In this work, we investigate the atomic structure of the interface between crystalline ZnO and amorphous HfO_2 and the electronic properties of defects near the interface through first-principles density-functional calculations. The amorphous phase of HfO_2 is generated by performing *ab-initio* molecular dynamics simulations. Crystalline HfO_2 is first melted at 4000 K and then quenched with the cooling rate of about 500 K/ps. In reliable amorphous phase, the average coordination numbers of the Hf and O atoms are estimated to be about 6.8 and 3.3, respectively. We generate various interface models where amorphous HfO_2 is placed on several wurtzite ZnO surfaces, such as (2110), (0001), and (0001). The conduction band offset between ZnO and a-HfO_2 is calculated to be about 2.0 eV, while the potential barrier for hole carrier conduction is nearly zero. We present the details of calculations for the defect properties of O-vacancy and dangling bond defects in the interface region and the role of these defects in device performance.

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Thu-7.14po

On the nature of donor states at interfaces of InAs/AlSb quantum wells

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Keywords: quantum wells, interface states

InAs/AlSb quantum wells (QWs) are characterized by a large electron population, even without intentional doping. This electron population is ascribed to three sources: donor-like states at the sample's free surface, bulk defects in barriers and donor states of the well interfaces [1]. The interface states have been discussed in several articles and are the subject of the present study.

Experiments with InAs/AlSb QWs demonstrate that the mobility of a two-dimensional electron gas is increased with electron density and accordingly with ionized impurities. To overcome such an inconsistency, the interface Tamm states have been proposed as sources of electrons [2] which describes experimental data in assumption that the Tamm state energy equals approximately 40 meV measured from the bottom of the InAs QW. However, numerical calculations give considerably lower value of energy of such states.

We report direct measurements of the interface state energy. In our experiments we have evaluated the energy of the interface states from cyclotron resonance experiments. We assume that a resonant interaction between the electrons in the well and interface donor states in the barrier affects the CR spectra. The penetration of the electron wave functions into the barrier increases when a Landau level coincides in energy with the interface donor level. This affects the spin-orbit interaction [3] and leads to oscillatory behavior of spin splitting as the Landau levels sequentially align the donor level at increasing magnetic field. The role of the Fermi energy for such oscillations would play the energy between the bottom of the conduction band and the donor interface level. From the CR line width oscillations we have determined the energy of the interface states as 30–35 meV for various samples.

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Thu-7.15po

Swift heavy ion irradiation effects at the interface of Zirconium/silicon

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Keywords: irradiation, interface, swift heavy ions

Zirconium silicon interface has been investigated using high energy Au ions in the present work. Zirconium was evaporated on silicon substrate in UHV at a pressure of 10^{-8} Torr by electron beam evaporation technique and the final layer was Au to avoid oxidation of zirconium. The Zr/Si system was irradiated by 350 MeV Au^{26+} ions at liquid nitrogen temperature at different fluences (0.46×10^{14}, 1.85×10^{14} and 4.62×10^{14} ions/cm^2). Rutherford backscattering spectroscopy using 2 MeV He ions was used to monitor the concentration profile and interdiffusion at the interfaces. The irradiation at the Zr/Si interface showed mixing. X-ray diffraction measurements confirmed the formation of nanosized $ZrSi_2$ phase. Thermal spike and melting in the tracks was found to be the dominant process at the interfaces.

Thu-7.16po

Point defects generated by oxidation of silicon crystal surface

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Keywords: silicon, oxidation, vacancy, hydrogen

One of the greatest problems in the field of defects in semiconductors is experimental determination of the formation energy of a vacancy (V) and an interstitial (I). We succeeded in determining the vacancy formation energy with the use of a quenching method, namely, heating specimens in hydrogen gas atmosphere followed by quenching into water and subsequent annealing of specimens at 450°C. In the last procedure, quenched-in vacancies form VH_4, i.e., a cluster of one vacancy and four hydrogen atoms. We studied the optical absorption intensity of VH_4, instead of the V concentration, after quenching from various temperatures [1].

The next problem is to determine the interstitial formation energy for which we applied the above quenching method. We first studied specimens under oxidation since it is usually said that interstitials are formed during oxidation [2]. Hence, we expected a high concentration of interstitials and a low concentration of vacancies in those specimens. Contrary to our expectation, we found the vacancy concentration to

be high in those specimens as shown below.

Specimens were prepared from a floating-zone grown p-type Si crystal. After chemical polishing, specimens were sealed in quartz capsules together with a drop of water and hydrogen gas. The specimen size was about $6 \times 6 \times 11$ mm^3. They were heated at high temperatures for various periods and then were quenched into water. Oxidation temperatures were 1250, 1283 and 1325°C. We observed their optical absorption spectra.

We did not detect the 1987-cm^{-1} peak which is due to IH_2, the most stable complex of an interstitial and two hydrogen atoms. So instead, we attempted to detect vacancies. After annealing at 450°C for 1 h, we measured optical absorption of specimens at about 7 K and detected a peak at the 2223 cm^{-1}, which is due to VH_4. The intensity of this peak is proportional to the vacancy concentration.

The peak intensity, and hence the vacancy concentration, increases with the oxidation time for short periods and then slightly decreases. We define the degree of supersaturation as the ratio of peak intensity under oxidation to that of thermal equilibrium without oxidation. The degree of supersaturation is greater than 1. It means that the apparent formation energy of a vacancy is smaller than that without oxidation.

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Tue-8.1po

Reduced photoluminescence from InGaN/GaN multiple quantum well structures following 40 MeV Iodine ion irradiation

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Keywords: semiconductor materials, heavy ions irradiation, photoluminescence, x-ray diffraction

There is limited knowledge on the effects of radiation on GaN-based devices. It is believed that defects are generated as a result of radiation in III-V semiconductors. In this work we have studied the effect of irradiation by high energy heavy ions on the quality of InGaN/GaN quantum well structures. Quantum well (QW) structures based on InGaN/GaN material system have been grown by using metalorganic vapor phase epitaxy (MOVPE). The active layers in the samples have an indium content of 6% and 10%. Apart from this 5 and 10 MQW structures were grown and analyzed after irradiation. Iodine and bromine ions have been used as irradiations ions. The irradiation fluences of these ions were varied from 10^9 to 10^{12} ions/cm^2.

After irradiation of various structures X-ray diffraction measurement were performed to investigate the effect of irradiation on the crystal structure of the quantum wells. Our X-ray diffraction measurement results have indicated that there is no major damage to the overall crystal structure of the quantum wells.

Apart from this, various types of photoluminescence experiments including continuous wave PL, low temperature PL and time resolved PL were also used to study the effect of various ions and radiation fluences on optical quality quantum well structures. The PL measurements show that the properties of samples irradiated with both ions have a strong dependence on the fluences of heavy ions. Continuous wave photoluminescence results at room temperature indicate that there is a degradation in the PL intensity for irradiated irradiated samples. Low temperature PL results indicate that the activation energy and internal quantum efficiency of the samples also show a dependence on the fluences of irradiation. We have also observed an increase in the decay time of the irradiated samples.

We believe that exposure to radiation causes the formation of point defects or cluster of point defects. We propose that the degradation of the optical quality of the InGaN/GaN quantum wells is linked to the formation of such type of defects.

Tue-8.2po

Defect structure of MBE grown GaMnSb/GaAs (111) layers

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Keywords: GaMnSb, spintronics, defect, X-ray diffraction

Ferromagnetic semiconductors have recently received much interest, since they hold out prospects for using electron spins in electronic devices Among materials that can be used in spintronics, just the these created by introducing ferromagnetic inclusions into a semiconductor matrix, seem to be especially promising. MnSb is one of the candidate materials. It has been shown that bulk MnSb indicates the Curie temperature, T_C of 587 K while the $Mn_{1-x}Sb_x$ layers grown on GaAs reach T_C of about 620 K [1, 2].

We report results concerning the defect structure of the $Ga_{1-x}Mn_xSb$/GaAs (111) system in dependence on the Mn concentration, x, ($x = 1\%$, 3% 6%, 8%). Temperature of substrate during layer growth was maintained at 770 K. Distribution of elements in the layers was determined by SIMS. Structural characterization of the layers was performed at the W1.1 beamline of DESY-Hasylab synchrotron as well as by high resolution X-ray diffraction methods using standard laboratory source. Two modes of measurement were applied with synchrotron radiations: the symmetrical $w - 2q$ and coplanar $2q$ scans in the glancing incidence geometry. Such measurements allow to detect the lattice planes of the layers parallel to the crystallographic orientation of the substrate and to obtain information concerning very thin polycrystalline inclusions. For these layers the inclusions of hexagonal MnSb phase were found. The lattice parameter and defect structure of the layers were studied using the X-ray high-resolution diffractometer. The strain state of layers was determined from the in-plane and out-of-plane lattice parameters and from reciprocal space mapping performed for the symmetrical and asymmetrical reflections. Defect structure of the samples was estimated from the analysis of diffuse scattering near Bragg reflection as well as from FWHM values of rocking curve. Correlation between the Mn concentration and the $Ga_{1-x}Mn_xSb/GaAs$ defect structure has been found.

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Tue-8.3po

Quantum-cascade laser design based on impurity-band transitions of donors in Si/GeSi(111) heterostructures

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Keywords: nanostructures, impurities, resonant states, lasers

The concept of quantum cascade laser based on impurity-band transitions in n-type Si/GeSi heterostructures has been analyzed. Silicon-germanium heterostructures are attractive for development of devices emitting in the terahertz spectral range, where the use of III–V compounds is limited by their reststrahlen band. The mechanism of population inversion is based on fast ionization of donor centers into continuum of the lower neighboring subband by phonon-assisted tunneling [1]. The fast tunneling is caused by hybridization between the impurity ground state and the 2D continuum in the neighboring quantum well. It is essential that the mentioned subband is closely matched with the ground state level of donor. A population of the ground state therefore is smaller than that of 2D continuum of the higher subband. Peculiar features of silicon-germanium heterostructures are related to multivalley character of the conduction band. It involves a lot of intra- and intervalley acoustical and optical phonons in tunneling and relaxation processes.

The laser scheme is analyzed for n-type selectively doped Si/GeSi(111) heterostructures. The choice of the growth plane arises from two circumstances. First, the quantization effective mass, $m = 0.26m_0$, is fairly small. This enables one to use thicker layers in heterostructures that reduces the sensitivity of the laser scheme to a dispersion of dopants through the period and to a fluctuation of heterostructure parameters. Second, build-in strain in the Si/GeSi(111) heterostructures leaves the Δ-valleys degenerate that eliminates additional relaxation channels. An undesirable impact of the remaining degeneracy is the decrease of filling factors of continuum states in the upper (working) subband.

Four- and six-layer-period-superlattice cascade laser are treated. Taking into account electron heating up to 100 K amplification coefficient is of the order of 10 cm^{-1} for doping concentration of 5×10^{11} cm^{-2} per period in the range of 24–29 μm wave lengths. Selective doping is assumed to be in the centre of a quantum well of the period. For comparison, uniform dopant distribution reduces the amplification coefficient by more than five times.

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Tue-8.4po

Defect study of light-emitting thermally treated porous SiO_x films

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Keywords: nanocrystals, EPR, point defects

Thermal evaporation of silicon monoxide on a substrate obliquely oriented to the direction of evaporated substance flow leads to the formation of porous SiO_x films with the columnar structure. Thermostimulated Si nanocrystal (nc-Si) formation in such films takes place in a limited volume of silicon suboxide columns resulting in smaller dimensions of nc-Si than in continuous films with the same value of x. In this report the results from an electron paramagnetic resonance (EPR) study of porous SiO_x films are presented. The low intense symmetrical and featureless EPR line with a g-value $g = 2.0054$ and a linewidth of 0.77 mT has been detected in as-sputtered films and attributed to dangling bonds of amorphous Si precipitates. Following anneals in vacuum at 950°C during 15 min result in decrease of this line and appearance of an intense EPR line with $g = 2.0025$, linewidth of 0.13 mT and hyperfine doublet with 1.6 mT splitting. According to its parameters this spectrum has been attributed to the EX center, a hole delocalized over four non-bridging oxygen atoms grouped around a Si vacancy in SiO_2 [1]. The effect of chemical treatment before annealing and time of annealing on defects and photoluminescence intensity of the films is discussed.

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Tue-8.5po

Deep levels investigation of AlGaN/GaN heterostructure transistors

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Keywords: GaN, high electron mobility transistor (HEMT)

High electron mobility transistors (HEMTs) based on AlGaN/GaN heterostructures are of great interest for microwave applications due to the very high electron density and mobility in the two dimensional electron gas (2DEG), high breakdown voltage, and large bandgap allowing high temperature operation [1]. However the mobility in the 2DEG is expected to be strongly dependent on the crystalline quality of the AlGaN/GaN interface and on the presence of deep traps related to defects in the structure [2].

In this work we investigate AlGaN/GaN HEMTs structures grown by metalorganic chemical-vapor deposition on SiC substrates. They consist of a 22 nm thick undoped AlGaN barrier with Al mole fraction $x = 0.24$ on top of a 1.7 μm unintentionally doped GaN buffer layer. In this paper, we report anomalies observed in temperature dependent output characteristics ($I_D - V_{DS}$) and capacitance-voltage ($C_G - V_{GS}$) curves such as variation of the drain current upon voltage sequence (drain lag) and kink effects. Consequently in order to determine if these phenomena are related to trapping of charge carriers in the transistors, structures with large gate are analysed by deep level transient spectroscopy (DLTS) between 100 K and 450 K. The dominant traps are found to be electron traps with activation energies of 0.12, 0.15, 0.21, 0.40, 0.49 and 0.94 eV. Various parameters of the DLTS measurements have been changes in order to determine the nature of these traps (reverse bias, pulse bias, pulse duration). The detailed analysis of DLTS spectra shows a strong dependence on the electric field in the space charge region of the Schottky contact. The traps location in the structure: either at the surface, at the heterointerface or in the buffer layer will be discussed. The nature of the deep levels will be further examined in order to determine if those traps are associated with extended defects, point defects or dislocation core sites.

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Tue-8.6po

Simultaneous effects of hydrostatic pressure and temperature on donor binding energy in Pöschl–Teller quantum well

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Keywords: Pöschl–Teller, donor impurity, quantum well, hydrostatic pressure, temperature

There are a lot of works related with the study of impurity states in semiconductor heterostructures which show the great possibility of useful manipulation of the impurity center characteristics by means of external electrical and magnetic fields, hydrostatic pressure, and temperature [1]. In semiconductor heterostructures, in contrast to massive sample, the binding energy, as well as other characteristics, depends on the shape and the size of the sample, on the shape of the confining potential, and also on the external hydrostatic pressure and temperature [2–3]. Using a variational procedure and the effective-mass approximation we have calculated the effects of hydrostatic pressure and temperature on the impurity binding energy for on-center donor impurities in Pöschl–Teller quantum well. The binding energy dependency on the hydrostatic pressure, for different values of temperature and parameters of confining potential, is investigated. The results show that with increasing pressure, for fixed values of temperature and of confining potential parameters, the binding energy increases linearly. We have also observed that with the increases of temperature and confining potential parameters the binding energy decreases. Thus, the results obtained specify the opportunities of efficient control of binding energy in a semiconductor quantum well by changing hydrostatic pressure, temperature and profile of confining potential.

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Tue-8.7po

Hydrogenic impurity binding energy in vertically-coupled GaAs-Ga$_{1-x}$Al$_x$As quantum-dots under hydrostatic pressure and applied electric field

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Keywords: quantum dot, donor impurity, hydrostatic pressure, electric field

In this work we perform a theoretical study, using a variational method and the effective mass approximation, for the ground state binding energy of a hydrogenic donor impurity in vertically-coupled quantum-dot structure under effects of hydrostatic pressure and growth-direction applied electric field. The low dimensional structure consists of three vertically coupled cylindrical shaped quantum-dots. For the hydrostatic pressure we have considered the Γ-X crossover in the barrier material. Our results consider different structure size values (well width, barrier thickness, and dot radius), the impurity position along the z-direction, applied electric field, and hydrostatic pressure.

We found that for both, symmetrical and asymmetrical dimensions of the structures, the binding energy as a function of the impurity position has a similar shape to that shown by the electron wave function without the Coulomb interaction. Also, the presence of the electric field changes dramatically the binding energy profile destroying (favoring) the symmetry in the structures. In the case of hydrostatic pressure our results show that the binding energy increases due to the diminishing of the Coulomb interaction mainly related to changes in the static dielectric function. Also, depending on the impurity position the binding energy can increase or decrease with the hydrostatic pressure mainly due to increases or decreases of the carrier-wave function symmetry by changing the height of the potential barrier.

Tue-8.8po

Photoluminescence energy transitions in GaAs-Ga$_{1-x}$Al$_x$As double quantum wells: electric and magnetic fields and hydrostatic pressure effects

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Keywords: double quantum well, electric and magnetic field, hydrostatic pressure, photoluminescence

Within the framework of the effective mass and parabolic band approximations and using a variational procedure we have calculated the photoluminescence energy transitions in coupled double quantum wells under simultaneous effects of electric and magnetic fields and hydrostatic pressure. The electric field is taken to be oriented along the growth direction of the heterostructure whereas for the magnetic field both in-plane and in-growth directions have been considered. The results show that hydrostatic pressure is an useful tool to tune the direct and indirect exciton transitions in coupled double quantum well systems. It is shown that the photoluminescence peak energy transitions strongly depend of the external fields and hydrostatic pressure here studied. Furthermore, our numerical outcome is in good agreement with previous experimental findings at zero pressure in double quantum wells under applied electric and magnetic fields.

Tue-8.9po

Hydrogenic donor impurity in parallel-triangular quantum wires: Engineering of the quantum confinement under hydrostatic pressure and applied electric field

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Keywords: donor impurity, triangular quantum wire, hydrostatic pressure, electric field

The combined effects of the hydrostatic pressure and the in-growth direction applied electric field on the binding energy and on the density of the hydrogenic shallow-donor impurity states in symmetrical and asymmetrical GaAs/Ga$_{1-x}$Al$_x$As parallel-triangular quantum wires are calculated using a variational procedure within the effective-mass approximation. The trial wave function for the ground state of the hydrogenic donor impurity is chosen as in Refs. [1–3]. The density of impurity states

is calculated for a homogeneous distribution of donor impurities within the barriers and in the triangular well-wires. Results are obtained for several wire and barrier widths, shallow-donor impurity positions, hydrostatic pressure, and applied electric field. This is an engineering of the quantum confinement which may be import in device constructions under suitable conditions.

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Tue-8.10po

Capacitance investigation of Ge nanoclusters on a silicon (001) surface grown by MBE at low temperature

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Keywords: quantum dots, nanostructures, capacitance-voltage technique

Unique optical and electrical properties of the germanium quantum dots (QDs) in silicon provide wide possibilities for nanostructure device fabrication. Electron structure of these objects is determined by the QD concentration, layer quantity and interaction between electron states of the different layers. Low temperature growth conditions lead to the formation of dense arrays of nanometric germanium islands in silicon matrix. So far as an electron structure determines properties of the QDs, the electrical investigations of these objects are very important.

In the present work, multilayer Ge/Si heterostructures with Ge nanoclusters grown on atomically clean (001) surface of the silicon substrates at temperature of 350°C by ultra high vacuum molecular beam epitaxy (MBE) method were studied. Three groups of structures with different effective thicknesses of Ge layers ($h_{\mathrm{Ge}} = 0.6$, 1 or 1.4 nm) containing the quantum dots were investigated. Each structure contained five Ge layers, silicon barriers with the thickness of 50 nm, buffer and cap silicon layers with the thicknesses of 100 and 50 nm, respectively. Silicon layers were grown at temperature of 530°C. Parameters and concentration of the QDs formed on silicon (001) surface at the mentioned temperature were determined in the samples-satellites by ultra high vacuum scanning tunneling microscopy (STM). It was found that the size and the concentration of the QDs depend on effective thickness of germanium layers.

Capacitance-voltage (CV) and deep level transient spectroscopy (DLTS) measurements were curried out on Schottky barriers in the temperature range from 77 to 300 K. The plateaus of nearly constant capacitance, which corresponds to recharging of the QDs, and corresponding peaks of effective concentration profiles were observed for all groups of samples. The hole concentration captured in the QDs was estimated and a correlation between the QD concentration and the charge accumulation was revealed. It was found that the capacitance plateau value depends on a temperature. The hysteresis was observed in the CV characteristics at low temperatures, which is caused by an emission rate decrease. In the sample with $h_{\mathrm{Ge}} = 1.4$ nm the apparent peak of effective charge concentration did not correspond to geometrical position of the QDs. This effect is discussed taking into account the λ-layer effect. The DLTS spectra were found to be essentially different for the sample groups studied. The DLTS peaks located near surface and probable caused by the presence of the QDs were revealed.

Tue-8.11po

Laser modification of MBE grown SiGe/Si multilayers

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Keywords: Ge dots, laser treatment, TEM

Stranski-Krastanov growth passes through the stage of 3D islands formation due to the strain relaxation in lattice mismatched heteroepitaxial systems [1]. The islands are formed on the top of a wetting layer — flat pseudomorphic layer of one or two monolayers thick. A negative feature of Stranski-Krastanov growth mode is a wide size distribution of the islands. One possible approach to solve a problem is to use a post-grown laser treatment. As it is reported in [2], laser treatment improves the size uniformity of Ge nanoislands. This talk will present some new results on structural investigation of laser treatment of Si/Ge multilayers.

