Institute of Solid State Physics RAS

RAS Council on Low Temperature Physics

RAS Council on Condensed Matter Physics

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Abstracts

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PREFACE

The CC-2010 conference is organized by the Institute of Solid State Physics RAS, RAS Council on Low Temperature Physics, and RAS Council on Condensed Matter Physics in Chernogolovka, Moscow region, Russia. The scope of CC is wide, including, but not limited to, films, nanoscale systems, charged species in cryocrystals, spectroscopy of cryocrystals, ultra-low temperature and high-pressure studies, matrix isolation in cryocrystals, ultrafast dynamics in crystals, order-disorder phenomena, technological applications and instrumentation. The general approach of the Conference aims at organizing a forum for exchange ideas on various aspects of physical, chemical and technological properties of solidified gases, and gathering together the best experts in the field.

Conference on Cryocrystals and Quantum Crystals (CC) has a long history that was started in 1979 when the first seminar on cryocrystals and quantum crystals was organized in Viljandi, Estonia by V.G. Manzhelii (B.Verkin Institute for Low Temperature Physics and Engineering NASU, Kharkov, Ukraine) and A.F. Prihod'ko (Institute of Physics NASU, Kiev, Ukraine). The next seminars took place in Kharkov (Ukraine), Donetsk (Ukraine), and Odessa (Ukraine). Since the meeting in Almaty (Kazakhstan) in 1995, the Conference has had international status and has been the important international forum for presenting new results on physics and chemistry of atomic and molecular solids such as rare gas solids, hydrogen, nitrogen, oxygen, methane, helium isotopes, water ice, etc.. The next two international conferences took place in Poland, in September 1997 in Polanica Zdroj and in August 2000 in Szklarska Poreba. In 2002 the conference was held in Friesing (Germany), in 2004 - in Wroclaw (Poland), in 2006 - in Kharkov (Ukraine), and the last 7-th Conference was organized in 2008 in Wroclaw (Poland).

School of Young Scientists is planned to be held in frames of the CC-2010, where a few Public Lectures will be presented by the top-level experts.

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50 Years of Matrix Isolation of Atomic Free Radicals

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In the late 1950s, a broad program was initiated at the US Bureau of Standards to investigate matrix isolated free radicals at low temperatures for possible applications to efficient rocket fuels. N atoms and molecules or H atoms and molecules were condensed onto liquid helium surfaces and measurements were made by electron spin resonance (ESR), optical spectroscopy, a c susceptibility, X ray diffraction and thermodynamic measurements. Interesting results were obtained, but the atomic free radical concentrations were too small (<1%) to be useful in energy storage applications, particularly rocket fuels [1].

Activity in this area increased in 1974, stimulated by the discovery of a new sample preparation technique at Chernogolovka, Russia, by Gordon, Mezhov-Deglin and Pugachev, who dissociated a beam of N_2 molecules and projected it onto the surface of superfluid helium [2]. Later work by Gordon *et al.* led to extremely high concentrations of N atoms in N_2 matrices (ranging up to $[N]/[N_2]$ of 30%), as determined by ESR. H in H_2 and mixed deuterium/hydrogen samples were also studied via ESR [3], and evidence for the tunneling reactions $D+H_2 \rightarrow HD+H$ and $D+HD \rightarrow D_2+H$ was obtained [4]. Optical spectroscopy and X ray diffraction techniques were also employed. The latter method established that the samples were composed of network of nanoclusters (with linear dimension ~ 10 nm) containing the atomic free radicals and surrounded by layers of solid helium.

Lukashevich *et al*. condensed H atoms and molecules onto helium cooled surfaces and performed elegant mm wave studies in high magnetic fields [5]. They studied the exchange tunneling chemical reactions in hydrogen deuterium mixtures. The mm wave studies were continued at Turku University by S. Vasiliev and S. Jaakola. A group led by Miyazaki in Japan studied H and D atoms in solid hydrogen via ESR. The atoms were obtained by using γ rays to dissociate the molecules [6].