A Si/Ge multilayer consisting of six bilayers of (0.9 nm Ge + 10 nm Si) were grown by MBE on (001) n-Si substrates at 550°C. A VG Semicon V80 MBE system was used. The Si/Ge multilayer was then treated using a Q-switched Nd:YAG laser operating at a wavelength of 1.06 μm and a pulse duration of 15 ns at 25 Hz. The diameter of laser beam was 50 μm and a beam overlapping was 50%. An energy density was varied between 0.8 and 1.3 J·cm^{-2}. The structure was investigated by TEM in plan-view and cross-section geometries. A EM-125 instrument operating at 100 kV was used.

As observed by TEM, rectangular and square base Ge nanoislands are typically created after MBE growth in above mentioned conditions. The average size of nanoislands was 60 nm and the surface density was (2–3)$\times 10^{10}$ cm^{-2}. The shape of nanoislands was typically classified as either "*hut*" or "*pyramid*". It is found that laser treatment results in strong modification of island morphology. Namely, the nanoislands are transformed from *huts* and *pyramids* to *domes* after laser treatment at 0.8–1.0 J·cm^{-2}. Accordingly, the islands are enlarged up to 90–110 nm with decreasing of surface density down to 8.5×10^9–5.3×10^9 cm^{-2}. However, further rise of laser energy density up to 1.3 J·cm^{-2} results in disappearance of the islands. The results are discussed in terms of liquid phase recrystallization of Si/Ge layers activated by laser treatment. Strain situation around Ge layers and segregation are also taken into account.

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Tue-8.12po

The structural properties and stoichiometric defects of anodic Ag(I) oxide nanofilm

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Keywords: silver oxide, photocurrent, photopotential

Photoelectrochemical measurements allow to investigate some structural-sensitive characteristics of semiconducting films. Carrier density and, consequently, defect concentration, directly influences on magnitude of photocurrent (i_{ph}) and photopotential (E_{ph}). Hence, photoelectrochemical methods are used to get the *in situ* information about the oxide film structure, its stoichiometry and role of chemical and structural state of substrate. It is important, that information can be obtained under condition of anodic formation of oxide layer on metal substrate in electrolyte solution, i.e. *in situ.* However, we have to be convinced, that photoresponse arises in oxide phase, but not because red-ox processes on the oxide/electrolyte interface.

Ag(I) oxide anodically formed in 0.1 M KOH on polycrystalline Ag_{poly}, single crystalline Ag_{100}, Ag_{110}, Ag_{111} and polycrystalline Ag–Au alloys (with gold concentration up to 15 at.%) were the object of investigation.

Photoelectrical measurements were performed by means of the set of light-emitting diodes. Photopotential E_{ph} was measured in open circuit after the polarization switching off. The role of potential of oxide Ag(I) formation (0.52–0.56 V s.h.e.), film thickness L (6–22 nm), light intensity (0.8–3.0 mW cm^{-2}) and wavelength l (385–875 nm) was examined. Photocurrent i_{ph} was measured under polarization at the potentials of oxide Ag(I) formation.

It was found that $E_{\text{ph}} < 0$ and $i_{\text{ph}} > 0$ independent of Ag_2O formation conditions. It proves the n-type conductivity connected with excess of metal. The photopotential and photocurrent arise in oxide volume but not in the surface electronic states. This conclusion results from the difference in E_{ph} and i_{ph} for oxides grown on $\mathrm{Ag}_{\mathrm{poly}}$, single crystals $\mathrm{Ag}_{\mathrm{hkl}}$ and alloys.

E_{ph} and i_{ph} depend on film thickness L, it means, that the anodic film is thin (its thickness is less than the space charge region). After the polarization switching off, photopotential decays in time in exponential manner. The decay is caused by the film dissolution.

The concentration of donor defects decreases in the row $\mathrm{Ag}_{\mathrm{poly}} > \mathrm{Ag}_{\mathrm{hkl}} >$Ag–Au. Hence, more stoichiometric oxide is formed on alloys. As a result the photoconductivity drops in the same order. The shape of $i_{\mathrm{ph}} - l$ dependences, hence, the band gap does not noticeably change at transition from $\mathrm{Ag}_{\mathrm{poly}}$ to $\mathrm{Ag}_{\mathrm{hkl}}$ and Ag–Au alloys, and its value is 2.23 ± 0.14 eV.

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Tue-8.13po

Defects in nanothin crystalline layers and multilayer structures formed of them

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Keywords: nanothin layers, multilayer structures, defects

Thermally deposited nanothin films are usable as effective buffer components of photovoltaic devices [1]. It is also established that near surface nanothin layers of crystals, irradiated and/or annealed, distinguish oneself by structural and optical properties different from those of bulks [2]. The defects in nanothin films and near surface crystalline layers of dielectrics and semiconductors is not discovered well due to complication of testing the properties of so small objects. The situation can be changed in the case of formation the relatively thick multilayer structures composed of high quantity of the nanothin layers. Since thermally deposited nanothin films and multilayers formed of them have been studied only in a limited way [3], in this paper we carried out the following procedures to investigate them.

The samples are multilayer nanostructures [3] and reference glasses, crystals, powders and films produced in a standard way. Each nanostructure unit is a nanothin layer with (111) ordered nanocrystal array inside it. Samples with various sensitizing nanocrystals were grown by multi-step deposition of alternate nanolayers, and by using special techniques for nanocrystal ordering. The geometry of the nanostructures was tuned by controlling the thicknesses and the compositions of the sensitizing and complementary, buffer, nanolayers. Every nanolayer can be designed of one material and as composition of nanocrystals, clusters of two materials. Sensitizing nanolayers were prepared with thicknesses equal to nanocrystal sizes [4]. After the growth some samples were ^{60}Co-γ-ray irradiated at room temperature up to 83 kGy.

Optical spectra of multilayer structures of nanothin films with nanocrystals of defined size and undoped crystals with given content of the impurities were compared. Relationships among the content of impurities, colloids and properties of initial crystals, and multilayer structures were examined. The influence of surface effects on size-dependent properties of nanothin layers with LiF and CdS nanocrystals were investigated. Microstructure testing, optical absorption, photoluminescence and nonlinear optical experiments indicate that the possible origins of nanothin layers peculiarities are their purification and the metal excess accumulation in their boundaries.

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Tue-8.14po

Diffuson-type relevant quantum corrections to coherent impurity scattering

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Keywords: disorder, impurities, weak localization, integer quantum Hall effect

It is well-known since 1979 [1, 2] that low-temperature conductivity of 2D electronic systems is strongly suppressed due to the coherent backscattering of carriers by the defects and impurities. Quantum correction to conductivity of the first order in $1/(k_{\mathrm{F}}l)$ due to Cooperon channel is given by

$\delta\sigma_1(\omega) = 1/\pi \ln \omega\tau e^2/h.$

Corresponding localization length can be easily derived from the condition $\delta\sigma_1 = -\sigma_0$ [2], $\xi_0 = l \exp(\pi g/2)$, where $g = k_F l$ is Drude conductivity σ_0 expressed in the units of e^2/h.

However, $\delta\sigma_1$ ceases to diverge in non-zero magnetic field due to magnetic length cut-off giving rise to negative magnetoresistivity [2]. In the present study we focus on intermediate range of magnetic fields where Cooperon channel is already suppressed but Landau quantization still can be neglected therefore quantum correction to conductivity of the second order in $1/(k_{\mathrm{F}}l)$, $\delta\sigma_2(\omega)$, comes to the front.

We apply usual short-range impurity diagram technique at $T = 0$ and pick out relevant diagrams of the second order in $1/(k_{\mathrm{F}}l)$ following Refs. [2–4]. As it was first stated if Ref. [2] all terms containing $\ln^2(\omega\tau)$ cancel out up to the second order in $1/(k_{\mathrm{F}}\mathrm{l})$. In Refs.[3, 4] the problem was treated using diffusive non-linear σ-model and mutually contradictory answers for the $ln(\omega\tau)$ prefactor were obtained. However, so-called diffusion approximation adopted in Refs. [3, 4], i.e. substitution of exact Diffuson by approximate expression $1/[(kl)^2/2 - \imath\omega\tau]$ is obviously incorrect for arbitrary values of k resulting in convergent answer for $\delta\sigma_2(\omega = 0)$ in line with Ref. [3].

Correct calculation of $\delta\sigma_2(\omega)$ requires accurate taking into account of ballistic contributions and results in the following answer:

$$\delta\sigma_2(\omega) = \Sigma/\pi^2 \ln(\omega\tau)(1/k_{\mathrm{F}}l)e^2/h, \qquad \Sigma = 11/12 + 3\ln 2 \approx 2.996.$$

So-called unitary localization length is related to Σ via

$$\xi_u = l\exp(\pi^2 g^2/2\Sigma).$$

Previously it was argued [5] that $\xi_u = l\exp(\pi^2 g^2)$ that corresponds to $\Sigma = 0.5$. We have shown that the actual value of Σ is almost one order of magnitude higher. Let us estimate ξ_u in the limit of high magnetic field using "bare" σ_{xx} peak values due to Ando, $g_n = (2n + 1)/\pi$:

$$\xi_0 \approx 1.2a\_H, \qquad \xi_1 \approx 4.5a\_H, \qquad \xi_2 \approx 65a\_H.$$

This estimation confirms reliability of linear growth of σ_{xx} peaks with Landau level number n in the integer quantum Hall effect regime stated in Ref. [6].

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Tue-8.15po

Evolution of luminescent Si nanostructures under irradiation by swift heavy ions

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Keywords: Si, nanostructures, swift heavy ions

When swift heavy ions (SHI) penetrate in solid-state targets, their stopping in thin near-surface layers occurs mostly at the expense of ionization losses. If the stopping rate exceeds ~1 keV/nm, tracks are forming with the nm-scale diameters, where the carrier concentrations may reach $\sim 10^{22}$ cm^{-3}. Temperature inside the tracks may exceed 5000 K for 10^{-13}–10^{-11} s. Thus, defect formation and ultra-short pulse annealing should proceed in the targets.

In our study thin SiO_2 layers were implanted with 140 keV Si ions to the dose of 10^{17} cm^{-2}. Two types of the samples were employed for irradiation with 130 MeV Xe ions: as-implanted with Si, and those subjected to post-implantation annealing at 1100°C to form Si nanocrystals. The doses of Xe ions were ranging from 3×10^{12} to 10^{14} cm^{-2}. HREM and photoluminescence were used for the characterizations. In the as-implanted layers HREM revealed after Xe irradiations the 3–4 nm-size dark spots, whose number and size grew with increase in Xe ion dose. In some of them lattice fringes may be distinguished, indicating their crystal character. The interplanar spacing matched those of silicon. Photoluminescence band at 660–680 nm was found in such samples. At first its intensity dropped with the Xe dose, but more prolonged bombardment caused the emission to grow. Passivation by hydrogen quenched the band and promoted emission at $\sim$ 780 nm, typical of Si nanocrystals. In spectra of 1100°C-annealed layers strong $\sim$ 780 nm peak was observed at once. Under Xe bombardement its intensity fell rapidly, followed by appearance and growth of the 660–680 nm band. Passivation partly restored the emission at $\sim$ 780 nm. The obtained results are interpreted as the emission at $\sim$ 660–680 nm belongs to the damaged Si nanocrystals. It is concluded, that ionization losses of Xe ions are mainly responsible for the formation of new Si nanostructures in hot ion tracks, whereas nuclear losses mainly introduce the radiation defects, which quench the luminescence. Changes in spectra with growth of Xe ion dose are accounted for the difference in the diameters of Xe ion tracks ($\sim$ 5 nm) and the displacement cascades ($\sim$ 50 nm).

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Tue-8.16po

Investigation of electrical properties of carbon nanotubes and polystyrene composites

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Keywords: carbon nanotubes, polystyrene, composites, conductivity

Carbon nanotubes (CNT) have been extensively studied since their discovery due to their excellent comprehensive mechanical, thermal, and electrical properties for a variety of applications. Their mechanical robustness, high thermal and electrical conductivity are invaluable in material engineering to create composite materials with controllable properties, assuring mechanical stability, high power dissipation and resistivity ranging in wide regions. In recent years, single-walled (SWNTs) and multi-walled (MWNTs) carbon nanotubes have been actively pursued in both fundamental and applied research aspects. Compared to single-walled carbon nanotubes, multi-walled carbon nanotubes are currently receiving more attention for commercial applications, because of easy large-scale production via the chemical vapor deposition synthesis.

We report investigation of electrical conductivity of the high resistivity polystyrene/carbon nanotube composites. The samples have been spin-coated onto sapphire substrates on which gold electrode structures have been deposited. Four electrodes were arranged to perform four-point resistivity measurements. The polymer/CNT films consist of a thiol-bonded network of singly wrapped MWNTs within a polystyrene matrix. We have investigated samples with the CNT/polystyrene mass ratio raging from 0% to 1%. The conductivity measurements were performed in the temperature range from 15 K up to 400 K.

The well expressed dependence of the electrical properties of samples on the doping level was evidenced experimentally. Resistance of the samples with the highest content of CNTs was about $10^6-10^7\,\Omega$. Their conductivity was nearly temperature-independent with the thermal activation energy value being as low as 0.013–0.016 eV. Properties of the samples had changed drastically with the reduction of the CNT amount down to 0.6%. Resistance of these samples at 300 K had jumped up to about $1 \times 10^{13}\,\Omega$, and thermal activation energy values increased up to 0.53 eV. By further reduction of the doping level conductivity measurements at the room temperature and below it became impossible because of the RC-effects of rapidly growing resistivity and sample capacitance. The well expressed current relaxations took place that lasted of several thousands of seconds. Nevertheless these relaxations were not exponential with the instantaneous relaxation time constant growing with time. This evidences that the observed effects cannot simply be ascribed to the effects of ohmic conductivity and geometric capacitance, but are related to the percolation and polarization phenomena in inhomogeneous media formed by "islands" of CNT in polystyrene matrix.

The observed peculiarities could be explained by the inhomogeneous distribution of CNT in polystyrene matrix. It was found that the most homogeneous distribution takes place in the samples having 0.7% of CNT. At higher percentage CNT forms interconnected clusters. Meanwhile if amount of CNT is equal or less than 0.6%, "islands" of CNT become separated by the layers of polystyrene, which govern charge transport.

Tue-8.17po

Influence of irradiation by neutrons on the properties of p^+-n-n^+ Si radiation detectors

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Keywords: silicon, radiation defects, energy levels, photoconductivity spectra

The photoconductivity spectra and thermally stimulated currents (TSC) were investigated in p+–n–n+ Si detectors according to the WODEAN project of CERN-RD50 collaboration. The samples were irradiated by neutrons up to the fluencies 1×10^{13}–1×10^{16} cm^2. The irradiation created deep levels below the middle of the bandgap that were observed by the extrinsic photoconductivity spectrum and by the temperature dependence of the dark current. The extrinsic photoconductivity edges corresponding to the optical activation energies of the defect levels were observed at 605 meV, 651 meV, 772 meV, 885 meV and 1072 meV. The shallower defect centers in the upper part of the bandgap were identified by TSC. Deep levels with activation energy of 0.10–0.11 eV, 0.25–0.26 eV, 0.34–0.36 eV and 0.40–0.42 eV were observed. The concentration of these levels was depending on the fluence and on the isochronal thermal treatment at low temperatures (80°C, 120°C, 150°C and 180°C). Also, change of donor and acceptor type center concentration was identified by the I-V characteristics fitting. It was found that the isochronal annealing up to 120°C results in the increase of the acceptor concentration. An increase of donor concentration after annealing at 150°C was observed, which is correlated to the current injection upon forward bias. The population changes of the defect centres determined by annealing have been compared with the steady state lifetime and photoconductivity decay constant.

Tue-8.18po

Characterization of epitaxial Al layers grown by MBE on GaAs (001)

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Keywords: MBE, Al, GaAs, TEM, Schottky barrier

Metal-semiconductor heterostructures can be used to produce epitaxial junctions, semiconductor-superconductor devices, as well as some optical elements. Recently Al/GaAs heterostructures have been examined as resonant tunnel heterostructures with Schottky barrier [1].

In the present work we present the results of *in situ* and *ex situ* structural characterization of these Al/GaAs heterostructures.

Al/GaAs(001) heterostructures were grown by molecular beam epitaxy (MBE) in CNA-25 MBE machine at growth temperature $< 100°$C and residual pressure $< 10^{-9}$ Torr in the growth chamber. Aluminum layers of $\sim 0.2\mu$ m thick were deposited on GaAs buffer layer. *In situ* reflection high energy electron diffraction (RHEED) indicated 3D mode of Al layer nucleation followed by further 2D growth of Al epilayer. The growth regime transformation from 3D to 2D mode occurred at Al layer thickness ≈450 Å, when a spotted diffraction pattern transformed into a highly streaked one. Atomic force microscopy (AFM) topography images indicate a plateau-valley morphology of the resulting Al layer, clearly proving the perfect coalescence between adjacent islands. Transmission electron microscopy (TEM) examination of the plan-view samples show that the Al layers studied are single crystal continuous (110) Al layers consisting of large enough domains. Epitaxially grown domains fit to the GaAs substrate so that the $\langle 110 \rangle$ in-plane direction coincides with one of the two $\langle 110 \rangle$ directions in GaAs substrate, $\langle 110 \rangle$Al/$\langle 110 \rangle$GaAs. An analysis of the transmission electron diffraction patterns show that the Al layers consist of two sets of domains oriented perpendicular to each other. Despite the domain structure of the resulting Al layer, the fine quantum effects of Al/GaAs Schottky-barrier structures were observed in samples with quite large surface area [1]. This fact implies that Schottky barrier properties do not depend dramatically on Al film orientation.

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Tue-8.19po

Molecular nanostructures as basic elements of spin electronic devices fabrication

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Keywords: molecular nanotechnology, information theory, entropy, spin-polarized transport

Modern molecular nanotechnology implies the design, modeling, and fabrication of molecular machine and molecular devices. Information may be described as patterns shared between structures.

If information is to be stored or transported, it must have a physical form. The device that stores the bit must have two distinct states, and bit is stored by putting the device in one or another of these states, and when the bit is needed the state of the device is measured. When the device has moved from one place to another then communications has occurred. In case when device has persisted over some time then it has served as a memory, if it has had its state changed in a random way then it has forgotten its original value.

We are naturally interested in physical devices, which are small. The limit to how small an object can be and still store a bit of information comes from quantum mechanics. A quantum bit, or qubit is object, which can store a single bit but is so small that it is subject to the limitations quantum mechanics places on measurements. In particular, a measurement cannot be made without possibly altering the object being measured. On the other hand, if a bit is represented by many objects acting together, a measurement can be made and enough objects left unchanged so that the same bit can be measured again. And if not all objects measure in the same way the result might be intermediate between the two possible Boolean values.

The most relevant physical phenomena, which should be basis of molecular device fabrication is spin polarized transport in diluted semiconductors. In these materials it is possible to transfer spins coherently in a spin-aligned state across interfaces with different magnetic properties. That physical effect allows building novel molecular (quantum) devices that exploit electron spin, and magnetic storage of the computing machine relies on the magnetic properties created by electron's spin.

Link between matter and information is most evidently manifested by the molecular constitution in building molecular phrases, where molecules are connecting in given order. The initial formation directs the synthesis of sequences, which logically are not random; there is an optimization of structure within the system. Such optimization of may be expressed in terms of Shannon's and fuzzy entropy and relates directly to the definition of information. Formation of the model system is based on two types of bindings between atoms and structural elements (molecules). Usage of appropriate molecular CAD software, molecular modeling software and related tools are the most promising way to explore and analyse of design of molecular manufacturing systems.

Tue-8.20po

Investigations of Si-implanted silicon nitride based on fotoluminescence and EPR methods

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Keywords: fotoluminescense, ion implantation, nanocrystallite, dielectric matrix

Silicon nitride (Si_3N_4) is widely used as engineering ceramics and insulators in the semiconductor technology. Si_3N_4 has attracted much attention in microelectronic related studies due to its excellent mechanical, thermal, and electronic properties and the importance of these amorphous materials is continually increasing. Moreover, Si-enriched Si_3N_4 are reported to display strong room-temperature luminescence in visible spectral region and can be used in all-Si-based optoelectronics technology.

In this work for silicon enrichment of Si_3N_4films ion implantation method has been used. Photoluminescence (PL) measurements were performed on a series implanted amorphous silicon nitride films with different irradiation dose and the annealing temperature. Our spectra were distorted by interference, therefore for correct interpretation of obtained data we use computer simulation taking into account interference effects. Finally the main PL peak was determined by fitting the data to Gaussian curve that is centered at 480 nm. Spectra of our samples is not vary up to $T = 1000$°C, but for more high temperature their intensity is monotonously decreased. Analyzing results, we suppose, that observed PL is due to the mechanism of band-tail recombination. EPR data of irradiated films is described as superposition of several spectra, corresponding to K-, N- centers and most probable nitrogen vacancies.

During Si ion implantation, many of structural defects of type of the displaced atoms are produced and part of introduced Si ions is built in to Si_3N_4 matrix. This processes result in the quenching of the intrinsic PL and the generation of paramagnetic defects, which is related to dangling bond of Si. Silicon ions stimulated by annealing have to form chemical bonds with an environment, as result the optical gap decreases and we can observe red shift of PL peak.

Simultaneously with Si-incorporation to silicon nitride matrix, nucleation of the silicon fraction is generated. For the temperature before 800°C these inclusions has crystalline structure and nanosizes. Thus they should be responsible for appearance of PL peak at 680 nm, which is in a good agreement with numerical simulation. At the more high annealing temperature we have been observed the growth of the inclusions size due to the coalescence and diffusion processes.

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Tue-8.21po

Effects of thickness of InGaZnO channel layer on device performance in oxide thin-film-transistors

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Keywords: IGZO, TFTs, Al:ZnO

Thin-film-transistors (TFTs) that can be prepared at low temperatures have attracted much attention due to the great potential for transparent and flexible electronics. One of the mainstreams in this field is the use of organic semiconductors such as pentacene. But device performance of the organic TFTs is still limited due to low field-effect mobility and rapid degradation after exposing to air. Alternative approach is the use of amorphous oxide semiconductors as a channel. Amorphous oxide semiconductors (AOSs) based TFTs showed the fast technological development, because AOS films can be fabricated at room temperature and exhibit the possibility in application such as flexible display, electronic paper, and large solar cells. Among the various AOSs, a-IGZO has many advantages because it has high channel mobility, uniform surface roughness and good transparency. [1] The high mobility is attributed to the overlap of spherical s-orbital of the heavy post-transition metal cations.

This study demonstrated the effect of the variation in channel thickness from 30 nm to 200 nm on the TFT device performance. When the thickness was increased, turn-on voltage and subthreshold swing was decreased. The a-IGZO channels and source/drain metals were deposited with shadow mask. The a-IGZO channel layer was deposited on SiO_2/p-Si substrates by RF magnetron sputtering, where RF power is 150 W. And working pressure is 3 MTorr, at O_2/Ar (2/28 sccm) atmosphere. The electrodes were formed with electron-beam evaporated Ti (30 nm) and Au (70 nm) bilayer. Finally, Al (150 nm) as a gate metal was thermal-evaporated. TFT devices were heat-treated in a furnace at 250°C and nitrogen atmosphere for 1hour. The electrical properties of the TFTs were measured using a probe-station.

The TFT with channel thickness of 150 nm exhibits a good subthreshold swing (SS) of 0.72 V/decade and on-off ratio of 1×10^8. The field effect mobility and threshold voltage were evaluated as 7.2 and 8 V, respectively.

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Tue-8.22po

Defect-related yellowish emission of undoped ZnO/p-GaN:Mg heterojunction light-emitting-diodes

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Keywords: ZnO, heterojunction, LED, deep-level emission

ZnO with a large band gap ($\sim$ 3.37 eV) and exciton binding energy ($\sim$ 60 meV) is suitable for optoelectronic applications such as ultraviolet (UV) light-emitting-diodes (LEDs) and detectors. However, the ZnO-based p–n homojunction is not readily available because it is difficult to fabricate reproducible p-type ZnO with high hall concentration and mobility. In order to solve this problem, there have been numerous attempts to develop p–n heterojunction LEDs with ZnO as the n-type layer. The n-ZnO/p-GaN heterostructure is a good candidate for ZnO-based heterojunction LEDs because of their similar physical properties and the reproducible availability of p-type GaN. Especially, the reduced lattice mismatch ($\sim$ 1.8%) and similar crystal structure result in the advantage of acquiring high performance LED devices. In particular, a number of ZnO films show UV band-edge emission with visible deep-level emission, which is originated from point defects such as oxygen vacancy, oxygen interstitial, zinc interstitial [1]. Thus, defect-related peak positions can be controlled by variation of growth or annealing conditions.

In this work, the undoped ZnO film was grown on the p-GaN:Mg film using RF magnetron sputtering method. The undoped ZnO/p-GaN:Mg heterojunctions were annealed in a horizontal tube furnace. The annealing process was performed at 800°C during 30 to 90 min in air ambience to observe the variation of the defect states in the ZnO film. Photoluminescence measurements were performed in order to confirm the deep-level position of the ZnO film. As a result, the deep-level emission showed orange-red color in the as-deposited film, while the defect-related peak positions of annealed films were shifted to greenish side as increasing annealing time. Furthermore, the electrical resistivity of the ZnO film was decreased after annealing process. The $I-V$ characteristic of the LEDs showed nonlinear and rectifying behavior. The room-temperature electroluminescence (EL) was observed under forward bias. The EL showed a weak white and strong yellowish emission colors ($\sim$ 575 nm) in the undoped ZnO/p-GaN:Mg heterojunctions before and after annealing process, respectively.

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Tue-8.23po

Impurity photoconductivity in strained p-InGaAs/GaAsP heterostructures

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Keywords: nanostructures, impurity, photoconductivity

Till now the resonant lines of the impurity photoconductivity (PC) in quantum well (QW) heterostructures were observed in QWs of elementary semiconductor (Ge) and of binary compound material (such as GaAs) only. In far IR photoconductivity spectra in p-type $\mathrm{Si}_{1-x}\mathrm{Ge}_x$/Si QWs a broad PC band was observed instead of narrow lines in bulk Si already at Ge content of 1% in the solid solution [1]. In another material system InGaAs/GaAs with strained QWs of InGaAs solid solution the shallow acceptor binding energies were probed by band-gap photoluminescence technique [2] and by the thermal activation of the conductivity [3]. In the present work we report on the first observation of optical transitions from the ground shallow acceptor state into excited localized and resonant ones in strained QWs of InGaAs solid solution.

The sample under study was multiple QW (30 periods) $\mathrm{In}_{0.06}\mathrm{Ga}_{0.94}\mathrm{As}/\mathrm{GaAs}_{0.9}\mathrm{P}_{0.1}$ heterostructure #5189 grown on semi-insulated GaAs(100) substrate by atmospheric pressure MOCVD technique. Two delta-layers of carbon were introduced into each InGaAs QW 200 A wide 50 A apart from the heterointerfaces. In observed photoconductivity spectra strong PC band at photon energies in between 20 and 30 meV is clearly seen. Within this band two narrow lines at 19.8 meV and 21.8 meV are resolved in the spectrum as well as a broader line corresponding to photon energies 25 to 28 meV. Also the narrow PC line is observed near the GaAs LO-phonon energy 37 meV.

To analyze the data obtained we calculated the shallow acceptor energy of states in the structure. The calculations were made using the approach developed in [3]. This method allow to calculate energies of the ground and excited p-like states of acceptors confined in a QW as well as probabilities of optical transitions between these states. The calculation results shows that the transition into the third excited state and into continuum should dominate in the long wavelength part of PC spectrum. Calculated energies of these transition are in a good agreement with narrow lines at 19.8 meV and 21.8 meV in observed PC spectra. The broad PC peculiarity at photon energies 25 to 28 meV can be related with transitions from the ground acceptor state into resonant states pertained with the second subband of size quantization. The observed spreading of these transitions could results from fluctuations of QW width that strongly affects the position of subband edges in contrast to the localized state energies. At last, the short wavelength line observed in the spectra seems to be Fano resonance, which is asymetric feature in PC spectrum of photoconductivity, observed at energies close to LO phonon one (see, for example, [4]).

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Tue-8.24po

Formation of intermediate layers between ZnSe quantum wells and ZnMgSeS barriers in the periodic structures grown on GaAs substrates misoriented by 10° from (001) to (111)A

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Keywords: x-ray diffraction, nanostructures, II-VI compounds, MOVPE

Using of ZnMgSSe quaternary compounds to achieve both high band gap (3–3.1 eV) and lattice period matching with the GaAs substrate is important condition to obtain low defect periodic structures with resonance-periodic gain for effective lasers with longitudinal optical and electron-beam pumping, radiating in blue spectral range (460 nm). Emission line of ZnSe quantum wells (QWs) undergoes short-wave shift due to unintentional doping by Mg atoms with concentration up to 1% when the structures are grown by metal-organic vapor-phase epitaxy (MOVPE) at temperature 480–500°C. In order to tune the emission line to required wavelength of 460 nm, one adds Cd with concentration of 1–2% in the QWs. This leads to increasing crystal lattice misfit between the ZnMgSSe and QW layers that can be the factor of degradation, especially for the structures containing 20–30 QWs required for such lasers.

For reduction of this misfit it is possible to add S in the QW also. Low temperature cathodoluminescence of these structures reveals doubling of QW emission line that finally worsens characteristics of the laser. The reason of this doubling, apparently, is connected with peculiarities of QW formation, as is an object of the given research.

In this work, ZnSe/ZnMgSSe structures with one, two and three identical QWs are investigated by high resolution x-ray diffraction methods in standard and grazing geometries, and by reflectometry. Thickness of the QW layers was varied from 8 to 20 nm while thickness of top, barrier and bottom ZnMgSSe layers was identical in each structure, but varied from 26 to 170 nm in different structures. GaAs substrates were misoriented by 10° from a (001) plane to a (111)A plane. Thin ZnMgS layer was used as the buffer.

Interference fringes due to the structure period and total structure thickness are observed on x-ray reflectometry curves, but there are no any fringes from thickness of the barrier layers. This fact is explained by absence of any sharp interface between the QW and following ZnMgSSe barrier (top QW interface). The sharpness of the bottom QW interface is higher but worsens for the deeper QWs because of mutual diffusion of Mg and Zn. Two dimensional scans at symmetrical and asymmetrical reflections reveal diffuse scattering near substrate and barrier peaks. The intensity of this scattering increases with adding S in the QWs.

Based on simulation of the obtained results we conclude that composition of the barrier layers at the top QW interface is essentially nonuniform. Heterogeneity is connected with dependence of barrier composition on lattice parameters of the QW. At an initial stage of barrier growth, thin layer with smaller concentration S and Mg is formed in order to match its lattice parameter with QW one. Misorientation of growth substrate stimulates composition nonuniformity along the interface that leads to formation of structural defects and nonuniform strain distribution. These structural defects stimulate mutual diffusion of atoms and result in a partial relaxation of elastic strain. Elastic strained and relaxed parts of the QW layers radiate at different wavelengths.

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Tue-8.25po

Irradiation effects in CaF_2: ZnO nanostructured crystals

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Keywords: radiation effects, ZnO nanoparticles, optical properties, luminescence

Effects of β, X, UV and vacuum-ultraviolet (VUV) radiation were studied in CaF_2:

ZnO single crystals in which ZnO was imbedded as nanoparticles. Absorption measurements of these crystals showed a steep increase in optical density below 250 nm and a weak absorption peak at about 320 nm, while pure CaF_2 crystals are transparent from the near infrared to the vacuum ultraviolet (UV) region. After β irradiation at room temperature (RT), additional absorption bands were recorded at 395 and 595 nm. The irradiated samples showed during heating several thermoluminescence (TL) peaks. The main TL peaks appeared after VUV irradiation at the same temperatures and with the same thermal activation energies as after β irradiation, indicating that the same defect levels were excited by the different radiations. Samples which had previously been exposed to β-irradiation at RT and subsequently been illuminated at LNT with light in the 390 nm region, showed during heating to RT several TL peaks. No such TL could be excited by 390 nm light in CaF_2: ZnO samples that had not been previously irradiated by any ionizing radiation and this TL emission is therefore attributed to a process of photo-transferred TL (PTTL).Measurements of Photoluminescence (PL) showed main emission bands at 320 and 340 nm and excitation maxima near 250 and 300 nm. These emission bands were also observed during X-irradiation (XL) at RT as well as additional emission bands near 355 and 400 nm. The fact that some of the same emission bands appeared in the XL, PL, TL of this crystal indicates that the same luminescence centers are involved in these emissions. In pre-irradiated samples, luminescence could also be excited by wavelengths that could not excite any PL in non pre-irradiated samples and showed also an emission maximum at 320 nm with stimulation maxima at 395 and 468 nm. The 320 nm emission band is of higher energy than the excitation light and this emission is therefore attributed to a process of optical stimulation (OSL). This emission could not be excited by 395 nm light in pre-irradiated samples that were heated after irradiation to above 550°C. The stimulation maxima of the OSL and PTTL in the 390 nm region are apparently due to the observed absorption band at 395 nm induced by the β irradiation.

Tue-8.26po

Local and quasi-local electronic states in graphen with short-range defects

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Keywords: potential and mass perturbation, resonance

We consider in this work forming of the bound states of the 2 + 1 gapped and zero-gap Dirac equation due to the short-range perturbation. The pristine graphene is gapless, but violation of symmetry between the sublattices can induce opening of the gap. The symmetry violation can be triggered by the substrate or be developed dynamically.

Notice that "short-range" stands here for the lack of a long-range tail of the potential. At the same time, the perturbation radius remains finite that is equivalent to the large quasi-momentum cut-off. This cut-off makes the quasi-momentum space form-factors of the perturbation small enough for the quasi-momentum transfer of the order of the reciprocal lattice vector and, therefore, mixing of K and K' states can be done non-effective. Particular attention to the short-range perturbation case stems from the effectiveness of short-range scatterers in contrast to the long-range ones: an effect of the latter is suppressed by the Klein paradox [8]. Our work takes into account the obvious fact that the Kohn–Luttinger matrix elements of the short-range perturbation calculated on the upper and lower band wave functions are not equal in a general case. This means that in the perturbed Dirac equation not only the potential, but also the mass perturbation can be present. The characteristic equation for the bound and resonance states energy E was derived and analyzed both qualitatively and numerically. This allowed us to investigate all-important features of the electronic spectrum for various amplitudes of the potential and mass perturbation.

Tue-8.27po

Optical properties of PbI_2 quantum dot in a polyvinyl spirit solution under of hydrostatic pressure

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Keywords: experiment, modeling

Now the quantum dots (QDs) are the perspective material for optoelectronic devices.

We have investigated PbI_2 quantum dots embedded in a polyvinyl spirit solution [1]. This QDs have a layer structure with size of square 3×3 nm and thickness 1 nm. Pressure was created by the high pressure box. The box allowed to create pressure in a range from 0 to 30 Kbar and to carry out measurements of absorption spectrum at temperature 77–370 K [2].

At zero pressure the absorption line with half-width 0.5 eV is observed at 2504, 2750 and 3004 meV. According to the simple effective mass approximation this absorption line corresponds to a condition of weak confinement. It corresponds to exciton quantization as the whole.

At $T = 300-77$ K no-change in absorption spectra was revealed in the interval of pressure 0–30 Kbar. It is allows make a conclusion that contact besides microcrystals and a matrix no exist.

It could be suggested that one of reason of contact absent is defects of polymer-polyvinyl spirit matrix. This absence of contact besides QD and matrix corresponds to model of QD with infinite barrier. It results in energy dependence on $1/R^2$ deviates from linear behavior.

Acording to Efros, it is very important to take into account the presence of such contact in theoretical calculations. From calculations follows [4], dependence of transition energy from $1/R^2$ deviates from linear behavior at presence of contact for QDs with smaller sizes.

This experiment have shown absence of contact between crystals and a matrix. It can be important for the further specification of the theory.

Thus, our baric investigations are actual for calculation of levels structure.

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Tue-8.28po

Charge transfer through localized defect states with no change in on-site total spin and population

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Keywords: two-electrons correlations, two-electrons defects, spin-correlated transport

There has been considerable interest in the role played by deep level defects in charge transport through nanostructures. Tunneling transitions to and from localized defect states at surfaces and quantum contacts appear to occur by way of coherent two-charge-carrier quantum jumps. Much previous work has been done on the basis of constructing the amplitude of a coherent two-electron transition by combining single-electron transition amplitudes within perturbation theory. This perturbative procedure leads, however, to a significant reduction in the magnitude of resulting tunneling probabilities. In the present paper, another approach to two-electron or two-hole transition amplitude is proposed and developed within the narrow-energy-band model (or even in the pseudo-atomic limit) with correlation. In addition to well-known Hubbard-Anderson two-electron single-site correlation, this new model includes specific spin-spin double-site electron correlation between the defect and its nearest neighbors only. This allows one to derive an explicit expression for the quantum amplitudes for the most important simultaneous coherent two-carrier and even four-carrier tunneling transitions. It is demonstrated that two and more charge carriers can be transferred between lattice sites in a single correlated quantum process with no loss in the probability magnitude due to perturbative consideration. The presented model of extended two-electron correlation reveals a significant reduction of the on-site fluctuations in total spin projection and total number of electrons at the defect site, in comparison with the narrow-energy-band theory without correlation or with only single-site correlation. This phenomenon is interpreted as a correlation-induced partial conservation of the defect spin state during the transfer processes.

Tue-8.29po

Resonantly enhanced defect formation in single walled carbon nanotubes induced by soft X-ray illumination

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Keywords: carbon nanotubes, defect, soft X-ray spectroscopy, syncrotron radiation

Single walled carbon nanotubes (SWNTs) have unique electronic and physical properties that are strongly affected by their structures. Recent studies showed that the electronic transport and the electronic structures are significantly affected by the presence of defects [1–3].

We have investigated the defect formation in SWNTs induced by intense soft X-ray illumination in the C1s core-excitation energy range that was detected by X-ray absorption (XAS) and micro Raman scattering spectroscopy. The SWNT samples deposited onto Si substrates were illuminated with a 0th-order X-ray from a synchrotron radiation source for 1 hour. The efficiencies of defect generation were quantified by broadening of the C–C π^* peak at 285 eV and the degree of G/D ratio degradation in micro Raman spectroscopy. The illumination effects observed in these spectra were resonantly enhanced around 289 eV.

We also have investigated ionic desorption from SWNTs induced by soft X-ray illumination in the same energy range. The desorption efficiency spectra exhibit a similar resonant structure near C1s core absorption edge independent of ion species.

Plausible mechanisms for the defect formation are discussed, including the core exciton mechanism, a spectator Auger mechanism, and secondary-electron effects which might be the origin of the resonant nature of ion desorption efficiency.

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Tue-8.30po

Research of the intermediate layer from the firm solution on heteroborder nCdS/pCdTe

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Keywords: Heterotransitions, influence, i-layer, gradient

Results of research of disintegration of phases of firm solution CdS_xTe_{1-x} on structure border nCdS/pCdTe are resulted by a photo-electric method. It is shown that phases the structure and a thickness of intermediate layer CdS_xTe_{1-x}, strongly depends on selection of temperature of a substrate. Influence of ultrasonic influence on the properties, the given layer is investigated.

The structure x layer CdS_xTe_{1-x} depending on the substrate temperature, important $x = 0.68$ from outside CdS is defined. And $x = 0.13$ from outside CdTe. By research of element structure of an i-layer on heteroborder CdS/CdTe a method mikrozonds the analysis by means of installation “Komeka” it is shown that on heteroborder the maintenance of atoms S and Te sharply changes and there is a penetration of atoms S in CdTe and atoms Te in CdS on depth ~ 1 μm. Photosensitivity corresponding edges of fundamental absorption are defined. Depth of penetration of a field in the volume, depending on level, indemnifications, concentration of the deep centres, can exceed diffusion length and lead to increase in factor of collecting. Maintenance of continuity FS CdS_xTe_{1-x} on heteroborder creates favourable effect. The width of forbidden zone HS increases to the irradiated surface, the built in electric field caused by a gradient of width of forbidden zone E_g, leads no basic carriers of a charge from volume of films. Depth of penetration of a field in the volume, depending on level, indemnifications, concentration of the deep centres, can exceed diffusions length and lead to increase in factor of collecting. Recession of photosensitivity in short-wave area of a spectrum is defined by thickness of layer heterotransitions and energy of photons since which essential there is an absorption in n — a layer on a structure surface. To the vacuum chamber sedimentation CdTe on a substrate of molybdenum received a layer with the area 1 cm^2 and thickness 5 μm, heterotransitions nCdS/pCdTe were made by authors on technology [8]. Then without vacuum infringement at various temperatures of substrate Ts films CdS 0.4 μm were besieged by thickness. As the top contact on CdS served indiy, put in the form of a comb. The calculated values and a(x) for firm solution CdS_xTe_{1-x}, formed on heteroborder nCdS/pCdTe in a range of temperature of $Ts = 180{-}240$°C, lie between values $a(x)$ sulphide and cadmium telluride. The non-uniform intermediate layer caused by formation of met stable conditions firm solution CdS_xTe_{1-x}, on border firm solution, can be to break up under influence Ouse irradiations or at a heat.