Subsequent X ray diffraction studies by Kiryukhin *et al.* determined the structure of the nanoclusters. The Cornell group also performed ultrasound studies of the superfluid contained in pores between the clusters to measure pore size. Further studies at Cornell were devoted to the kinetics of the tunneling exchange reaction. Very large concentrations of H atoms in Kr clusters were also studied via ESR. Collaboration between Turku University and Cornell University was devoted to mm wave studies of H atoms embedded in molecular hydrogen films down to ~ 100 mK. Interesting effects observed included a large deviation from the Boltzmann distribution for the two lowest hyperfine states of atomic hydrogen [7], Overhauser effect aided pumping between states and almost completely negligible recombination rates at the lowest temperatures. H atom concentrations of ~ 10^{19} cm^{-3} were obtained.

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New Findings in Simple Molecular Systems under Pressure

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The behavior of simple molecular systems under extreme pressures and temperatures is important fundamentally because of the large compressibility, marked changes in bonding and electronic properties, and dramatic alterations in physical and chemical behavior leading to novel phases in this class of materials. Hydrogen-rich molecular systems are of particular interest because their quantum properties can induce intriguing phenomena at high densities. Experimental techniques for studying these materials up to megabar (>100 GPa) pressures continue to evolve, and a growing variety of measurements are possible, including x-ray and neutron diffraction and inelastic scattering, optical and infrared spectroscopies, and transport methods. Recent results for pure hydrogen, related diatomic molecules, and hydrogen-rich and van der Waals compounds and alloys are described.

Vibrational Raman spectroscopy used in combination with laser and resistive heating has been employed to probe phase transitions and melting behavior to above 140 GPa [1]. Laser heating/x-ray diffraction experiments show that ε-O_2 above 1000 K reversibly transforms above 44 GPa to a new phase which has a melting curve that increases monotonically with pressure [2]. Recent spectroscopic studies of SiH_4 show that the material remains in an insulating state to megabar pressures [3], in contrast to earlier observations. The H_2 sublattice in the initial SiH_4-H_2 compound formed at low pressure exhibits a vibron spectrum that reveals strong intermolecular interactions as a function of pressure; new results constrain the crystal structures and the higher pressure behavior. Remarkable compounds in the Xe–H_2 binary system include a unique hydrogen-rich structure that can be viewed as a tripled solid hydrogen lattice and xenon dimers, a phase that can be stabilized at low pressures and temperatures [5]. The vibrational spectra indicate a weakening of the intramolecular covalent bond as well as persistence of semiconducting behavior in the compound to multimegabar pressures. A variety of studies of carbon-bearing systems have been carried out. The non-molecular form of CO_2 is stable over a broad range above 25 GPa; the phase dissociates in the fluid with a transition line having a negative *P-T* slope above 34 GPa [6]. New molecular compounds have been found in simple mixtures with carbon-bearing species at very modest pressures.

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Topological Media: Quantum Liquids, Topological Insulators and Quantum Vacuum

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The ether of the 21-st century is the quantum vacuum. The quantum ether is a new form of matter. This substance has some peculiar properties, different from the other forms of matter (solids, liquids, gases, plasmas, Bose condensates, radiation, etc.). But it shares many common properties with condensed matter. Quantum vacuum can be viewed as a macroscopic many-body system [1]. According to Landau, though the macroscopic many-body system can be very complicated, at low energy and temperatures its description is highly simplified. Its behavior can be described in a fully phenomenological way, using the symmetry and thermodynamic consideration. Later it became clear that another factor is also very important for the low energy properties of a macroscopic system – the topology.

Many quantum condensed matter systems are strongly correlated and strongly interacting fermionic systems, which cannot be treated perturbatively. However, topology allows us to determine generic features of fermionic spectrum. Momentum space topology determines the universality classes of fermionic vacua. In particular, the quantum vacuum of Standard Model of particle physics belongs to the same universality class as superfluid 3He in phase A and in planar phase. These topological superfluids have topologically protected gapless fermionic quasiparticles. At low energy these quasipaticles behave as relativistic massless Weyl fermions. Gauge fields and gravity emerge together with Weyl fermions at low energy. This allows us to understand the origin of physical laws and the hierarchy problem in Standard Model. The masses of elementary particles are very small compared to the Planck energy scale because the natural value of the quark and lepton masses is zero. The small nonzero masses appear in the infrared region, where the quantum vacuum acquires the properties of the fully gapped topological media: superfluid 3He-B and topological insulator.

In the limit of low temperatures, the main role in dynamics and thermodynamics of condensed matter systems and of quantum vacuum is played by zeroes in fermionic spectrum. The gapless fermions in topological media are protected by topology and thus survive deformation and interaction. The topologically stable gapless fermions arise:

(i) in topological superfluid 3He-A, in quantum vacuum of Standard Model in its semi-metal state, etc;
(ii) on the surface of the fully gapped topological medium, such as superfluid 3He-B, topological insulators and quantum vacuum of Standard Model in its massive state, and as edge states of systems which experience intrinsic quantum Hall and spin-Hall effects;
(iii) in the core of topological objects, such as different types of quantized vortices in 3He-B.

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Molecular Semiconductor Fullerite C_{60}

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The review deals with the electrical and other relevant properties of fullerite C_{60}. Being a typical superconductor, C_{60} differs cardinally in many respects compared to other semiconductor due to the fact that this solid is not only comprised of molecules but also has a rotational subsystem. Presence of molecular rotations changes drastically current-carrying characteristics if compared with traditional semiconductors. In particular, conduction is determined by a competition between disorders of two types.

Other properties, which might affect the current-carrying application characteristics of fullerite C_{60}, are also reviewed, including the kinetics of doping with chemically neutral species, material strength parameters, thermodynamics, etc.

Experiments with Ultracold Neutrons

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Ultracold neutrons (UCN) form a tiny low-energy fraction in the Maxwelian spectrum of thermal neutrons in moderators of nuclear reactors and spallation sources. Their energy is extremely small (~10-7 eV), their velocity equals a few meters per second only, and their effective temperature is as low as ~1 mK. The specific of UCN consists in their nearly total elastic reflection from the nuclear-optical potential of many materials at any incidence angle; therefore they could be stored in closed traps for extended period of time, thus used for extremely sensitive measurements. As the fraction of UCN in the thermal neutron flux is as low as 10^{-11}-10^{-12}, serious effort are undertaken all over the world to produce UCN in larger amounts, using super-thermal UCN sources or even equilibrium cooling of neutrons. UCN are widely used in precision particle physics experiments, such as, for instance, searches for additional fundamental short-range forces, searches for non-zero neutron electric dipole moment, precision neutron lifetime measurements, and constrains for the neutron electric charge.

Applications of UCN are emerging in surface and nanoparticle physics. We will focus on recent advances in the field, consisting in observation of the centrifugal quantum states of neutrons, providing, when combined with the observation of the gravitationally bound quantum states of neutrons, the first demonstration of the weak equivalence principle for an object in a quantum state. Also we will present a new spectrometer GRANIT constructed for precision studied of the gravitationally bound quantum states of neutrons and for other applications in particle physics, quantum optics, and in surface studies.

Finally, a promising methodical development in the field consists in building neutron reflectors based on nanostructured materials. Recently, powders of diamond nanoparticles have been used efficiently as the first reflectors for Very Cold Neutrons (VCN) in the complete velocity range from UCN to up to ~160 m/s, thus bridging the energy gap between efficient reactor reflectors for thermal and cold neutrons, and optical neutron-matter potential for UCN. Moreover, VCN could be stored in traps with nanostructured walls in some analogy to storage of UCN in traps.

A Mystery of Giant Growth Rate for the ^{4}He Crystal Facets

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Crystals of ^{4}He are best objects for studying fundamental problems of the thermodynamics and growth dynamics of phase interfaces. The factors, which determine these aspects, are as follows: high purity of a matter, contact with the superfluid liquid, and the lack of crystallization heat. The quantum nature of a helium crystal is manifested in the tunneling motion of elementary steps at the crystal surface [1]. This results in fast crystallization at the superfluid-crystal interface. Thus there has appeared a possibility for experimental study of the roughening transitions under equilibrium conditions as well as the growth dynamics governed by the interface processes alone, see review [2].