Tue-8.31po

Influence *g*-irradiations on heterostructures nCdS/pCdTe

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Keywords: radiations, heterotransitions, acceptors

Other perspective direction of practical use of polycrystals CdTe creation on their basis of detectors rigid X-ray and g-radiations. Very much frequently heterostrukturs nCdS/pCdTe is used as solar elements, interest which it is connected by dearness silicon and arsenide gallium's analogues. It has been shown, that FS $\mathrm{CdTe}_{1-x}\mathrm{S}_x$ on heteroborder it is formed strongly non-uniform, it has been established, that a firm solution also non-uniform and on structure. It is known, that an irradiation g in quantum's generates dot defects on all nCdS/pCdTe heterostrukturs, but they are especially sensitive in the high-resistance, strongly compensated layers of a firm solution. Research of influence therefore is of interest g-irradiations on the $I-V$ the characteristic nCdS/pCdTe heterostructures. As the current in heterostructures nCdS/pCdTe is limited to resistance of thickness $\mathrm{CdTe}_{1-x}\mathrm{S}_x$. An irradiation g by quantum's Co^{60} it was carried out. it was spent, at temperature 500°C with the help of installation by capacity 1700 R/s and energy of quantum's $E \gg 1.2$ MeV.

For carrying out of research are made nCdS/pCdTe heterotransitions on the technology described in. The top contact on the part of which illumination is carried out, is made from india, raised dust in vacuum $\sim 10^{-5}$ torr as a comb. Resistance films are equal $\rho \approx 10^2 - 10^3$ Om cm, and thickness made $d \approx 70\,\mu$m. The sizes of grains are in limits from 100 up to 150 μm so grains cover all thickness of a film. Naturally the height of a potential barrier raises at a congestion additional charged acceptors the centers on border of the unit, for example, radiations stimuli - active negatively charged local acceptors the centers and she (it) goes down at a congestion active positively charged donor the local centers. Therefore concentration negatively charged recombination centers of acceptors type increases, and it causes reduction of time of a life and diffusion lengths of no basic carriers of a charge (holes), as occurs on experiment. And then with the further increase in a doze of an g-irradiation in quantum's concentration radiation's, negatively charged deep acceptor centers in a base layer of structure decreases, that causes increase value L_p and t the river.

Tue-8.32po

The mechanism of carrying over of a current of heterostructure nCdS-pCdTe with a transitive layer from a firm solution in the thickness $\sim 1\mu$m

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Keywords: firm solution, heteroborder, heterostructure, binary connections, geometrical capacity

Very often heterostructures n-CdS/p-CdTe are used as solar elements. Therefore the big attention is given to processing methods of creation of heterostructures n-CdS/p-CdTe and to studying of electronic processes in such structures. By authors of works it has been shown, that semiconductor binary connections CdS and CdTe, cooperating among themselves, form a firm solution $\mathrm{CdTe}_{1-x}\mathrm{S}_x$ with continuous change of maintenance CdS ($0 < x < 1$). After an establishment of possibility of formation firm solution $\mathrm{CdTe}_{1-x}\mathrm{S}_x$ on border of section of heterostructure n-CdS/p-CdTe intensive research of properties of this layer has begun. In works it has been shown, that $\mathrm{CdTe}_{1-x}\mathrm{S}_x$ on heteroborder it is formed strongly non-uniform, and in it has been established, that the firm solution is non-uniform and on structure. For achievement of the best efficiency heterostructure the firm solution should possess continuous structure at thickness $d < 1\mu$m, change from CdS to CdTe. It is the difficult technological problem connected with application of a heat. In the given work it is resulted results of researches on role revealing highly-Om layer firm solution $\mathrm{CdTe}_{1-x}\mathrm{S}_x$ by thickness $\approx 1\mu$m. In structure FS easily flying components atoms of cadmium are. Therefore in atoms of cadmium are easily formed one and two charge vacancies of atoms of cadmium, and components atom Cd_i. Two charge vacancies of atoms of cadmium in most cases form complexes with positively charged impurity of type $(\mathrm{V}^2_{\mathrm{Cd}}\,\mathrm{D}^+)^{-1}$ and with neutral between knot atoms of tellurium of types $(\mathrm{V}^2_{\mathrm{Cd}}\,\mathrm{D}^+)^{-2}$. These complexes are deep acceptors the centre. In structure FS are available as the donor Cl, In, Al, and acceptors impurity P, Li, Ag, Au, Cu. Atoms of silver (Ag), copper (Cu), gold (Au) give the deep acceptor centres. The investigated heterostructure works as p–i–n structure where a p-layer is CdTe, as a i-layer $\mathrm{CdTe}_{1-x}\mathrm{S}_x$, an n-layer CdS. It can, will prove as MDS structures as CdS a layer practical semimetal, is alloyed atom Indy (In) as it should be $\sim 10^{18}$ cm^{-3}. Really experimental $C-V$ curve removed on frequency $f = 1$ MHz at a room temperature shows the MDS structure characteristic. Concentration $P_o \approx 4 \cdot 10^{14}$ cm^{-3} on the size is very close to equilibrium concentration of holes of a base film p-CdTe, therefore it is used for construction of the settlement $C-V$ characteristic. An experimental $C-V$ characteristic lays to the right of the settlement $C-V$ characteristic. It means that in MDS-structure is available three type's dielectric which differs on geometrical capacity. In n-CdS/p-CdTe to structure a role dielectrics play FS $\mathrm{CdTe}_{1-x}\mathrm{S}_x$, forming on border of section of layers CdS and CdTe.

Tue-8.33po

Nanolayer structure of an element with reconstructed logic function for computers

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Keywords: thin film structures, logic elements, displacement, neyristors

As is known, the element base modern digital electrons-computers are based on logic elements which it is realized on semiconductor diodes, transistors, etc. Therefore since the third generation of electronic computers (COMPUTER) the basic efforts is directed on working out of improvement of technology for compact placing in particular logic elements on one crystal. Now, when the COMPUTER of the fourth generation with elements of the big integrated schemes (ENCORE) on the basis of thin semiconductor films the maintenance $\approx 10^5 - 10^6$ widely uses Elements on one crystal, it is developed the fifth generations of the COMPUTER on the basis of the super big integrated schemes.

At the decision of such problem the density of integration of microcircuits undoubtedly increases on some ($\approx 10^5$) usages in comparison with the ENCORE. In the present work some experimental results found out for the first time rather to data of world references till today are presented.

Thin film structures CdTe–Al of 40–80 nanometers received in vacuum 10^{-4} torr in kvazi the closed volume are investigated by thickness. The investigated structures have "N" figurative the $I-V$ characteristic. However unlike diodes Hannah who has the same characteristic at positive V_{cm} in the first quadrant two-dimensional Cartesian system, and passes through "0" coordinate axes, "N" the figurative characteristic of the investigated structures covers I, II, III quadrants. The further increase at V_{am} leads to sharp growth of a current through structure which reaches to 5000 μkA. The found out properties nanolayer structure in the form of thin film CdTe–Al opens new possibilities by working out of base logic elements for digital computers.

That if to the integrated scheme one logic element is capable to carry out all basic logic functions as NOT, And, OR and their combinations, undoubtedly density of packing of elements increases.

We spend an example use of the mentioned characteristic for realization of some logic operations.

Apparently from the resulted dependence $I-V$ characteristic the investigated structure pressure of displacement V_0, -V_4, -V_5, V_6 for an element and, and V_{cm}: -V_3, -V_1 for an element OR with a negative input, $+V_7 + V_9 + V_{11}$ with a positive input; and forlements with a double input or with a threefold input accordingly, i.e.

2 OR, 3 OR. It is necessary to pay attention to this fact, that all mentioned logic operations: NOT, And, OR it is possible to realize on one element executed in a kind nanostructures. For example the structure in the beginning can function as a logic element and, then as inversion, further as a logic element OR for performance of such logic functions usually it is required, at least, at separate discrete elements. At use for a structure food by bipolar saw tooth pressure with higher frequency the density of packing of elements increases at the expense of minimizations of the $I-V$ characteristic.

Tue-8.34po

Lattice dislocation in Si nanowires

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Keywords: Si nanowire, crystal structure, dislocation, Gruneisen parameter, nanowire layers

The dislocation of lattices were calculated for Si nanowires having diameters of 115, 56, 37 and 22 nm from the data of lattice thermal conductivity, Gruneisen parameter, lattice thermal expansion, bulk modulus and specific heat.

Lattice thermal conductivity for Si nanowires were calculated by using the Debye-Callaway model through the method of trial and error on fitting the calculated date to that of the experimental curve. While a standard formula were used to calculate each of lattice thermal expansion, specific heat and Bulk modulus for the four Si nanowire diameters above. From these results, mean lattice volumes were found to be as 20.03 $Å^3$ for the bulk and 23.63, 29.91, 34.69 and 40.46 $Å^3$ for Si nanowire diameters mentioned above respectively. The mean bonding length was calculated to be as 0.235 nm for the bulk and 0.248, 0.269, 0.282 and 0.297 nm for the nanowires diameter mentioned above respectively. By dividing the nanowires diameter on the mean bonding length, number of layers per each nanowire size were calculated and found to be as 230, 104, 65 and 37 for the diameters mentioned above respectively. However if the structure of central wire has properties belongs to the bulk then it's mean bonding length will be 0.235 nm while the nanowire surface layer which is a size dependent properties were calculated and found to be as 0.2616, 0.3025, 0.3294 and 0.3592 nm for the above wires diameter respectively. Then from the numbers of layers and values for both central and surface mean bonding length with the dependence on the diameter dependence Gruneisen parameter, the bonding length were calculated for each of the layers for the nanowires interested in this work. These layers found to be increases systematically beginning from the central nanowire to that of the surface layer and that found to be also a nanowire diameter dependent which gave an empirical relation.

Tue-8.35po

ZnO Nanocrystals/SiO_2 multilayer structures fabricated using RF-magnetron sputtering

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Keywords: nanocrystals, zinc oxide, interface defects

Zinc oxide (ZnO) is currently a popular semiconductor material; one of the reasons is its potential as a base material for optoelectronic devices operating in the UV spectral region. Compared to other semiconductors, ZnO has a large exciton binding energy, which leads to strong excitonic emission in a wide temperature range. However, the luminescent properties of the excitonic emission in nanocrystalline ZnO depends strongly on nanocrystal size, due to quantum confinement effects, and on surface defects. Despite the plethora of papers on nanocrystalline ZnO published during the last years, only a limited number of reports have appeared which deal with the fabrication of high-quality ZnO nanocrystals with highly efficient and predictable luminescent properties.

In the present study ZnO nanocrystals embedded in a SiO_2 matrix were successfully produced by means of radio frequency magnetron sputtering deposition. Multilayer structures consisting of 10–15 ZnO/SiO_2 bilayers were deposited on Si substrate wafers using ZnO and SiO_2 sputtering targets. The samples were grown either in vacuum or in an oxygen ambient. Subsequently, the structures were heat-treated at different temperatures and in different atmospheres. The size and size distribution of the ZnO nanocrystals were controlled by transmission electron microscopy. Stoichiometry and multilayer profiles were characterized by means of secondary ion mass spectroscopy and Rutherford backscattering techniques. The crystalline structures and lattice constant of the ZnO nanocrystals were determined using X-ray diffraction analysis. Photoluminescence properties of ZnO nanocrystals were studied by means of steady-state luminescence spectroscopy under excitation in the blue-UV spectral range. It is found that intensities, shapes and positions of excitonic emission peaks from ZnO nanocrystals can be distinguished from those from for the bulk material. Correlations between the luminescence properties of the ZnO nanocrystals and the synthesis parameters will be demonstrated in detail. The role of surface defects for the luminescence properties of nanocrystalline ZnO will be discussed.

Tue-8.36po

Optical studies of A^{+}-centers in GaAs/AlGaAs quantum wells. Energy structure of the isolated centers, and their collective behavior.

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Keywords: charged defects, quantum wells, GaAs

In our report we present a systematic study of the positively charged acceptors (known as A^{+}-centers) in GaAs/AlGaAs quantum wells. The A^{+}-center is a neutral acceptor that has captured an extra hole, and it is similar to the negative hydrogen ion H^{-}. We have used a zero radius potential model to describe a hole captured on a neutral acceptor. In article [1] this model was used to calculate an energy structure of the A^{+}-center, the expressions for the wave functions of the outer hole in dependence on quantum well width being obtained. According to the results of the calculation, this hole has two states splitted by the quantum well potential: the ground state with spin $3/2$ and the excited state with spin $1/2$. To test the theoretical model the GaAs/AlGaAs samples with 15–18 nm width quantum wells, selectively doped both in wells and in barriers, were studied. This doping makes the holes go down from the barrier acceptors to the wells, and localize on the neutral acceptors in quantum wells at low temperatures, producing the thermal equilibrium A^{+}-centers.

In photoluminescence spectra of the samples with such a doping geometry a line of radiative recombination of free electrons with A^{+}-center outer holes prevails at low temperatures. Other photoluminescence lines are suppressed, because the photocapture cross-section of the attractive coulomb centers is by 2–3 orders of magnitude bigger than the cross-sections of the other radiative processes. The excited $1/2$ state of the A^{+}-center is by approx. 2 meV higher than its ground $3/2$ state at liquid helium temperature and is not occupied at equilibrium. However at the pump light intensity increase this line appears in photoluminescence spectra due to the “phonon bottleneck effect”. This effect occurs as the time of relaxation from the excited to the ground states of A^{+}-centers is greater than the time of photo-capture on the charged attractive center.

To analyze experimentally the fine structure of A^{+}-center a degree of circular polarization of the photoluminescence depending on the magnetic field applied perpendicularly to the quantum well plane have been studied, as well as a degree of the linear polarization of photoluminescence depending on the uniaxial pressure applied in the plane of the quantum well. The results obtained under pressure and in the magnetic field show unambiguously that the higher energy line in A^{+} spectra corresponds to the recombination of the light hole, while the lower energy line that of the heavy one.

Tue-8.37po

Non-linear optical response of metal-nanocluster composites prepared by the method of dynamic ion mixing of polymers

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Keywords: ion mixing, polymers, metal nanoparticles, non-linear optical properties

Metal nanocluster composites (MNCs) based on polymers are promising for future ultra-fast optical devices, electronics and biomedical applications. Heavy-ion implantation of polymers is a powerful tool for fabrication of MNCs. However, high kinetic-energy ions striking the surface of polymer target are slowed down by electronic and nuclear stopping mechanisms, resulting in chain scission, cross-linking, bond disruption, formation of free radicals and so on. Ablation and sputtering processes may also cause considerable damage of polymer surfaces. Consequently, the controllability of metal precipitation and the damage resistance of polymer substrates dominate the applicability of ion implantation for fabricating MNC in polymers. Aimed at diminishing the effects of sputtering and damage on MNC, we developed a method of dynamic negative ion mixing (DNIM) for polymers. We found that the method of DNIM is suitable for fabrication of the polymer-based MNCs with an improved ultra-fast non-linear optical response.

Ion mixing methods mostly employ light-ion bombardment and excess point defects enhance non-equilibrium diffusion of surfaces or interfaces of a material. We employed intense negative Cu or Ag ions of 60 keV to introduce mass precipitation, as well as vacuum evaporation of the polyethylene (PE) matrix. PE was deposited on a silica glass substrate in a vacuum chamber, and simultaneously negative ions were implanted into the deposited film. Silica glass substrate used for DNIM worked as an efficient heat sink: it enabled us to conduct DNIM at ion fluxes as high as 10 mA/cm^2, though fluxes lower than 3 mA/cm^2 were allowable for ordinary ion implantation of PE. Excellent transparency of the substrate was also important, for further non-linear optical measurements.

Optical absorption spectra of MNCs fabricated by the DNIM method consisted of a peak of surface-plasmon resonance (SPR) of metal nanoparticles and a wide band of color centers induced in polymer by irradiation. The SPR peak emerged at around 2.2 eV and 3.1 eV for Cu- and Ag-implanted specimens respectively. The SPR peaks were much more pronounced than those observed after ordinary Cu- or Ag-ion implantation of PE. In particular, strong SPR peaks were observed at effective ion fluences below $6e^{16} \times$ ions/cm^2 for DNIM, whereas they were hardly distinguishable at $1e^{17} \times$ ions/cm^2 for ion-implanted polymers. Defect absorption, which usually dominates the optical spectra after ordinary ion implantation, was not strong for DNIM-samples.

Measurements of negative non-linear optical absorption (transient bleaching) of MNCs obtained by DNIM were carried out by the Z-scan method with a laser pulse of $<$ 200 fs, repetition rate of 1 kHz, photon energy from 1.9 to 4 eV and intensity up to 200 GW/cm^2 at the laser beam waist. The non-linear optical response consisted of contributions from (a) metal nanoparticles and, possibly, (b) a polymer matrix. The contribution, which was tentatively ascribed to polymer, was observed in the range from 1.9 to 2.5 eV for Ag-ion-implanted specimens. For Cu-ion-implanted ones, the contribution from the polymer matrix superimposed with that from Cu nanoparticles, in the range of SPR.

Tue-8.38po

Kinetics of reverse resistance recovery of silicon diodes with different distance between metallurgical pn-junction and the defect layer formed by krypton implantation

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Keywords: ion irradiation, carrier lifetime, reverse resistance recovery time

The implantation of light ions (hydrogen and helium with the energy of about the unities of MeV) is used to optimize the reverse resistance recovery time and direct voltage drop in fast-operating diodes [1]. As it shown in the work [2] irradiation with heavy ions possessing the energy of about the hundreds of MeV allows to achieve similar results and provides the principal possibility to control the distribution of irradiation-induced defects in the plane parallel to pn-junction [3]. However the question about the optimal arrangement (occurrence depth relative to pn-junction) of the defect layer introduced by implantation of heavy ions requires additional investigations.

The diodes under study were fabricated on the uniformly phosphorus doped silicon (111) wafers with resistivity of 90 Ohm·cm. The change in the distance between pn-junction and the defect layer formed by krypton ion implantation was achieved by variation of the depth of pn-junction occurrence and the thickness of aluminum layer on the contact to heavily doped p-region. Manufactured diodes were implanted from the side of p-region with krypton ions (energy 250 MeV, fluence from 10^8 to 10^9 cm^{-2}). According to the simulation results in the TRIM program the distance between metallurgical boundary of the abrupt asymmetric pn-junction (defined disregarding the compensation of n-Si by irradiation-induced defects) and the maximum of distribution of primary vacancies for the two groups of examined diodes was amounted of 25.7 μm (group 1) and 13.9 μm (group 2).

It has been established that in the transient process of diode switching along with the phase of high reverse conductance and the phase of reverse resistance recovery an additional phase is observed. During this phase the holes injected beyond the bounds of irradiation damaged silicon layer are vanishing. The duration of high reverse conductance phase is practically the same for both groups of diodes. The duration of reverse resistance recovery phase is longer in the case of the closely spaced pn-junction and the layer of irradiation defects in the n-region.

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Tue-8.39po

The investigation of the structural and electrophysical properties of carbon nanotubes with controlled dopant and defect composition

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Keywords: carbon nanotubes, structural defects

The carbon nanotubes (CNT) layers are the nanostructured material with unique electric properties which able to change their electrophysical characteristics at adsorption and desorption of chemical reagents. This property of CNT lets us to use them as sensing element in gas sensors. The CNT layers may be synthesized on the Si–SiO_2 substrates in the ordinary silicon technology, so one can create the integrated microsensors. The doping of CNT (by N, B, F etc.) changes the electronic properties of the nanotubes. Particular the doping by N (1...2 %) leads to increasing of semiconducting phase in the CNT layers [1]. The CNT layers containing a large amount of metallic and semiconducting phases are suitable to use in resistor-type gas microsensors.

The structures on the basis of carbon nanotubes (CNT) produced by thermal decomposition of acetonitrile on the Si–SiO_2 substrates and metal layers are investigated by SEM, AFM, STM, XRD, Raman scattering. The CNT layers grown on the silicon oxide with volumetric catalyst (Fe) show predominantly perpendicular to substrate growth of the nanotubes. In the area of the metallic layers (Ni catalyst film and buried metal layer) the CNT bundles parallel to substrate form with graphite and amorphous carbon. The activation character of the temperature dependence of the conductivity of the CNT layer is observed and discussed.

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Tue-8.40po

Binding energy of magnetoexitons bound to donor impurities in GaAs/Al$_x$Ga$_{1-x}$ quantum wells

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Keywords: magnetoexcitons, impurities, quantum wells

Excitons bound to impurities or imperfections have been study for a long time, first in bulk semiconductors and lately in low dimensional systems both theoretically and experimentally [1–4]. The magnetic field has been one of the best proves to find how the new energy channels originated by this interaction behave in low dimensional systems. Despite there have been several efforts to understand this fact, there are not conclusive results on this subject. In this direction we investigate the binding energy of Wannier's excitons bound to donor impurities in GaAs/Al$_x$Ga$_{1-x}$As quantum-wells, using the effective mass approximation within a variational approach. Our calculations are performed as a function of the barrier height, the well width and the concentration of impurities. We have considered the magnetic field applied in the growth direction. We compare the binding energies of light- and heavy-hole magnetoexcitons bound to impurities with previous experimental reports.

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Tue-8.41po

Spin-dependent recombination of defects in bulk ZnO crystals and ZnO nanocrystals as studied by optically detected magnetic resonance

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Keywords: nanocrystals, ODMR, defects, recombination, afterglow

ZnO is a direct wide-band-gap semiconductor (energy gap of 3.35 eV at room temperature) and crystallizes in the wurtzite structure. Since it is a strong emitter, it attracts considerable attention for applications as ultraviolet (UV) light-emitting diodes and laser diodes. The confinement of the electronic wave function in ZnO nanocrystals allows the tuning of the optical and electronic properties. In the present note, we report on the optically detected magnetic resonance (ODMR) study of spin-dependent recombination of defects, which gives rise to the long-lasting afterglow in ZnO nanocrystals and ZnO:Li bulk crystals. These results are compared with the photoluminescence-detected ODMR and allowed to identify the recombining defects.