At the small deviations from equilibrium the facets grow in a full accordance with the classic models [3]. However, above some critical overpressure the crystal facet growth rate increases drastically by two or three orders of the magnitude [4]. At high overpressure a crystal grows at first with a small rate in the usual manner. Later, after some time interval the transition to the state of high growth rate occurs. The transition is observed simultaneously at the crystal facets of various orientations having different roughening transition temperatures. The build-up time and phase diagram of anomalous state are measured. The growth rates for the crystal facets of various orientations are determined as a function of the overpressure and temperature. The reentrant behavior of facets to the normal state with low growth rates is studied as well. The effect of facet growth acceleration is confirmed by the experiments on the dislocationless facet ("burst-like growth") [5].

The phenomenon observed has no explanation within the framework of the known models for the crystal facet growth. The search of qualitatively new mechanism has led to the development of the facet growth model based on the kinematics multiplication of steps [6]. Unfortunately, the numerical estimates show that the mechanism proposed is effective only at low temperatures but cannot be responsible for the phenomenon at high temperatures. So far, there is no theory describing all the experimental features of the phenomenon. A new qualitative approach is necessary.

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CC-2010 Oral Reports

Quantum Crystals and Formation of Supersolid from Excitations in Solid Matter

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Strong correlation regime and quantum phase transition into crystal phase controlled by the density are studied for 2D dipole Bose atom and dipole exciton systems by *ab initio* quantum simulations. The condensate fraction is calculated as function of the density. The collective excitation branch and appearance of roton minima is analyzed. 2D exciton and polariton traps are analyzed. We show using quantum Monte Carlo simulations that dipole excitons which are under experimental study now actually are strong interacting systems. This manifest itself in essential peculiarities in excitation spectra, in structure and condensate depletion which we discuss in the talk.

We have studied also the possible existence of a supersolid phase of a two-dimensional dipolar crystal using quantum Monte Carlo methods at zero temperature. Our results show that the commensurate solid is not a supersolid in the thermodynamic limit. The presence of vacancies or interstitials turn the solid into a supersolid phase even when a tiny fraction of them are present. The residual interaction between vacancies is repulsive making a quasi-equilibrium dipolar supersolid possible.

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Dust Liquids and Crystals at Cryogenic Dusty Plasma

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Dusty plasma is a unique laboratory tool for the investigation of the physics of systems with strong Coulomb interaction. This is due to the fact that the interaction of micron-sized dust particles 0.1-10 μm with charges up to 10^2-10^5 elementary charges may form the ordered structures of liquid (dust liquid) and crystal (dust crystal) types accessible to observe them at kinetic level, i.e. at level of behavior of separate particles of medium.

In present work the results of experimental and theoretical investigations of structural and dynamic properties of dusty plasma in dc glow discharge at the temperatures of 4.2-300 K were presented. The experiments were conducted in a gas-discharge tube cooled by cryogenic liquids (LN_2 and LHe) and their vapors. It was shown that “cooling” of thermal motion of ions down to cryogenic temperatures leads to decreasing of ion Debye radius and formation of super dense dust structures where density of dust grains can be of the order of plasma density and ion Debye radius can be close to grain size. The dependence of dust particle’s density on discharge temperature in dust structures was obtained. The kinetic processes of interaction of dust particles with the plasma component at cryogenic temperatures were analyzed with consideration for the ion-atom collisions. This analysis made possible to determine main mechanism responsible for the observed increase in the dusty plasma density. New data on correlation functions, particle velocity distribution functions and diffusion coefficient for dusty plasma at cryogenic temperature were obtained. The experimental observations of the waves and vortices under cooling the discharge down to cryogenic temperatures were presented.

This work was supported by the CRDF Grant RUP2-2891-MO-07, by NWO Grant 047.017.039 and by Research Program of the Presidium of the Russian Academy of Sciences “Thermophysics and Mechanics of Extreme Power Actions and Physics of Highly Compressed Matter”.