Two types of samples were studied: (i) dry powder of both undoped and Al doped ZnO nanocrystals, 3 to 6 nm in size, obtained by colloidal chemistry methods and (ii) ZnO:Li bulk crystals grown by a vapour phase method and doped with Li during growth. ODMR experiments were carried out at 2 K on a home-built ODMR spectrometer operating at 35 GHz and 94 GHz.

Long-lasting afterglow (up to 3 hours) was observed in ZnO nanocrystals after switching off the UV excitation. A quenching of the afterglow intensity in magnetic field at low temperatures was found, which appears because of the preferential orientation of the recombining spins along the field. ODMR was detected as resonance increase in the afterglow intensity at EPR of defects, which take part in the recombination. Shallow donors and different types of acceptors were identified. In ZnO:Al nanocrystals, ODMR signals of Zn-vacancy acceptors and Na acceptors were resolved in 94 GHz ODMR spectra due to the increased resolution. A g-factor shift of shallow donors relative to the shallow donor g-factor in bulk ZnO appears because of spatial confinement effects. It should be pointed out that observation of ODMR via the afterglow in UV-irradiated ZnO nanocrystals provides a simple way to characterize the nanocrystal size using the experimental size dependence of g-factor measured by high frequency EPR. In bulk ZnO:Li crystals, ODMR of donors and Li acceptors was recorded via the afterglow which could last for about an hour. In photoluminescence-detected ODMR spectra exchange-coupled DA pairs were observed in addition to the Li acceptor and donor signals. Exchange-coupled pairs dominated the ODMR spectra recorded on the photoluminescence of ZnO nanocrystals.

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Tue-8.42po

Connection between electronic properties of ZnO defects and the low power threshold of the optical non-linearity in inverted opals

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Keywords: ZnO defects, emission, oxygen chemosorption

Photonic crystals are designed for efficient light transformation due to strong light-to-matter interaction. However, initiating the non-linear optical behaviour of photonic crystals, such as photonic bandgap (PBG) switching or lasing, still requires very heavy optical pumping.

We prepared the inverted ZnO opals templated in thin opal films by low-temperature atomic layer deposition of ZnO. After removing the opal spheres, the remaining 2.2:1 value of the refractive index contrast ensures strong light confinement and high bandgap sensitivity to minute changes in the refractive index. We discuss two effects, for appearance of which the low pumping power threshold is facilitated by the electronic properties of ZnO defects.

Under continuous wave ultraviolet pumping, the photo-induced chemodesorption of oxygen from the ZnO surface leads to the decrease of the material polarisability. The corresponding 40% relative shift of the transmission at the photonic bandgap edge occurs. This effect was achieved at 3 W/cm^2 pumping, whereas the similar magnitude of the bandgap shift due to photogenerated free carriers requires gigawatt/cm^2 pumping. However, the speed of the PBG recover is limited by the diffusion of the oxygen in nanopores of the inverted opal, i.e., the process requires hundreds of milliseconds to complete versus femtosecond-range recovery time inherited to the electronic mechanism.

In photoexcited ZnO inverted opals the broadband green emission of ZnO defects is centred at 2.35 eV. Due to fast non-radiative relaxation of photoexcitations from the conduction to the defect band, the long radiative lifetime of excitations in the defect band and the limited capacity of the defect band with respect to the density of excitations, the emission from ZnO defects becomes very sensitive to the environment. In such tree-level light emitting scheme, the positive feedback provided by distributed Bragg resonance at opal lattice results in strong emission modification at very low optical pumping, moreover, only 10 lattice periods in this high contrast grating form the effective resonator. As a result, the threshold needed for spontaneous emission amplification becomes as low as 1 W/cm^2. This value is 100-1000 times lower than the threshold, which is necessary to achieve the amplification of the bandedge luminescence in the ZnO inverted opal, if the PBG is tuned to the ZnO excition band. The diffractive nature of the feedback was proved by observation of the similar angle dispersion for the emission and PBG bands.

Tue-8.43po

Effects of impurity charge occupation in silicon single electron transistors

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Keywords: heavily doped silicon, single electron transistors, charge localization, spatial Rabi oscillations

We investigate the effect of DC bias and high frequency radiation on heavily doped Si-based single electron transistors measured at cryogenic temperature. We observe typical Coulomb Blockade features (i.e. non-linear $I-V$ characteristic and Coulomb oscillations) although there is no inclusion of deliberately engineered tunnel barriers in the nanostructure and the doping density is sufficient to expect metallic behavior. Furthermore, by applying microwave radiation, we find changes in the device current that take the form of resonances [1], as the frequency is swept. These resonances include positive and negative going features and their amplitude does not increase monotonically with power. In order to explain the device behavior both at DC and under irradiation, the effect of charge traps at the Si–SiO$_2$ interface and the probability of occupation of single donors (phosphorus) in the n-type silicon by an electron must be taken into account.

A high density of traps at the sidewalls [2] is expected due to the fabrication method employed [1]. Wherever the width between sidewalls scales down to few tens of nm, the depletion of free carriers leads to the formation of tunnel barriers with resistance much greater than the resistance quantum. This effect is also seen to be enhanced by the application of an external DC electric field which can force more electrons into traps. This explains the observed Coulomb Blockade-based behaviour at DC.

Depletion of charges and random distribution of dopants cause electrons localization at donor sites; this results in transport taking place as variable range hopping between impurity sites via tunnelling events [3, 4]. An externally applied AC electromagnetic field resonant with the energy separation between two sites can lead to spatial Rabi oscillations [5] which modify the impurity occupation densities by inducing charge delocalization. This is consistent with the observed spectroscopic features and the non-linear dependence on high frequency excitation power.

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Tue-8.44po

Optical quenching of photoconductivity in Al$_x$Ga$_{1-x}$N/GaN epilayers

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Despite impressive progress in GaN-based devices, the physical properties of various impurities and native defects in GaN and related compounds are still far from being fully understood. Defects acting as deep recombination centers are cited as possible causes of slow relaxation processes in these materials. Also, quenching of photoconductivity has been reported in several materials including GaN [1–2]. Hence, it appears that a basic understanding of deep defects and their complex recharging kinetics resulting in persistent, metastable, and quenching effects is essential both from the point of view of fundamental research and device application.

In this work we report results from photocurrent measurements on MOCVD-grown Al$_x$Ga$_{1-x}$N materials. Using a UV background illumination along with a secondary below-bandgap illumination with variable wavelength the optical quenching of photoconductivity has been investigated. We observe a quenching of the photocurrent for a range of wavelengths of the secondary light beam. It was found that the intensity of the background illumination and the temperature of the sample affect the magnitude of the optical quenching. Furthermore, measurements of the spectral distribution of the quenching effect indicate the existence of multiple hole traps located in the range between Ev and Ev+1.25 eV which are believed to be responsible for the optical quenching.

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Tue-8.45po

Multiparticle electron-hole complexes localized on quantum wire lateral dimensions fluctuation

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Keywords: quantum wire, ecxiton, trion

Experimental and theoretical studies of the bound states of the electron-hole complexes in semiconductor quantum wires (QWRs) are of significant interest [1–3]. It is known that experimentally determined values of trions (three particle complexes) binding energies can exceed significantly the theoretical predictions [1]. This effect can be attributed to localization of the charge carriers on fluctuations of the QWRs lateral dimensions as it happens in quantum wells [4]. Our goal is to describe the localization of electron-hole complexes on QWR fluctuations in much the same way as it had been done in our work [5] for 2D systems with lateral inhomogeneity, by using variational functions with a small number of trial parameters.

We assume QWRs to be quasi-1D and describe the Coulomb interaction between the charge carriers by widely used soft-core potential: $V_{\text{eff}} \sim (a^2 + z^2)^{1/2}$, where z is the relative coordinate and a is the effective QWR radius. We characterize the interaction of electrons and holes with a fluctuation by independent single-particle attractive 1D potentials for electrons and holes. One can separate only two qualitatively different limiting cases, where electron-hole complex Schroedinger equation can be reduced to several independent equations with smaller number of variables [5]. In the first case the fluctuation potential is weak compared to the Coulomb interaction and the complex wavefunction reduces to the product of the center-of-mass function and the wavefunction depending on the relative coordinates. In the limit, where fluctuation potential is strong for at least one type of particles, the whole wavefunction can be recast as a product of wavefunctions of electron and hole subsystems.

We represent the following trial function for localized 1D electron-hole complex: $Psi = [\Psi^{C.M}]^{\alpha R}[\Psi^{int}]^{\alpha\rho}[\Phi^{e}]^{\alpha e}[\Phi^{h}]^{\alpha h}$. Here $\Psi^{C.M.}$ is the wavefunction of the complex center of masses, Ψ^{int} is the function of carriers relative motion in a free 1D complex, $\Phi^{e(h)}$ is the wavefunction of the ground state of electrons (holes) in the sum of the fluctuation potential and the averaged effective Coulomb potential of the holes (electrons), α_R, α_ρ, α_e, α_h are the trial parameters, see Ref. [5] for details. The general form of our trial function is independent of the specific form of the fluctuation. To illustrate our approach, we consider the case of 1D exciton, X^+ and X^-trions localized on the parabolic fluctuation. We demonstrate that the strong increase of trion binding energies can be achieved by the localization of electron-hole complexes on quantum wire fluctuations with realistic parameters.

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Tue-8.46po

Two channels of non-radiative recombination in InGaN/GaN LEDs

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The non-radiative carrier recombination in InGaN/GaN blue Light Emitting Diodes (LEDs) with multiple quantum well (MQW) is studied extensively for more than ten years. However the relative role of point defects and extended defect system in quantum efficiency (QE) restriction of these diodes has not yet been clarified until now.

The aim of this paper is to clarify the contribution of point defects and the extended defect system in non-radiative recombination process in InGaN/GaN LEDs.

Integrated studies including measurements of current low frequency noise (CLFN) in the range from 10 Hz to 10 kHz of I-V characteristics over the range 10 mV–5 V forward bias V and 10^{-12}–1 A forward current I of current and QE(I) temperature dependencies were carried out with the set of InGaN/GaN LEDs with different active region design and different values of maximum (QE) from 16% to 37%.

The following regularities were established for all structures studied independently on the width and height of the potential barriers the number of quantum wells and on the structure design:

i) At relatively small current densities $j \leq 1$ A/cm^2 the main contribution to the total current comes from the tunneling assistance current which depends weakly on the temperature. In this region of j the CLFN increases heavily with j growth.

ii) In the range of 1 A/cm$^2 \leq j \leq 10$ A/cm^2 which corresponds to maximum QE values the main contribution to the total current comes from the Shockley-Read recombination current. The strong temperature dependence of current and relatively weak CLFN dependence on j is very characteristic for this region of j.

The results obtained can be apparently related with the filling of trap levels located close to the bottom of conduction and top of valence bands. The presence of such traps correlates with Albrext's model of dislocation in GaN.

One can assume that there are two non-radiative recombination channels in LEDs under study. One of them is related to the extended defect system piercing the LED active region. Its influence on QE is indirect and consists mainly in electric field redistribution in the active region. This recombination channel acts "active shunts" which changes their parameters under the current injection. The other non-radiative recombination channel is caused by presence of point defects. This channel is especially effective in the range 1–10 A/cm^2 corresponding to the maximum QE values.

Tue-8.47po

Effect of impurity potential range on a scaling behavior in the quantum Hall regime

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Keywords: Quantum Hall effect, impurity potential

The quantum Hall effect (QHE) regime may be regarded as a sequence of quantum phase insulator–metal–insulator transitions when the density of states of 2D system in quantizing magnetic fields is scanned by the Fermi energy. In the theoretical framework of scaling [1] as the temperature approaches zero the width of the transition regions between adjacent QHE plateaus δB should go to zero as T$^{\kappa}$ with the critical index $\kappa = 0.43$. We have analyzed magnetoresistance data in transition region between the first and second QHE plateaux in n-In$_x$Ga$_{1-x}$As/GaAs and p-Ge/Ge$_{1-x}$Si$_x$ samples.

The dominant contribution to disorder for investigated InGaAs/GaAs samples is of short-range character: an alloy scattering in solid solution InGaAs. For n-InGaAs/GaAs heterostructure we see a rather good power-law scaling in the temperature range from 0.4 K to 4.2 K with a critical exponent $\kappa = 0.48 \pm 0.04$.

For p-Ge/Ge$_{1-x}$Si$_x$ heterostructures with long-range impurity potential (a scattering on remote impurities at GeSi barriers) the data cannot be satisfactorily described by a scaling law but they are much more compatible with a linear dependence $\delta B = \alpha T + \beta$ for finite β. The answer on the question about the finite $T \to 0$ widths of QHE transitions may be found in the works treating the influence of Coulomb interactions on the screening of smooth disorder potential [2].

Thus, qualitatively different temperature dependences of QHE transition width are observed for heterostructures with short-range or smooth impurity potential. As the real scaling behavior, with exponent κ close to the theoretical value, has been observed at the former, the semiclassical in nature linear temperature dependence of $\delta B(T)$ takes place at the latter.

Our results are in accordance with conclusions of Ref. [3] that the dominant scattering mechanism of electrons should be of a short-range character in order to experimentally observe the true low-temperature asymptotic behavior for the quantum phase transition — the scaling behavior of $\delta B(T)$.

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Tue-8.48po

Hybrid-impurities resonances in quantum dots

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Keywords: quantum dot, ionized impurity

Optical electron transitions in quantum dots (QD) are widely studied [1] since QDs can be used in new or improved optoelectronic devices [2], such as QDs lasers or infrared photodetectors [3]. What is more, the investigation of the intraband optical transitions offers an efficient method for studying many fundamental physical phenomena.

QDs support several types of intraband resonances. The hybrid and hybrid-phonon resonances in parabolic anisotropic quantum dots were studied in our preceding papers [4, 5]. However, it is important to investigate the influence of the impurity scattering on the absorption because these processes can modify the selection rules in the optical transitions and lead to losses in optical devices based on QDs. The study of these processes is crucial for the development of technology of QDs production.

Modern nanotechnology enables one to fabricate QDs of different shapes. In the past years the significant interest has been given to semiconductor quantum wells and QDs that are characterized by an asymmetric confining potential [6].

In this theoretical report we study optical electron transitions in quantum dots taking into account the processes associated with simultaneous scattering from ionized impurities. We consider anisotropic dots placed in a magnetic field arbitrarily directed with respect to the potential symmetry axes of the QD. We have obtained simple analytic formulae for absorption coefficient of a high-frequency electromagnetic field. We have shown that the scattering of electrons by impurities leads to the resonance absorption. The positions of the resonances peaks are found. The dependences of absorption on the position of the impurities, the shape of a dot, the frequency of the electromagnetic radiation and the magnetic field are studied. We have shown that changing the magnitude of the magnetic field we can strongly decrease losses of electromagnetic radiation in the QDs. What is more, the analysis of the experimental dependence of the absorption on the magnetic field can be effective instrument to determine the degree of anisotropy of QDs.

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Tue-8.49po

The association of halogen radiation defects in alkali halide crystals (AHC) symmetry lowering by point defects and elastic stress

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Keywords: alkali halide crystals, elastic stress, radiation defect

The creation process of the initial radiation defects in alkali halide crystals (AHC) is well studied; the main cause of the process is nonradiative annihilation of self trapped electronic excitations [1]. It is known that thermally stable radiation defects in AHC are resulted from the interaction between interstitial halogen atoms in regular lattice sites. However, this interaction efficiency is very low because the lattice transformation is required with emission of both cation and anion.

The present work offers experimental reaction facilitation techniques of interstitial halogen atoms' interaction in the field of cation-homologs of minor radius and vacancy defects by elastic stress.

A unique pattern was experimentally created in KCl-Na, KCl-Li and KCl-Sr crystals activated by one univalent cation-homologs of minor radius (Na, Li), and bivalent cation (Sr); it allows cation site gradual emission-Na; it serves as a base for efficient association of two H-centres with transformation to thermally stable-centres.

According to the experimental results the elastic stress in crystals creates mainly divacances [2, 3]. In this case not only cation site emits but also anion site does, it results in maximum facilitation of two H-centre interaction with transformation to -centres because their association takes place in the field of divacancies.

Elastic low temperature (80 K) stress in KCl and KBr crystals leads to the redistribution of halogen radiation defects between the -and -centre bands without efficiency change of F-centre creation by radiation, and in KI and RbI crystals — to the creation efficiency decrease of both- centres and F-centres.

At AHC lattice symmetry lowering by point defects the efficiency of -centre creation increases, and at low temperature elastic stress - sharply decreases (KI, RbI). The reason of this phenomenon could be connected with either probability reduction of exciton decay to F, H-pairs, or the probability reduction of the H-centre association in the field of elastic stress [2].

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Tue-8.50po

Deep-level transient spectroscopy studies of light emitting diodes (LEDs) based on multiple quantum well (MQW) InGaN/GaN structure

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Keywords: LED InGaN/GaN, superlattice, multiple quantum wells, DLTS, C-V

In the present work we report the investigation by means of capacitance-voltage ($C - V$) and deep level transient spectroscopy (DLTS) of electron and hole emission from the states of MQW in p–n InGaN/GaN heterostructure in relation to the amplitudes of the recording voltage pulse U_b and filling voltage pulse U_f. The MQW InGaN/GaN structures studied in this work were grown by metalorganic chemical vapor deposition under standard conditions. According to the wafers manufacturer the structure consisted of an n$^+$-GaN, a five period superlattice (SL) of GaN/InGaN (2 nm/3 nm), and a p$^+$-GaN contact layer. From the $C-V$ data, we determined the regions of bias voltages, so that the signals associated with the emission of carriers from the states of SL should be observable in the DLTS spectra. These measurements have shown that, when recording the DLTS signal at $U_b = 0$, the SL lie in the space-charge region. Thus, when performing DLTS measurements, it appears to be necessary to investigate electron emission from QWs, varying the amplitudes of U_b and U_f in the range of positive values. For this structure we measured $I-V$ curves, which showed that values of the current (≈1E-12, A) very slightly dependent on voltages in the range up to 2.3 V. We observed three DLTS peaks (E1, E2 and H1) related to the emission of electrons and holes accumulated at states of SL. For identifying the origin of the levels responsible for these DLTS peaks, we studies how the DLTS spectra depended on conditions of preliminary isochronous annealing both under application of and without a bias voltage ($U_b = 0$). For all DLTS peaks were observed a strong shift in the position of the DLTS peaks toward higher temperatures and change of their amplitudes in the case of annealing with $U_b = 0$, which is due to a shift of the quasi-Fermi level for electrons and holes resulting from recharging of deep-level defects in the GaN layer. This effect is attributed to the emission of carriers from the localized states in SL. The shift in the position of the DLTS peaks is due to the built-in piezoelectric field bringing to spatial separation of the electron and hole ground-state wave functions and defined as manifestation the quantum confined Stark effect for SL. The spatial separation of injected carriers induces electrostatic potential screening the piezoelectric field. Profiles of the surface density of electrons and holes trapped on the states of the SL have shown their localization with maximum shifted one another. It is found that the positions of the maxima for all of the three DLTS peaks depend on of the bias pulse voltage applied to the sample in the DLTS measurements and U_f. It is believed that changes are determined by a localization of the electron wave functions in one QW which is called Wannier-Stark localization.

Tue-8.51po

Optical absorption and photoluminescence spectra of ZnMnO and ZnO nanopowders

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Keywords: absorption, photoluminescence, ZnMnO, nanopowders

Diluted magnetic ZnMnO semiconductors have become particularly attractive because of the potential spintronic device application. Apart from this, nanopowders may be considered as new effective catalysts and photoluminescence materials. In this report we present luminescence and optical absorption spectra of ZnO and $Zn_{0.95}Mn_{0.05}O$ nanopowders obtained by gas-phase synthesis in the oxygen contained argon atmosphere.

For ZnO nanocrystals at room temperature a broad absorption peak with the maximum at the light quantum energy of 3.30 eV was observed. With the decrease of the temperature to 77.3 K the peak became narrower and shifted towards the energy of 3.36 eV. The second peak appeared at 3.42 eV as well. For $Zn_{0.95}Mn_{0.05}O$ nanocrystals at 77.3 K two broad lines were distinctly seen at 3.37 eV and 3.42 eV. The direct observation of exciton lines (inherent in single crystals) in the absorption spectra indicates that the crystal structure of ZnO and $Zn_{0.95}Mn_{0.05}O$ nanopowders is quite perfect and close to the structure of ZnO and $Zn_{0.95}Mn_{0.05}O$ single crystals.

The photoluminescence spectrum of $Zn_{0.95}Mn_{0.05}O$ nanocrystals at the temperature of 90 K consists of two broad peaks at 2.1 eV and 2.9 eV. The first peak arises due to transitions forming the yellow–orange band of the luminescence in ZnO. The appearance of the second peak at 2.9 eV is caused by the presence of Mn impurities due to the generation of the Dangling Bond Hybrid state which is splitting from the valence band top. The $Zn_{0.95}Mn_{0.05}O$ photoluminescence excitation spectrum of the Mn related peak exhibits broad profiles at 3.9 eV, 4.5 eV and 5.3 eV. The $Zn_{0.95}Mn_{0.05}O$ photoluminescence and photoluminescence excitation spectra are discussed in comparison with PL and PLE ZnS:Mn spectra on the basis of the hybridization between the Mn^{2+} ions d-states and the deep valence sub-bands.

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Tue-8.52po

Detection and identification of nitrogen defects in nanodiamonds as studied by EPR

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Keywords: nanodiamond, EPR, defect, nitrogen

The properties of carbon nanostructures are of the great interest. Nanodiamond (ND) doping processes, formation and structure of intrinsic and impurity defects differ from those in bulk diamonds. In particular, the theoretical studies have shown that nitrogen impurities in ND are metastable in contrast to bulk diamonds.

Continuous-wave (cw) electron paramagnetic resonance (EPR) and electron-spin echo (ESE) at both X-band (9.3 GHz, cw) and W-band (94 GHz, cw and ESE) were used to study nitrogen impurities in natural nanodiamond powder with characteristic size of a particles of about 150 nm and detonation nanodiamonds (after pressure sintering) with a size of ~ 8.5 nm.

Observed X-band EPR signals in natural nanodiamond powder were similar to previously observed in natural diamond microcrystals. The EPR spectrum consists of a strong central line of surface centers and small intensity satellites. A number of the EPR signals in microdiamond powder occur in approximately the same magnetic fields, and the EPR signal of the surface centers masks the main EPR lines. The interpretation of the satellite lines remains contradictory even in diamond microcrystals and this was not yet discussed in nanodiamonds.

In this report the problem was solved by measuring the EPR and especially ESE spectra at high frequency. In the ESE experiments central line of the surface centers was suppressed due to short relaxation time and all the EPR lines of two types of nitrogen centers: isolated nitrogen donor N^0 (P1 in bulk diamond) and nitrogen pair N_2^+

(W24) have been observed in the natural nanodiamond powder with spin Hamiltonian parameters $g|| = g_+ = 2.0024$, $A|| = 40.7$ G, $A_+ = 29$ G (N^0) and $g|| = 2.00245$, $g_+ = 2.0030$, $A|| = 55.38$ G, A_+=29G (N_2^+).

EPR studies in detonation nanodiamonds showed the presence of N^0 centers for the fist time. The appearance of the EPR signals related to N^0 center suggests that single nitrogen atoms occupy stable position inside nanodiamod particles with a size of less then 10 nm produced by pressure sintering of nanodiamond powder.

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Tue-8.53po

Use of SRIM for analyzing nanocrystal damage statistics in ion-irradiated nanocrystalline systems

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Keywords: silicon nanocrystals, silicon dioxide films, ion irradiation, atomic displacements, recoils

In the examination of radiation processes in nanocrystalline (nc) systems under ion irradiation, grasping the detailed picture of primary radiation damages done to nanocrystals often becomes desirable. Such an approach, used in [1], implies making numerical SRIM simulations of recoil cascades in the ion-irradiated target followed by subsequent analysis of the statistics of atomic displacements introduced inside spherical regions chosen to represent nanocrystals. As for nc systems made up by Si nanocrystals embedded in a SiO_2 matrix, with the ion stopping power of SiO_2 being close to that of Si, SRIM calculations can be performed assuming the target to be bulk silicon, i.e. by replacing the SiO_2 matrix with Si.

In the present report, we show, in addition to [1], that a computer analysis of SRIM simulation data contained in the recoil cascade data file *collision.txt* makes it possible to evaluate, apart from average damage characteristics of nanocrystals (such as the mean number $< f >$ of primary displacements produced in Si per one damaged nanocrystal), the distribution of damaged nanocrystals over parameters of interest, for instance, over nanocrystal damage factors f.

In our calculations, Si nanocrystals were assumed represented by spherical regions having certain chosen sizes. Using SRIM-simulated data, we assessed the number of displacements introduced in each nanocrystal. The nanocrystals in the calculation domain were arranged so that to imitate their random position with respect to ion tracks. Initially, all nanocrystals were places at cubic-lattice sites and, then, each nanocrystal was shifted in three dimensions over random fraction of half the separation between adjacent nanocrystal grains. Using the described procedure, we were able to calculate, for instance, the distribution of nanocrystals over f in nc systems irradiated with low ion doses (the case of non-overlapping displacement cascades). In order to reveal regularities in gained distributions, such calculations were made for ions of different types and various energies. The dependence on structural parameters of nc systems, such as nanocrystal shape and size, was also examined. Next, by adding random displacements to the lateral coordinates of all vacancies introduced into the nc system by one and the same ion (or by the recoils produced by this ion), we were also able to directly model the case of a "distributed" ion bombardment of a sample with an arbitrary (not necessarily low) irradiation doze. It is shown that, in this way, it becomes possible to directly calculate the fraction of "survived" nanocrystals in irradiated samples versus irradiation dose without invoking additional statistical hypotheses about damaged nanocrystals similar to the hypotheses used in [1]. With an additional program module incorporated into the main program to calculate the formation of secondary defect complexes inside nanocrystals (such as, e.g. divacancies), the proposed approach will become useful for analyzing the accumulation of defect complexes in ion-irradiated nc systems. Due to small volume of nanocrystals, such calculations can be easily made, assuming some appropriate values for reaction cross-sections, by the Monte-Carlo method while performing the analysis of the damage statistics in nanocrystals.

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Tue-8.55po

Effect of thermal treatment on the photoluminescence and ESR of porous silicon

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Keywords: porous silicon, nanocrystallites, photoluminescence, ESR

Porous silicon (PSi) is a material with nanocomposite structure, which is include silicon nanocrystallites and surroundings phases of variable structure, containing significant amount of oxygen and carbon. It is known that properties of PSi are determined by quantum confinement effect in nanocrystallites. On the other hand, optical, electric and magnetic properties of the high-surface-area porous silicon structures are affected by the physical and electronic structure of the surface and Si/SiO_2 boundary conditions. In particular, charge carriers captured in SiO_2 or on Si/SiO_2 boundary can determine high-frequency conductivity of PSi and the luminescence features of PSi are strongly affected by post treatments of the samples. In this paper, we report the photoluminescence (PL) and electron spin resonance (ESR) study of PSi samples subjected to thermal oxidation in ambient air.

The PSi samples were prepared by standard electrochemical etching of high-resistance ($\sim$ 3 kOhm*cm) p-type Si wafers in a hydrofluoric acid/methanol solution. PL spectra were investigated in a range of 340–800 nanometers using the 325-nm line of the He-Cd laser. PL spectrum localized to the orange-red emission region is strongly modified after short-time thermal oxidation on air at 700–1000°C for 3–40 sec. The orange-red band almost completely disappears and the spectrum is shifted in short-wave region. Short-time annealing ($\sim$ 3 sec) gives rise to a green PL band 450–500 nm. Blue PL band peaked at $\sim$ 400 nm dominates after 40 sec annealing at 1000°C. The short-wave shift can be explained by oxidation of the PSi and decrease of effective nanocrystallite size.

ESR research of PSi samples shows that 3–15 sec annealing at 700–1000°C results in very strong absorption of microwave radiation by the thin (10–100 microns) PSi layer. It is revealed that the known P_b ESR center which is main paramagnetic defect in as-grown PSi disappears upon 700–900°C annealing, and an isotropic ESR spectrum ($g \sim 1.9980$) characteristic for disordered dangling bond emerges instead. Annealing at 1000°C results in the appearance of an additional isotropic ESR spectrum ($g = 2.0701$) of Dyson type which can be attributed to free carriers absorption. The high value of the g-factor indicates that the absorption can be hole-like, in contrast to the free electron absorption in silicon with $g = 1.9995$. Intensity of the ESR spectrum with high g-factor considerably changed upon rotation of the magnetic field H in the (011) plane, at the same time the shape and half-width of the spectrum line did not change. The intensity was maximal with H along $\langle 111 \rangle$ directions and decreased in 2–3 times with H along $\langle 011 \rangle$ and $\langle 001 \rangle$ directions when the intensity reached minimum. This effect can be explained by formation of layers with free holes on PSi surface for compensation of negative charged traps, which located in SiO_2 layer or Si/SiO_2 boundary. Variation of intensity of free hole absorption spectrum can take place due to confinement of free carriers in PSi quantum wires.

Tue-8.56po

Small-angle X-ray scattering study of interfacial roughness of MBE-grown CaF_2–CdF_2 superlattices on Si(111)

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Keywords: superlattice, diffuse X-ray scattering, roughness

Calcium and cadmium fluorides are wide band gap materials having the fluorite type of cubic crystal structure and the energy gaps of 12.1 and 8 eV correspondingly. Their lattice parameters are quite close to that of Si; this enables growth CaF_2–CdF_2 superlattices (SLs) on Si (111) substrates. Being doped by divalent rare-earth ions, these superlattices show interesting optical properties, attractive for applications in optical memory cells.

High-resolution X-ray diffraction study was carried out, and it was shown that the short period CaF_2–CdF_2 superlattices (with the period $t < 30$ nm) can be grown pseudomorfically. The curves calculated using model of an ideal SL disagreed noticeably, however, with the experiment. Only by introducing transition layers could one in some cases obtain the required accordance. These layers in our case could be due to roughness of CaF_2–CdF_2 inner interfaces (there is no interdiffusion at these interfaces because of the low growth temperatures).

In this work we have used small-angle X-ray scattering (reflectometry and diffuse scattering) measurements to investigate interfacial roughness in short-period ($t = 1.5-20$ nm)) CaF_2–CdF_2 SLs grown by MBE on Si(111). Diffuse scattering measurements are sensitive to the widest length scale of all the techniques that have been used. Structural characterization has been carried out by using X-ray diffractometer AXS D8 Discovery (Bruker Corp.).

Reflectometry and diffuse scattering curves have been simulated. The amount of interfacial roughness, its evolution, and the degree of correlation are obtained from a fit to the data.It has been found that roughness in all of SLs is vertically correlated. It has been shown that interfaces in SL with $t = 20$ nm can be described by rather small mean-square roughness ($s \approx 0.5$ nm). Vertical correlation in this SL related to of the stepped interfaces with large width. On the other hand short-period ($t < 10$ nm) SLs can be described by $s \approx 1$ nm. These SLs have partially vertical correlated roughness related to growth of CdF_2 epitaxial layer at low temperature. This conclusion is consistent with AFM measurements.

Possible mechanisms of inheritense of roughness have been considered.

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Tue-8.57po

Study of nanostructure and photo-luminescence in InGaN/GaN multiple quantum wells on silicon (111) substrates

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Keywords: gallium nitride, photo-luminescence, silicon substrate

The group III-nitride wide band gap semiconductors have attracted much attention due to many applications, such as red/green/blue/UV light emitting diodes (LEDs) and laser diodes (LDs). Some commercial applications have included LED back-light for liquid crystal displays, traffic signals and indoor illumination. It has also been noted that multiple quantum well LED grown on Si substrate has some advantages over that on sapphire substrate, such as lower cost, less hardness, and design flexibility in electronic circuits. However, some problems in InGaN/GaN quantum wells such as In-rich phase separation and the quantum confined stark effect can still influence the optical properties and need to be clarified. Ga (In)-Nitride multiple quantum wells (MQW) have been successfully grown on high quality Si (111) substrates using metal-organic vapor phase epitaxy (MOVPE). In this paper, we would investigate the nanostructure and optical properties of the InGaN/GaN MQWs. The full-width at half-maximum (FWHM) GaN (002) was about 600 arcsec from XRD rocking curves. The In-rich phase separation was studied by photo-luminescence (PL) and transmission electron microscopy (TEM). In the 20 K PL curves, the different emission peaks suggested the quantization effect and In-rich phenomenon in the multiple quantum wells. From our calculation, the quantum confined stark effect (QCSE) caused the potential well.

Tue-8.58po

Study of two-dimensional photonic crystal arrays for beam-splitters

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Keywords: photonic crystal, silicon, beam-splitter

In photonic crystals, periodic modulation of the dielectric constant leads to the formation of photonic band gaps, where light waves cannot propagate in the spectral regions. When a defect is introduced in an otherwise perfect photonic crystal, a localized effect may be found at frequencies within the photonic band gap. A line defect acts as a waveguide and a point defect can act as a resonant cavity. In this report, we demonstrate two-dimensional photonic crystal structures based on germa-

nium (n=4.0), silicon (n=3.49), titanium oxide (n=2.71), silica (n=1.50), and polymer (n=1.50) materials. Both square lattice array and triangular lattice array have been studied. The results exhibited the Mach–Zehnder interferometer function that could be applied to optical switches or optical integrators. The beam-splitter had the crossed linear defects shape, constructed by two orthogonal-line defects. We could reduce the pattern diameter to 200 nm and the lattice constant to 560 nm for the operation under 1.55 μm environment. In addition, the silicon based beam-splitter was defined by an e-beam writer and the semiconductor processing technology. As a result, the induction coupling ion etching machine (ICP) was employed for high aspect-ratio silicon column arrays.

Tue-8.59po

Defects of Ge quantum dot arrays on the Si(001) surface

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Keywords: Ge quantum dots, dense arrays, defects, scanning tunnelling microscopy

Ge clusters with parameters considerably different from the characteristic parameters of clusters in the array or areas with appreciable local deviation of array parameters from those typical for the conditions of the array formation will hereinafter be referred to as defects of Ge quantum dot (QD) arrays. The defects of Ge QD arrays may affect the electrophysical, photoelectrical or optical properties of Ge/Si heterostructures as well as the functionality of devices produced on their basis. The defects of Ge QD arrays formed at moderate temperatures on the Si(001) surface were investigated by the ultra high vacuum scanning tunnelling microscope (UHV STM) integrated with the UHV molecular beam epitaxy chamber. A preliminary classification of the defects was carried out. The revealed defects were subdivided into the following groups: (i) large hut or dome clusters with the sizes untypical for the growth temperature (large defects), (ii) extended clusters stretched along the $\langle 110\rangle$ direction (extended defects), and (iii) areas in which QDs did not grow (depleted regions). Morphological peculiarities of the defects were studied. Facets of the large and extended defects were investigated with atomic resolution. The $\{105\}$, $\{113\}$, $\{102\}$ faces as well as some additional facets were revealed. The surface densities of defects of different types were determined. The extended defects were investigated in detail. It was found that (i) the extended defects may arise on the extended structural defects of the initial Si(001) surface, (ii) the density of QDs dramatically drops in the vicinity of the extended defects, (iii) the extended defects may affect the QD array parameters and at high enough defect density sufficiently decrease the QD density throughout the array, (iv) the extended defects formation probability is increased as the array growth temperature is enhanced.

Tue-8.60po

Structural characterization and electro-physical properties for SiOC(-H) low-k dielectric films

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Keywords: SiOC (-H) low-k film, C-V characteristics, surface state conditions, (Si-CH3)+/(Si-O)- defects

The hybrid type SiOC(-H) film formed from organic and inorganic materials are very promising as low-k material because the spatial hindrance of the alkyl groups may produce abundant nano-pores in film and decrease the dielectric constant. It is well known that the physical properties of these low-k SiOC(-H) films are sensitive to the replacement of Si–O bonds with (Si–R) bonds [1]. One of promising methods of low-k SiOC(-H) film deposition is plasma enhanced chemical vapor deposition (PECVD) using organosilane molecules as source materials. Especially the decomposition processes of the molecules and the effects of the growth mechanism on structural and electro-physical properties are not fully understood well. In this study, low-k SiOC(-H) films with different structural orders were fabricated, and the influence of the replacement of Si–O bonds to the (Si–R) bonds on structural and electro-physical properties has been investigated. The films were deposited on p-type Si(100) substrates in the process of PECVD at various rf-power from 400 to 800 W using Methyltrimethylsilane (MTMS) and Oxygen as reagents. The structural characterization was performed by transmittance FT-IR in the ranges of 400–4000 cm^{-1}. These techniques provide us with valuable information of Si-CH, Si-O and C-H bonds. High frequency C-V characteristics of the Al/SiOC(-H)/p-Si structures were registered using standard method at the frequency of 1 MHz. The conduction mechanisms in the various types of film classified from the analysis of the current-voltage (I-V) curve dependences. These results are further analyzed in connection with the theoretical calculations. It was found that the excess $-CH_3$ or $Si–CH_3$ and Si-H bonds in SiOC(-H) films produced the effective positive charges coming from excessive interstitial defects. Flat band voltage (V_{fb}) shifts depended of the quantity trap centers produced the effective negative charges coming from excessive oxygen interstitial defects and they increased with increasing RF power. So the results suggest that the electro-physical properties of the deposited films, such as capacity, V_{fb} shifts, density of charges and mechanisms of conduction strongly depended of the excessive $(Si\text{-}CH_3)^+/(Si\text{-}O)^-$ bonds ratio and have been significantly changed (controlled) by the addition of oxygen.

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Tue-8.61po

Capacitance spectroscopy of CdTe self-assembled quantum dots embedded in ZnTe matrix

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Keywords: ZnTe, CdTe, quantum dots, DLTS

It has been already demonstrated that the CdTe/ZnTe quantum dot system allows to study a single magnetic atom in a solid state environment by doping of the CdTe quantum dot with a single Mn atom. However, for such a magneto-electric device applications the electrical characteristics of the carrier binding properties of the dot system has to be known. In this study the capacitance–voltage ($C-V$) and deep level transient spectroscopy (DLTS) measurements have been performed on ZnTe (p-type) Ti/Au Schottky diodes containing one layer of CdTe self-assembled quantum dots (QDs). The reference samples were the ZnTe–Ti/Au diodes without dots for comparison. Both kinds of investigated samples were grown by molecular beam epitaxy. The dots were formed during the Stransky-Krastanov growth mode. The C-V characteristics of the samples containing the QDs exhibit characteristic step related to discharging of the QDs. For the reference sample $C-V$ characteristics show solely bulk behaviour. DLTS measurements for the samples with QDs reveal the presence of two hole-related signals with thermal activation energies equal to $E_1 = 0.2$ eV and $E_2 = 0.4$ eV. For the reference ZnTe/Ti/Au diodes only the E_2 signal is observed. It may be concluded that the $E_1 = 0.2$ eV level can be assigned to the hole emission from the QDs. The 0.4 eV trap is attributed to the ZnTe bulk material. The quantum dot binding energy for holes of 0.2 eV combined with the commonly observed energy of the excitonic luminescence from the CdTe/ZnTe quantum dot system of around 2.0 eV and compared to the ZnTe bandgap of 2.4 eV allows to evaluate the quantum dot binding energy for electrons in the conduction band. Such an evaluation helps to conclude about the binding of electrons by the dots in a case of known difficulty to obtain n-type ZnTe.

Tue-8.62po

Neutron-Transmutation-Doping of Ge nanocrystals imbedded in Si-MOS structures: C-V characteristics

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Keywords: isotopically enriched Ge nanocrystals, neutron-transmutation doping, MOS structures, C-V characteristics

MOS structures containing ^{74}Ge and ^{70}Ge nanocrystals (NC-Ge) imbedded inside the SiO_2 layer were studied for their capacitance characterization. Ge atoms were introduced by implantation of $^{74}Ge^{+}$ or $^{70}Ge^{+}$ ions with energy of 150 keV into relatively thick (500–600 nm) amorphous SiO_2 films grown on a $\langle 100 \rangle$ surface of p-Si. In these samples, appearance of NC-Ge was observed, using TEM and Raman-scattering measurements, only after annealing the samples at 800°C. Typical diameter of the NC-Ge is shown to be in the range of 4–10 nm. The experimental characterization included measurements of the C-V dependences at room temperature and in response to the white light illumination. Three groups of samples have been studied: before ion implantation (“initial” sample, without Ge atoms), after Ge ion implantation but before annealing (“implanted” sample, with randomly distributed Ge atoms) and after annealing (“NC-Ge” sample). It is shown that in contrast with “initial” and “implanted” samples, “NC-Ge” samples have U-shape C-V characteristics and exhibit a hysteresis which indicates memory retention properties. The capacitance at low voltages is strongly affected by light illumination. The observed phenomena are explained on the basis of assumption that NC-Ge in SiO_2 matrix are “trapping centers” for charge carriers which can be delocalized in strong electric field or under light illumination.

In the next experiments, the NC-^{74}Ge and NC-^{70}Ge samples were subjected by an intensive neutron irradiation in a research nuclear reactor with the integral dose up to 10^{20} neutrons/cm^2 (“irradiated” samples), followed by the annealing of radiation damage introduced by fast neutrons (“annealed” samples). Capture of slow (thermal) neutrons by isotopes ^{74}Ge and ^{70}Ge leads to transmutation of these isotopes to donor (^{75}As) and acceptor (^{69}Ga) impurities respectively (Neutron-Transmutation-Doping). Changes of C-V characteristics observed in “irradiated” and “annealed” NC-Ge samples are also discussed.