Melting Behavior of Hydrogen at Megabar Pressures

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Investigation of the phase diagram of hydrogen at very high pressures and temperatures has been actively pursued in the recent years to explore occurrence of novel ground states in general and the melting behavior in particular [1-7]. Recent first principle molecular dynamics studies converge on the prediction of a reentrant behavior the melting curve at high pressure and temperatures [4,5]. Experimental efforts to determine the melting behavior have not been satisfactory so far owing to several factors that include indirect diagnosis such as variation of sample heater temperature with laser power, electrical conductance changes or speckle changes and possible chemical reactions between hydrogen and the heater material that can influence these [6,7]. Recently, we have developed a methodology to confine and study H_2 at extreme conditions, wherein, in situ Raman spectroscopy in conjunction with laser heating can be done over multiple heating-cooling cycles on a highly localized sample region (5 µm in diameter x 4 µm thick) that is well isolated from the diamond anvils [8]. Here we present direct observations of phase changes in hydrogen from use of *in situ* confocal Raman spectroscopy in a fully automated laser heating arrangement [9]. A pronounced molecular vibron discontinuity has been found at elevated temperatures above 30 GPa along with a large broadening of the roton bands and changes in the laser speckle pattern; these phenomena are clearly indicative of melting. The vibron frequency discontinuity and broadening at the transition show a nonmonotonous behavior with a maximum at 70-100 GPa. Using the appearance of a new vibron as a criterion of melting, we mapped out the phase diagram of hydrogen at high P-T conditions. Our results are in fairly good agreement with the extrapolations of the previously measured in the resistively heated DAC data [2] up to approximately 110 GPa. Our data are in odd with the recent pulsed laser heating data [6] in that we do not observe a narrow maximum in the melting line. Beyond 110 GPa the melting line goes down in temperature abruptly deviating from the extrapolation of the Ketchin fit and from the melting points reported by Eremets and Trojan [7]. The observation of nonmonotonous pressure dependence of the vibron discontinuity and its sharpening in the fluid phase suggest that the H_2 fluid changes with pressure along the melting line. It is conceivable to connect this with the presence of the maximum in the melting line predicted theoretically [5] and inferred in the previous experimental studies [2,7]. Theoretical calculations predict the presence of a short-range orientational ordering for the fluid above the pressure corresponding to a turnover of the melting line [10]. Our observations of the narrowing of the vibron band in the high-pressure limit are in line with these predictions.

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New Data on Shock Compression of Liquid Nitrogen in 1-3 Megabar Range

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Thermodynamic properties of strongly shock-compressed liquid nitrogen are under discussion. The base is new experimental data, obtained recently in VNIIEF (Sarov) using hemispherical shock wave generators [1,2]. These experiments covered nitrogen Hugoniots in pressure range 100–3500 GPa and temperature range 10–80 kK. A nearly isochoric behavior of nitrogen Hugoniots is observed in new experiments. Such a behavior indicates existence in nitrogen plasma of a significant range of nearly constant Gruneisen parameter, $\mathrm{Gr} \equiv V(\partial P/\partial E)_V \approx 0.62$. The thermodynamics of shock-compressed nitrogen have been analyzed theoretically using so-called quasi-chemical model (code SAHA-N) where nitrogen plasma is described as strongly interacting (non-ideal) equilibrium mixture of atoms, molecules, ions and electrons. This approach supplements in the high-P_high-T region previous calculations of shock-compressed nitrogen of moderate parameters ($P < 100$ GPa) as series of molecular and polymeric states [3] [4]. Present experiments and calculations lead to conclusion that approximately at $P \approx 100$ GPa, $T \approx 16000$ K, and $\rho \approx 3.3$ g/cm^3 shock-compressed nitrogen comes through new type of “pressure ionization” – not from molecular (like hydrogen) but from polymeric state to the state of strongly non-ideal plasma.