Tue-9.1po

Non-contact reaction between micropipes and correlated reduction of their cross sections in bulk SiC growth

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Keywords: silicon carbide, micropipes, dislocations, phase-sensitive radiography

Development of SiC-based power electronics has been hampered by insufficient quality and size of SiC ingots. Seeded sublimation growth techniques produce large-area SiC wafers, however, it is accompanied by the formation of cylindrical pores, called micropipes (MPs). As a rule, they represent the hollow cores of superscrew dislocations with giant Burgers vectors. MPs have deleterious effect on the properties of SiC such as large breakdown electric field strength, high thermal conductivity, etc. Therefore, the problem of growing bulk SiC crystals with low MP density is of special importance. The MP evolution during the crystal growth is a complex process that involves the formation of new MPs, the overgrowth of the existing MPs due to their various reactions with one another, and the coalescence of MPs, resulting in micropore formation. In the present work, we study one more form of MP evolution, namely, a correlated reduction in the cross sections of two neighboring MPs along their axes. Such variations in MP cross sections can lead to MP healing. We provide experimental evidence of this effect and discuss its reasons and a possible mechanism. Our main idea is that MPs can remotely interact with each other by the exchange of full-core dislocations. We propose a theoretical model describing the energetics of this process.

SiC sample was an axial-cut slice along the growth direction [0001] obtained from 4H-SiC boule grown in Ar by the sublimation sandwich method. The sample contained MPs located almost parallel to the surface. MPs were examined with the white beam phase contrast imaging method at the 7B2 X-ray Microscopy Beamline of the Pohang Light Source, Korea. The sample was sequentially placed at different distances from the detector. Three MPs forming a group were examined: two in contact, and the third lying remotely. For all sample-to-detector distances and for different points along the axis of MPs, the intensity profiles normal to the axis were measured. To determine the characteristic sizes of the MP cross sections in different points along the MP axis, we applied the method of computer simulation of the measured intensity profiles. For every MP cross section under investigation, the computer program calculated many profiles for various possible section sizes on the base of Kirchhoff propagation to find the profile which gives the best fit to the individual experimental profile registered for this section. As a result, we have revealed that MP cross sections drastically change during the crystal growth. Moreover, they demonstrate a correlated reduction. Since the cross section of a MP is tightly related to its Burgers vector, this effect can be explained by the corresponding changes in the Burgers vectors that need appropriate dislocation reactions.

Up to now, it has been generally accepted that any reaction between MPs requires their direct contact. An alternative for contact reactions is contact-free reactions that do not require a direct contact between MPs. These reactions can be realized through emission and absorption of full-core dislocations. Therefore, if two neighboring MPs demonstrate correlated reduction in their radii, one can suppose that, first, these MPs contain dislocations of opposite signs, and, second, they have remotely reacted through the exchange of a full-core dislocation: one of MPs has emitted this dislocation while the other has accepted it. We have considered a simplified 2D model of a contact-free reaction between two parallel MPs. To analyze the possibility of dislocation exchange, we have used the energy variation associated with dislocation emission and shown that the dislocation exchange is most energetically favorable if the MP Burgers vectors are opposite in sign. If the Burgers vectors of the two MPs are of the same sign, the emitted dislocation must overcome two energetic barriers on its way from one MP to the other. In this case, the possibility for the dislocation exchange between these MPs is governed by the difference of the Burgers vector magnitudes. This model helps in understanding the mechanisms which control the MP density in bulk SiC crystals.

Tue-9.2po

Pore growth by mechanism of micropipe absorption at foreign polytype boundaries in bulk SiC crystals

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Keywords: silicon carbide, micropipes, pores, phase-sensitive radiography

Silicon carbide is a promising semiconductor material for high-power, high-frequency, and high-temperature electronics. At the same time, in spite of significant progress in SiC seeded sublimation-growth technologies, SiC crystals still contain various structural defects, such as stacking faults, micropipes (MPs), small-angle grain boundaries and inclusions of foreign polytypes. Among these defects, MPs (hollow-core screw superdislocations) and micropores are considered to be the most dangerous for the performance of high-voltage devices because they cause microplasma. In the course of crystal growth, MPs can be accumulated at inclusion boundaries, which leads to their coalescence resulting in the formation of larger pores. The pores generated in such a way can continue their growth by virtue of the absorption of new MPs as it has been observed by means of phase-sensitive radiography. The aim of the present work is to reveal the conditions for pore growth at the boundaries of foreign polytype inclusions in SiC crystals at the expense of MP absorption.

The samples were prepared from a 4HSiC boule grown in Ar by the sublimation sandwich technique. The 0.4 mm thick wafers were cut perpendicular to the [0001] growth direction and mechanically polished on both sides. The morphology of pores and MPs in the interior of SiC wafers was studied by means of phase-sensitive radiography at the Pohang Light Source, Pohang, Korea. The foreign polytype inclusions located close to the surface were revealed with the aid of a photoluminescence (PL) microscope in visible as well as ultraviolet light. The polytype was identified by the color of PL as 6HSiC and $21R$SiC inclusions in the 4HSiC wafer. We have observed that pores of different sizes and shapes are always present at the boundaries of foreign polytype inclusions in SiC samples under study. The phase radiographs demonstrate slit shapes of the pores and separate MPs in the wafer interior. It is shown that that pores are produced by agglomeration of MPs. The pores spread over the inclusion boundary and propagate deeply inside the wafer. Near the inclusion boundaries, the

MPs remarkably deviate from the growth direction, which we attribute to the interaction of MPs with the polytype inclusion. As follows from these observations, MPs are attracted to foreign polytype inclusions and can initiate the growth of slit pores along the inclusion boundaries.

To theoretically analyze the conditions for pore growth at the expense of MP absorption, we have suggested a 2D model of pore growth along a polytype inclusion boundary by means of MP coalescence. The main assumption is that neighboring MPs are attracted to the inclusion to accommodate the orientation mismatch of the inclusion and matrix crystalline lattices. This orientation mismatch is described mathematically through the components of the inclusion plastic distortions. The growing pore is modeled as a cylindrical void of elliptic cross section which attracts and absorbs MPs from the neighboring area. The pore volume is supposed to be equal to the total volume of the MPs that merged to form the pore. To study the conditions for pore growth, we have calculated the force exerted on a MP by the inclusion containing the pore. The force analysis has shown that the pore attracts MPs until their number reaches a critical value. After that the MPs absorbed by the pore produce a repulsion zone for new MPs, and pore growth stops. The critical pore size is determined by the values of inclusion plastic distortions: at their small values isolated MPs form at the inclusion/matrix interface, at medium values MPs coalesce to form a pore of a certain size, at large values the pore occupies the whole inclusion boundary.

Tue-9.3po

Growth of GaN nanostructures by halide vapor phase epitaxy

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Keywords: HVPE, GaN, nanostructures

GaN and related group III-V nitride semiconductors are getting considerable attention during the last decade due to their strong potential for light-emitting and electronic applications. GaN nanostructures, such as quantum dots, nanorods, nanowires and nanocolumns have become interesting subjects because of their excellent optical properties due to their high crystal quality. Since such nanostructures are as small as several tens to hundreds of nanometers, crystal strain arising from the growth on a foreign substrate is expected to relax, resulting in the reduction in dislocation density. Thus, this type of nanostructures can be used for optoelectronics applications or as seed crystals for producing low density templates for growth of thick crack free GaN, which is highly desired for fabrication of GaN substrates. Although the growth of such nanostructures has been reported, the detailed growth mechanism for such structures has not been clearly understood.

We report here the results of growth and characterization of GaN nanostructures grown by halide vapor phase epitaxy (HVPE). The nanostructures size, shape, density and the selectivity of growth have been studied depending on process parameters and substrate material. The growth was performed in a vertical HVPE reactor at a temperature of 500°C using pure N2 or a mixture of N2 and H2 as a carrier gas. It is observed that the shape and density of the nanostructures is dependent on the partial pressure of GaCl and choice of substrate material, respectively. With increasing partial pressure of GaCl, the shape of the nanostructures is changing from dots to nanocolumn-like shape. The typical diameter of the nanostructures is in the range 50–500 nm; however, smaller structures with diameters down to 15 nm have been observed. The grown nanostructures have been characterized by scanning electron microscopy, μ-photoluminescence (PL), cathodoluminescence and time-resolved PL.

Tue-9.4po

Dislocation-related luminescence in oxygen-implanted silicon

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Keywords: dislocation-related luminescence, ion implantation, oxygen, silicon

A study of dislocation-related luminescence (DRL) in silicon is of a great interest due to its possible use for the fabrication of silicon-based light-emitting devices. There are contrary points of view on a role of oxygen in formation of centers with DRL. These experiments were carried out in samples prepared by the techniques of bending deformation and the formation of oxygen precipitates [1–3]. We have recently suggested a new way for the fabrication of light-emitting structures with DRL using the implantation of oxygen ions [4]. However, DRL was studied in oxygen-implanted p-Cz–Si after annealing at 900°C in a chlorine-containing atmosphere for 4 h, only. The aim of this paper was to study DRL in oxygen-implanted p- and n-Cz–Si after annealing over more wide ranges of temperatures and durations.

Multiple implantation by oxygen ions with energies of 0.1–1.5 MeV and doses of 7×10^{13}–2×10^{14} cm^{-2} and subsequent isothermal annealings at temperatures of 800–1000°C in a chlorine containing atmosphere were carried out. Results of photoluminescence measurements at liquid nitrogen temperature will be presented for the samples. Some additional results concerning chemical, electrophysical and structural properties were obtained using Secondary Ion Mass Spectrometry, IR absorption, the conductivity type, resistivity, Rurtherford Back Scattering, Transmission Electron

Microscopy and X-Ray Diffraction techniques. The experimental results allow us to receive some additional information about the nature of DRL centers and study an effeA study of dislocation-related luminescence (DRL) in silicon is of a great interest due to its possible use for the fabrication of silicon-based light-emitting devices. There are contrary points of view on a role of oxygen in formation of centers with DRL. These experiments were carried out in samples prepared by the techniques of bending deformation and the formation of oxygen precipitates [1–3]. We have recently suggested a new way for the fabrication of light-emitting structures with DRL using the implantation of oxygen ions [4]. However, DRL was studied in oxygen-implanted p-Cz-Si after annealing at 900°C in a chlorine-containing atmosphere for 4 h, only. The aim of this paper was to study DRL in oxygen-implanted p- and n-Cz–Si after annealing over more wide ranges of temperatures and durations.

This work was partly supported by the Russian Foundation for Basic Research (Grant 07-02-01462).

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Tue-9.5po

Al ions implantation and “defect engineering” in SiC

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Keywords: ion implantation, radiation defects, annealing, local cathodoluminescence

SiC is one of the most promising wide-bandgap semiconductors for high-power, high-voltage and high-speed electronic devices with stable operation under extreme conditions. A major difficulty encountered in fabrication of SiC devices is the high resistivity of the p-type material, which is due to the fact that the concentrations of acceptors are limited by their low solubility in SiC. A nonequilibrium method, implantation doping (ID), allows introduction of acceptors in concentrations exceeding their solubility limit in SiC. It has been shown that ID of SiC with high dose of Al, followed by a short high-temperature annealing, can produce p^+n junctions in which ID p^+-layers do not introduce any additional resistance in device structures. At the same time, the effects of far-action accelerated diffusion of radiation defects during Al ID and the gettering of various defects in the course of short high temperature thermal annealing were observed. As a result the improvement of the structural perfection of the starting material was observed. However, it is known that implantation of ions with different doses into semiconductors is the reason for different influence of the radiation defects on the quality of the starting material.

This communication reports the results of a study of the effect of different doses implantation of Al ions and subsequent short high temperature annealing on the effects of accelerated diffusion of radiation defects, the gettering of various defects and, as a result, on the quality of the starting 4H–SiC material.

4H–SiC epitaxial layers (9 μm thick) with a donor concentration of 3×10^{15} cm^{-3} were grown by the chemical vapor deposition (CVD) method on commercial n^{+}–4H–SiC wafers. After the CVD growth, ion implantation with 300 keV Al ions was performed at a doses in the range 5×10^{13}–5×10^{16} cm^{-2}. Then rapid thermal annealing for 15 s at 1700°C was used. The distribution depth profiles after Al ID and annealing were measured using secondary ion mass spectrometry (SIMS). Specific structural features of CVD epitaxial layers before and after the formation of the ion-implanted layers were examined by two cathodoluminescence (CL) techniques: local CL (LCL) and CL imaging on cross-sectional cleaved surfaces of the structures. The concentration of deep levels in CVD layers before and after Al ID and annealing were investigated by deep level transient spectroscopy (DLTS).

According different investigations the decrease in the defect centres concentration and increase in the diffusion length of minority carriers in the CVD layers were observed due to combined effects of high dose Al ID and followed short high-temperature annealing. The decrease of Al implant doses led to non linear reduction of the amount of radiation defect centers in CVD layers that is specific for SiC.

Mechanisms of the far-action radiation defects and gettering effects in the course of short thermal annealing in SiC, implanted with different Al doses, will be discussed.

Tue-9.6po

Silicon nanoclusters formation in silicon dioxide by high power density electron beam

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Keywords: luminescence, silicon dioxide, silicon nanocluster

Si/SiO_2 structures with silicon nanoclusters use in modern microelectronics. There are many silicon nanoclusters buried in SiO_2 growth methods. We suggest a new method for silicon nanoclusters formation. Silicon dioxide intrinsic defects and silicon nanoclusters can be produced by high power density electron beam. This method allows forming silicon nanoclusters at a different depth and studying a process of its formation by cathodoluminescent method.

Electron beam influence on silicon dioxide leads to heating of interacted microvolume of silicon dioxide. The overheating of silicon dioxide microvolume causes intrinsic defects formation. Depth of overheating depends on electron energy. The purpose of this work was study of CL properties change in the process of intrinsic defect and nanoclusters formation. In this work two types of bulk amorphous silicon oxide samples were studied (OH-group content was >2 ppm and 1000 pmm).

Spatial stationary distribution of loss energy density was amounted by Monte-Carlo method. The temperature of overheating was calculated for bulk silicon dioxide. The estimated temperature is about 1200°C, it is enough for nanoclusters formation in vacuum. The depth of silicon nanoclusters formation depends on electron energy (0.1 micron for electron energy is 2.5 keV; 1.0 micron for electron energy is 20 keV).

Modification of silicon dioxide was carried out at different power density and different time modification. At the result we can say four following stages during intrinsic defects formation at a depth of 0.3 micron (electron energy is 5 keV):

- increase of intrinsic defect (2.6 eV — “blue” luminescence)
- formation of region with oxygen deficit (2.0–2.3 eV — “green” luminescence)
- creation of silicon nanoclusters (1.6–1.7 eV — IR luminescence)
- formation of large silicon cluster (1.1–1.3 eV — IR luminescence; luminescent intensity is decreasing).

Tue-9.7po

Influence of the type of growth defects on the molecular structure of SiO_2 phase precipitated in Cz-Si single crystals

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Keywords: Cz-Si, oxygen precipitation, strained and relaxed SiO_2 phase

Si material undergoes thermal treatments on all stages of its production and use for semiconductor devices. The formation and transformation of different types of defects (vacancy-type, interstitial, and mixed-type) takes place at this, also due to the interaction with defects and impurities. Such universal impurity as oxygen participates practically always in these processes. It can be in different states in Cz-Si, such as interstitial state and extended regions of precipitated SiO_x and SiO_2 phases. As it was found, the release processes of interstitial oxygen and its precipitation in form of either phase depend significantly on the mechanical stress fields in the crystal and, hence, on the type of growth defects. This correlation is investigated in detail in the present work.Electronic- and solar-grade (100) oriented Cz-Si wafers with the thickness of $\sim$ 1 to 2 mm were investigated. The wafers were cut from different parts of ingots 40 to 300 mm in diameter. The concentration of interstitial oxygen was in the range of $(9–11)\times10^{17}$ cm^{-3}. For the determination of the concentration of oxygen in interstitial position and precipitated in SiO_2 phase as well as the structure of precipitated phase, IR spectroscopy with the analysis of the shape of adsorption band on the valence oscillations of Si-O bonds was used. The type and size of defects as well as related mechanical stress were determined from the diffraction scattering curves and the X-ray diffuse scattering measured using the high resolution X-ray diffractometer

"X'Pert PRO MRD". For the formation of precipitated SiO_2 phase in the Si lattice, the samples were annealed at 800°C during 20 h and then at 1050°C either in furnace or by RTA in the argon atmosphere.

It is shown that for the samples with high enough concentration of interstitial-type growth defects the precipitation of oxygen in SiO_2 phase was significant. At this, together with extended phase of amorphous SiO_2 having different structural modifications a significant concentration of SiO_2Si_2 molecular complexes, mainly at the precipitate/Si interface were observed. The microstructure of precipitated phase was characterized by a significant number of strained 4-member rings of SiO_4 tetrahedra, hence, appearance of strained Si material is probable.
Opposite to this, for samples with high enough concentration of large vacancy-type growth defects, the high-temperature stage of annealing almost did not change both the concentration and the structural state of oxygen. Precipitated oxygen in SiO_2 phase had a rather ordered structural state, mainly in the form of 6-member rings of SiO4 tetrahedra. Most likely, its structure reflects that of α-christobalite. This phase, unlike the mixed phase with SiO_4 rings, does not form significant mechanical stresses, i. e. favours the formation of relaxed Cz-Si material.

Tue-9.8po

Characterization of defect states in semiconductors

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The energy distribution of secondary ions indicates on atomic particles both in surface and "bulk" layers, and also on change of its states. The essential information of localization of an electronic charge on bonds can be received by secondary ion energy spectroscopy and X-ray diffraction methods.

In present work reports for a study of the channels of redistribution of energy are considered at ion and x-ray probing of semiconductor monatomic and polyatomic surface such as silicon, $Al_xGa_{1-x}As$, $Al_xGa_{1-x}Sb_{1-y}As$, and also GaP epitaxial structure of p-and n-type. Observable at ion flux the integrated maximum of continuous radiation of energy spectrum on length of a wave 400 nm was considerated as ion luminescence.

The role of chemical interactions of particles as in near coordination sphere on a surface, and in cluster formations is discussed. The distinction in a degree displacement of a charge on atomic bonds and formation moment dipole is considered. The transition from molecular to a crystal state is characterized by change of coordination number and it is possible to take into account by the correction to atom electronegative number or recalculation of distribution of electronic density of the nearest atoms of a matrix and impurity including implanted ions.

The researches of structure Si upper layers by mean of X-ray standing waves method observe the difference in distribution of an electronic charge on bonds on a surface and in a bulk. For units electron-volt appropriate to a maximum on secondary ion energy spectra the characteristic time is about 10^{-15} s. In the report it compares with characteristic time to time of the auger-transitions in free and surface atom structures, the excitation of particles and the processes of redistribution of energy.

On the unusual interaction the defects near a free surface is marked. For instance the point defects with the similar signs attract each other and against with the different signs push away ones. The formation of the surface vacancy and interstitial loops after different technological treatments are described.

Tue-9.9po

Structural change of graphite under intense thermal shock load

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Keywords: diamond, graphite, defect, irradiation, shock compression

We report the structural change of graphite under intense thermal shock load. A fine grain graphite grade, R6650 (SGL Carbon, Germany) was used as a sample for thermal shock experiments. The nominal grain size of the original grade was around 7 μm. Sample coupons were prepared in a size of $12 \times 12 \times 5$ mm^3. Thermal shock load was applied in the electron beam facility JUDITH, that is installed in the hot cell laboratory, Forschungszentrum Jülich, Germany. Due to the high acceleration voltage (120 kV), the electron beam penetrates about 100 μm in carbon. Homogenous heat distribution is realized by fast scanning of the electron beam (several tens kHz). The single thermal shock load was applied at a power density of 9.6 GW/m^2 for 5 ms at room temperature, over an area of 4 mm^2 in a vacuum. After the load, the graphite samples were investigated by micro-Raman spectroscopy, using a backscattering geometry with the 488.0 nm line of Ar-ion laser.

We observed the reduction of Raman intensity ratio of D and G peaks, contrary to the defect production process [1]. This indicates that the load caused ordering of graphite structure even for as short as 5 ms. The Raman spectra of the surrounding area generally exhibited features of amorphous carbon indicating a carbon deposits. The spectra showed a strong positional dependence related to the substrate surface temperature. The Raman spectra analysis clearly shows the graphitization of the amorphous carbon deposits, formation of nano-crystalline graphite layers, reflecting the depositing temperature. The structure evolution was summarized in terms of variation of Raman intensity ratio and peak width [2].

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Tue-9.10po

Thoughts about reactions in crystal lattices

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Keywords: defects, vacancies, interstitials, reactions

In mid of the previous century some important data on the point defects, generated by irradiation in Ge and Si crystals, have appeared. Their high mobility even at cryogenic temperatures, existence of the barriers for the recombination of the Frenkel pair components, and intense reactions of the defects on the atomic level, leading to modification of the defect — impurity sub-system, have been recognized. Today, those facts are approved by the whole complex of the experiments on the molecular-beam epitaxy, chemical treatments, ion implantation and deformation stresses. The obtained results point to the common character of the defects behavior and its validity for all the crystals. In general, up to date the reactions in the crystals are not well understood. The complexity of the huge problem, the variety of the crystalline materials, lack of the basic approaches, numerous disputable questions and dependence of the reaction rates on the charge states of the partners hinder the investigations and development of technology for creation of active nanocenters in crystals. The goal of this work is to draw attention to these long-lasting problem, yet not fully taken into account. The paper was initiated by the recent publication of G. D. Watkins, J. Appl. Phys. **103**, 106106 (2008).

Tue-9.11po

Influence of Si ion implantation and annealing conditions on luminescence centers and structural defects in silicon

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Keywords: dislocation-related luminescence, structural defects, ion implantation, silicon

The development of Si optoelectronics is hindered by the lack of efficient light sources compatible with Si technology. It seems promising to use the so-called dislocation-related luminescence (DRL), which appears in single crystal Si with a high density of extended structural defects. Laser recrystallization and uniaxial deformation techniques gave a possibility to fabricate structures with DRL [1, 2]. We have found a new way for the fabrication of light-emitting structures based on the implantation technique [3]. DRL arises in single crystal Si containing a high density of extended defects induced during high temperature annealing in an oxidizing ambiance of Si implanted by Er ions. It was recently found that the implantation of silicon ions and subsequent annealing introduce extended structural defects and centers with DRL [4, 5]. However, there is a little information about the nature of extended defects and luminescence centers in Si-implanted layers. The purpose of this paper was to study an influence of the conditions of ion implantation and annealing on the formation of structural defects and luminescence centers.

100 keV silicon ions were implanted at a dose of 1×10^{17} cm^{-2} into n-FZ–Si polished wafers. The target temperature was changed from 20 to 100°C. After the implantation, the samples were annealed at 900–1100°C in a chlorine-containing atmosphere (flow of oxygen saturated with 0.5 mol % carbon tetrachloride) for 8–240 min. Structural and luminescence properties were studied by TEM, XRD, RBS and photoluminescence techniques.

The variation of the target temperature gave us a possibility to change a depth of defect-containing layer and its defect structure. Amorphous layer was produced at low target temperature, and there is no amorphyzation at the higher temperatures. Subsequent annealing was followed by the transformation of the structural defects and the formation of luminescence centers. The so-called D1 center of DRL was a dominant luminescence center at our experimental conditions. The detailed investigations of luminescence centers and extended structural defects in dependence on the implantation and annealing conditions were carried out. A correlation between the extended defects and the DRL line intensity permits to clarify the nature of DRL centers.

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Tue-9.12po

Self-organizational behavior of point defects in ion irradiated semiconductors and its application to nano-cell fabrication

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Keywords: GaSb, InSb, Ge, point defects, ion irradiation

Fine cellular structure consisting of many cells develops on the Sn^+ ion irradiated GaSb surface at a low temperature (130 K∼150 K) [1–3], and this behavior is due to the self-organizational movement of the point defects induced by the irradiation of energetic ions [2–3]. The same or similar behaviors were observed in InSb and Ge.

The characteristics of the authors discovered cellular structure, fine dimensions, high aspect ratio and very thin partitioning wall (5–10 nm) may be exploited in nano-device processing. Therefore we proposed a new fabrication technique using focused ion beam to form an ordered nano-cell structure [4]. This nano-fabrication technique consists of two processes, the top-down and the bottom-up. The starting process is to create the voids orderly under the surface by scanning the focused ion beam at a constant interval. Ions are irradiated at designed points on the surface, by which a lot of vacancies and interstitials are created in the cascade. The vacancies with a low mobile remain in the implanted cascade, though the interstitials migrate far from the created site. Then, one void is formed from the oversaturated vacancies. As the ion beam is scanned at a constant interval, an ordered array of voids is obtained at uniform intervals under the surface. These voids are formed at the depth corresponding to the projected ion range, therefore the depth of the voids can be controlled by acceleration voltage and the volume of the voids can be changed by the ion dose. Ion species is also a factor for controlling these parameters.

The second procedure (bottom-up) is to develop on ordered cellular structure from the starting array of the voids by ion-implantation at an appropriate temperature depressing new void formation, i.e. at the temperature where the vacancies not recombined are absorbed by the initially formed voids. The initial voids develop by absorbing the remaining vacancies and by the interstitial atoms migrating to the walls partitioning voids during implantation. In this manner, an ordered cellular structure is fabricated self-organizationally. This procedure is possible by imaging mode in a FIB, since the beam dwell point spacing is very small compared with the void interval.

The nano-cell fabrication experiments were performed at room temperature using Ga ion FIB. The ion acceleration voltage, ion dose, and dot interval were varied as parameters, and the fabricated structures were observed by plan SEM, cross-sectional

SEM and cross-sectional TEM. The ordered nano-cell structure is developed between 50–150 nm dot interval and the partitioning wall thickness is realized, proving that the new technique is promising.

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Tue-9.13po

Iron-oxygen interaction in silicon: a combined XBIC/XRF-EBIC-DLTS study of precipitation and complex building

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Keywords: DLTS, EBIC, XRF

Iron and oxygen are common impurities in silicon that play an important role in the formation of its electronic properties. It is well known that both species can form complexes with other impurities or native defects or form precipitates. However the information of their direct interaction is scant. The appearance of a new iron-related level in oxygen-reach silicon was reported [1] indicating the creation of some Fe–O molecular complexes. It was established that the presence of iron, despite of its thousands times lower concentration than that of oxygen, can drastically accelerate oxygen precipitation in silicon [2]. The origin of such strong catalytic action of iron and its relation to the creation of Fe–O complexes remains unclear up to now.

In this work we followed the evolution of iron in oxygen-rich silicon starting from iron atomic state in the lattice to the iron–oxygen complexes and to its final stage in precipitates. We applied conventional techniques to define electrical levels and recombination activity of defects in a combination with the synchrotron radiation based techniques which are capable to provide information about the elemental content and chemical composition of arising defects: deep level transient spectroscopy (DLTS), electron beam induced current (EBIC), X-ray induced current (XBIC), X-ray fluorescence microscopy (μ-XRF), X-ray absorption spectroscopy (μ-XAS).

Our initial samples were p-type CZ Si and mc-Si wafers doped with boron (2.5×10^{15} cm^{-3}) and with the initial concentration of interstitial oxygen of 7×10^{17} atoms/cm^3. Iron in-diffusion was performed from a surface source at 1150°C.

The contaminated specimens were subjected to various single step thermal treatments at 850°C, 950°C and 1050°C for 2–16 hours.

We found that the shape and the magnitude of DLTS signal as well as the density and the sizes of electrically active defects in EBIC/XBIC images changed strongly depending on the temperature and the duration of the post-annealing. Thus, for example, the treatment at 850°C for 16 h or at 950°C for 2 h transformed the initially observed levels due to FeB pairs and interstitial Fe_i to the single level at $Ev + 0.32$ eV previously interpreted [1] as a complex of Fe with O. Besides, this thermal treatment was accompanied with the appearance of the dense array of EBIC (XBIC) contrasts caused by the recombination active extended defects. The annealing at the higher temperature led to the significant lower concentration of FeO complexes together with the appearance of new defects with the level at $Ev + 0.18$ eV. The recombination activity of the extended defects was higher but their density was significantly lower in this case. XBIC/XRF measurements revealed the presence of iron precipitates at the positions of recombination active defects. A good correspondence between the recombination activity and the sizes of the precipitates was found. More detailed description of the results and their discussion will be presented at the Conference.

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Bistable character of a deep level in polycrystalline Si substrate for solar cell

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Keywords: polycrystalline silicon, DLTS, grain boundary, copper, hydrogen passivation

Electronic levels in p-type polycrystalline Si substrate for solar cell made by cast method have been studied by deep level transient spectroscopy (DLTS) measurement. We have found a broad peak at around 250 K ($E_\mathrm{v} + 0.47$ eV) whose intensity showed interesting behavior. If we re-measured the sample after the first DLTS measurement, the peak intensity became smaller. It was supposed that this was due to application of reverse bias voltage (V_R) on Schottky electrode for DLTS measurement. In fact, the peak reduction was observed more clearly after annealing under V_R at 300 K. The reduced peak intensity was recovered after the sample was kept at room temperature without V_R. These reduction and recover of peak intensity could be observed repeatedly. In relation to the origin of this peak, we have obtained the following results. This peak was not observed in the case that the measured region did not contain grain boundaries (GBs). Even if measured region contained GBs, we could not detect the peak when we kept the sample clean carefully. Such a sample with clean GBs came to show the DLTS peak after intentionally contaminated by Cu. Therefore, the origin of the peak must be attributed to the electronic level of Cu-related contaminants that are trapped by a grain boundary. The activation energy of the level (0.47 eV) is close to the previously-reported values of Cu in p-type Si [1] and there is no contradiction of the conclusion. We tentatively interpret the change of DLTS peak intensity as follows. There are two or more stable configurations of Cu near a GB. The most stable one under V_R is different from that without V_R, and the former has no gap level. The energy barrier between these two states can be surmounted at 300 K. From the application viewpoint, we tried to passivate this electronic level and that was attained by hydrogen treatment at 573 K for an hour, which will be also reported in the paper.

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Thu-10.1po

The effect of δ-doping on light emitting properties of InGaAs/GaAs quantum size heterostructures

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Keywords: electroluminescence, ferromagnetic semiconductors

Doping of A^3B^5 semiconductors with Mn is well known method of obtaining materials with ferromagnetic properties [1]. Prospective option of this method is d-doping of InGaAs/GaAs quantum well (QW) heterostructures. Our previous investigations have shown that the light emitting devices Schottky diodes fabricated on the basis of mentioned structures demonstrate both circularly polarized electroluminescence (EL) [2]. In the present work we investigate the properties of Schottly diodes based on InGaAs/GaAs heterostructures with d-doped GaAs barrier.

The structures were grown by two-stage epitaxial growth method. An $In_YGa_{1-Y}As$/GaAs QW ($Y = 0.1-0.2$) and the thin (3 nm) spacer GaAs layer were grown on n^+-GaAs (or i-GaAs) substrates by MOCVD at 600°C. At the next stage the d-doping and a GaAs cap layer growth were carried out at 400°C in the same reactor by the laser sputtering of a Mn and GaAs targets, respectively. The details are described elsewhere [2]. The nominal thickness of d layer (Q_{Mn}) was varied from 0.1 to 1.8 monolayers (ML). Another variable parameter was the position of additional d-layer with respect to d-layer. Delta doping was carried out in order to increase hole concentration in quantum well. The reference sample contained no d-layer.

The type of conductivity and 2D concentration of carriers in the QW/d structure were determined by the Hall effect measurements of the samples grown on i-GaAs substrates. All samples have a p-type conductivity with concentrations of holes up to 1×10^{12} cm^{-2} at 77 K.

The forward bias EL at 77 K demonstrated strong enhancement of the EL intensity in comparison with that of the similar samples without d-doping. The EL intensity non-monotonously depends on the Mn content as well as on a spacer layer thickness. The maximum of the EL intensity was obtained for the sample with $Q_{\mathrm{Mn}} = 0.1$ ML. The best thickness of a spacer between d and a QW was found to be 10 nm. The enhancement of the EL is believed to be due to increased hole injection into the QW with the inserted acceptor d-layer. This supposition is approved by $I - V$ characteristics that show the peculiarities related with additional hole current flowing.

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Thu-10.2po

Influence of the growing and annealing conditions on the structural properties of $Zn_{0.95}Mn_{0.05}O/Al_2O_3$ nanostructures produced by pulsed laser deposition

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Keywords: diluted magnetic semiconductors, Mn- doped ZnO nanocrystals, thin films

Transition metal doped ZnO attracted considerable attention recently as a good candidate to diluted magnetic semiconductors for spintronics. Theoretical calculations predict that p-type ZnO with 5% Mn should be ferromagnetic at RT [1]. Since then, extensive efforts have been focused on producing ferromagnetic ZnO by several growth methods. The results are diverse and some of them are in the contradiction. The origin of ferromagnetism at low Mn concentrations is still under discussions. Among the main reasons of ferromagnetism are carrier-induced interactions between the separated Mn atoms in ZnO [2, 3] and oxygen vacancies [4].

In this work, $Zn_{0.95}Mn_{0.05}O$ layers (with thickness 4–20 nm) and multilayered $Zn_{0.95}Mn_{0.05}O/Al_2O_3$ thin films were grown on Si(100) substrates by Pulsed Laser Deposition. Post growing annealing at different atmosphere was performed to study the formation of $Zn_{0.95}Mn_{0.05}O$ nanocrystals (NCs) in the dielectric matrix.

The crystalline structure and morphology of the nanostructures were characterized by Raman spectroscopy, grazing incidence X-ray diffraction (GID), grazing incidence small angle X-ray scattering (GISAXS), and high resolution transmission electron microscopy (HRTEM). NCs shape, size distribution and spatial arrangement were estimated from GISAXS using IsGISAXS program [2].

Annealing conditions are shown to be influent significantly to the crystallinity, size, shape, and distribution of NCs array. Moreover, GISAXS and GID techniques demonstrate to be powerful tools for characterization of buried NCs arrays.

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Thu-10.3po

Magnetic properties of Mn-doped ZnO nanowires

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Keywords: first-principles, diluted magnetic semiconductors, ZnO

Diluted magnetic semiconductors (DMS) are the most promising materials for spintronic devices due to the use of both the electronic transport properties of semiconductors and the memory characteristics of magnetic materials. The origin of ferromagnetism in Mn-doped ZnO nanowires is still not clearly understood and could be affected by factors such as additional carrier doping and point defects. Experimentally, nanobelts, nanorods, and nanowires have been fabricated using different growth environments, however, the ferromagnetic (FM) state was not observed in these nanostructures [1]. Other experiments showed that the magnetic ordering of Mn-doped ZnO nanorods is very sensitive to growth temperature, and the room temperature FM may be obtained by native point defects [2, 3]. Recently, using first-principles calculations, Shi, *et al.* have shown that the antiferromagnetic (AFM) state is favored in Mn-doped ZnO nanowires with the passivated surface, while, for unpassivated nanowires, the FM state, which may be influenced by surface electronic states, appears between two nearest Mn ions [4].

In this work we present the results of first-principles calculations within the local-spin-density-functional approximation (LSDA) and LSDA+U approaches for the magnetic properties of Mn-doped ZnO nanowires, where U represents the Coulomb repulsion on the localized orbitals of the magnetic ion. We use the projector augmented wave potentials for the ionic potentials, as implemented in the VASP code. We find that no ordinary FM coupling state between the nearest neighbor Mn ions is energetically favorable in the pseudo H-passivated ZnO nanowire doped with the Mn ions. On the other hand, the FM state can be stabilized if the antibonding t^a state formed by two adjacent Mn ions is partially occupied, which leads to an energy gain. Our calculations suggest that a partial occupation of the anitbonding t^a state is realized by the hole carrier doping such as dangling bonds on the wire surface, zinc vacancies which act as acceptors, and nitrogen acceptors which substitute for the oxygen sites.

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Thu-10.4po

Electron *g*-factor in laser-dressed low-dimensional semiconductor systems under applied magnetic fields

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Keywords: g-factor, laser effects, low-dimensional system

The effects of a laser field on the conduction-electron effective Landé g factor in GaAs–$Ga_{1-x}Al_xAs$ quantum wells and quantum-well wires under applied magnetic fields are studied within the effective-mass approximation. The interaction between the laser field and semiconductor heterostructure is taken into account via a renormalization of the semiconductor energy gap and conduction-electron effective mass [1, 2]. Calculations are performed for the conduction-electron Landé factor and g-factor anisotropy by considering the non-parabolicity and anisotropy of the conduction band. Theoretical results are obtained as functions of the laser intensity, detuning, and geometrical parameters of the low-dimensional semiconductor heterostructures, and indicate the possibility of manipulating and tuning the conduction-electron g-factor in heterostructures by changing the detuning and laser-field intensity.

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Thu-10.5po

Potentiality of light scattering management in photovoltaic cells through defect engineering in colloidal crystals

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Keywords: light trapping, colloidal crystal

The light harvesting in thin film photovoltaic cells can be facilitated through purposive photon management in the spectral range of the material's low absorption. Ideally, the role of trapping architecture is to increase the light path in the absorber, e.g., by converting the transversely incident light into longitudinal flow. In practice, the enhancing of the light scattering without increasing the cell reflectance can be a plausible target. We consider the structural modifications of colloidal crystals that lead to increasing the light scattering keeping in mind that owing to open porosity these crystals can be integrated with virtually any absorber.

The existing solutions rely on photonic crystals as the back-reflectors or the directional filters or the deflectors, but these options require high degree of ensemble crystallinity and exploit spectrally narrow diffraction bands. Alternatively, we suggested to enhance the light scattering and, hence, to trap the light, by engineering the artificial defects in low-cost inhomogeneous 3-dimensional photonic crystals. Such materials were conveniently realised using the Langmuir–Blodgett (LB) method for forced layer-by-layer assembling the colloidal crystals. The major advantage of the LB method is the tuneability of disorder in a crystal. Moreover, the disorder can be introduced independently either within the monolayer of crystallised colloidal spheres or in the ordering of stack of such monolayers. The idea of combining order and disorder allows to select the spectral range of enhanced scattering and to achieve the broadband operation.

To characterise the scattering strength, we estimated the transport mean free path for photons in different crystals using angle-resolved transmission, reflectance and scattering spectra. Increase of the ensemble complexity, like formation of the stack of monolayers assembled from spheres of different diameters, allows to reduce the mean free path of photons to few micrometers. This method allows also to efficiently couple the light into the structure by depositing a layer that acts as the non-reflecting coating.

Another approach is to generate the scattered light at the interface between ordered and disordered photonic crystals and to couple this light to evanescent modes propagating transversely along the interface. The hetero-crystal composed from the disordered LB crystal assembled on top of the opal film was design to explore this idea. It was observed, that scattering becomes strongly enhanced in the photonic bandgap intervals of such hetero-crystal. Hence, tuning the high order bandgaps to the desirable spectral range, that is achievable through choosing the sphere with appropriate diameters, is preferable because of the high spectral density of bandgaps. In such crystal more than 90% of the incident light, which falls on the photonic crystal film at moderately oblique incidence, is scattered at the interface: moreover, the scattering enhancement band spreads over the range of several hundred nanometres in the visible and the near-infrared.

Thu-10.6po

Low-threshold up-conversion luminescence in $Zn_xCd_{1-x}S$ with oxidated surface

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Keywords: solid solution, UP-conversion luminescence, photostimulated flash of luminescence

Creating nonlinear materials possessing up-conversion luminescence (**UCL**) excited by low intensity light beam at the temperature 300 K is relevant for the achievement of a number of objectives of optoelectronics such as low threshold up-conversion of light frequency and intensity. In this work the results of study of the low threshold (10^{-2}–10^{-3} W/cm^2) UCL in $Zn_xCd_{1-x}S$ ($x = 0.5-0.9$) solid solution crystals with oxidized surface are present. The modification of crystal surface was carried out with annealing at temperature 1100 K with following etching in 20% CH_3COOH.

The information of UCL was gained from the spectrums of excitation. The change of the density of electronic states that appeared while oxidizing the surface of the specimens was judged by the method of photostimulated luminescence flash (**PSLF**). PSLF was excited under the long-wave radiation ionizing deep electronic states of preliminary photo-excited crystals with the modified surface.

The excitation spectrum of UCL was placed in the range 1.9–2.0 eV. Its intensity changed non-monotonously as a result of etching $Zn_xCd_{1-x}S$ surface with 20%

CH_3COOH. This acid is capable of dissolving ZnO and CdO, while it is inactive to $Zn_xCd_{1-x}S$. Etching in CH_3COOH during 24–48 hours gave the largest intensity of UCL. At the same time monotonous blue shift of the excitation spectrum occurred. By means of PSLF method it was shown that etching of $Zn_xCd_{1-x}S$ in the presence of oxigen resulted in increase of concentration of electron states with depth of 1.2–1.8 eV under the bottom of conduction band. It is important that annealing in nitrogen atmosphere did not stimulate creation of UCL centers and deep electronic states. The presented data confirm that UCL centers are adsorbed $(ZnO)_n$ and $(CdO)_n$ clusters arising as a result of oxidation of $Zn_xCd_{1-x}S$ surface. It should be noted that deep electronic states in range 1.2–1.8 eV under the bottom of conduction band appear under Cd^{2+} and Zn^{2+} adsorption from $CdCl_2$ and $ZnCl_2$ solutions on the $Zn_xCd_{1-x}S$ surface, but UCL does not occur in this case. Therefore we examined possibilities cascade two-quantum excitation mechanism of UCL via deep electron states and Auger process in heterocontact region $Zn_xCd_{1-x}S/(CdO)_n$.

The research of the spectrum of UCL excitation by two monochromatic sources displayed that the UCL intensity does not change if the quantum energy of one of the sources is less than 1.85 eV. This phenomena can be described as the mechanism of UCL excitation — cold Auger process, because UCL excitation takes place through the local states, the absorption spectra, caused by the electron transition from the valence band to the level and from the level to the conduction band, can hardly coincide.

Therefore, UCL excitation in the samples of $Zn_xCd_{1-x}S$ ($x = 0.5-0.9$), annealed in the presence of oxygen, is brought about as a result of the cold Auger process in the quantum well, caused by the clusters of oxidated metals $(ZnO)_n$ and $(CdO)_n$.

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