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Lattice Distortion and Raman Scattering in HCP Cryocrystals Under Pressure

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Among cryocrystals only quantum crystals - solid helium and *J*-even solid hydrogens (p-H_2, o-D_2 and HD) crystallize in the hexagonal close-packed (hcp) lattice at ambient or low pressure. The heavier or classical rare gas solids (RGS) - Ne, Ar, Kr, Xe - crystallize into the face-centered cubic (fcc) structure. Diamond-anvil-cell studies have shown that the hcp phase can be stabilized at high compression in Xe, Kr, and Ar, with the fcc and hcp phases coexisting over a broad range of pressures. Contrary to expectations, a high-pressure x-ray diffraction study of solid Ne at the pressure range up to 200 GPa found that the crystal structure of Ne remains fcc.

Unlike fcc, the hcp structure has optical branches in the phonon spectrum. At zone center, one of the branches, an LO mode, is polarized along the *c*-axis. The doubly degenerate TO mode (symmetry E_{2g}) is polarized within the hexagonal planes and is Raman active.

Another distinctive feature of the hcp structure is an additional degree of freedom associated with the *c/a* ratio. A lattice of closed packed hard spheres has $c/a = (8/3)^{1/2} = 1.63299\ldots$ (the ideal hcp structure). The quantity $\delta = c/a - (8/3)^{1/2}$, the lattice distortion parameter, describes the deviation of the axial ratio from the ideal value.

We report here results of calculations of the lattice distortion parameter and Raman frequencies of hcp cryocrystals in the pressure range up to metallization. The calculations were performed using semi-empirical and first-principle approaches which complement each other: the former works better for low pressures, the latter for high pressures. In these calculations we used a many-body interatomic potential. Is small

Our study shows that for He and for hydrogen isotopes δ is small (of the order 10^{-3}) and negative in the entire pressure range. For Ar, Kr, and Xe δ changes sign from negative to positive as the pressure range increases, growing rapidly in the magnitude at higher pressures.

Fluid-Fluid Phase Transition in Strongly Compressed Polymerizing Nitrogen

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The problem of molecular-to-polymer transitions in simple polyvalent molecular systems and disagreement between existing experimental and recent ab initio simulation data for highly compressed nitrogen fluid is discussed.

A new equation of state based on a simple model of polymerization is proposed and applied to prediction of fluid-fluid coexistence line. We discuss the position of the second critical point and effects of negative thermal expansion in condensed polymerized nitrogen.

Matrix Isolation – Almost 100 Years Old, but Still Hale and Hearty

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Even though the term “matrix isolation” was only coined in 1954, in the laboratory of George Pimentel, experiments which today could fall well within the scope of “matrix isolation” were actually being carried out more than fifty years earlier. Already before the turn of the 20th century, persistent, long lived light emission – phosphorescence - from a variety liquid and solid solutions after their being exposed to x-rays or other high energy radiation was observed and extensively studied. The fact that rare gas solids, as well as frozen simple molecular gases such as nitrogen or oxygen provide suitable media for spectroscopic studies was first realized by Lars Vegard in his studies starting around 1924. Their goal was in fact the understanding and elucidation of Aurora Borealis which he initially believed to originate in small particles of frozen nitrogen “dust”. In 1945 Lewis and Kasha Berkeley have shown in that the long lived “phosphorence” is due to the spin forbidden emission from the lowest triplet state to the ground state. George Pimentel realized in 1954 that the solid rare gases provide an ideal, inert and transparent medium for spectroscopic studies of reactive, transient species and free radicals. I became involved in matrix isolation after joining Pimentel’s group in Berkeley in 1969 as a graduate student, and remained then active in the field for several decades and could observe its development ever since. While over the more than sixty years since the early Vegard studies the techniques, range of problems studied, and the goals of the investigations have changed continually, a steady flow of papers dealing with matrix isolation, and a multitude of conferences dedicated to low temperature spectroscopy and show that it remains even today a lively, productive field. It keeps yielding an uninterrupted string of interesting results, and the objective of my talk will be to review and discuss some of this work.

Colloids as Model Systems for Condensed Matter

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Colloidal suspensions consist of small particles in (mostly) aqueous medium, which allow to model phenomena in condensed matter on a mesoscopic scale. Due to the dominant length and time scales such systems are readily accessible by means of video microscopy. In this talk examples for both the structure of colloidal particle ensembles and transport phenomena in colloidal systems will be discussed. In the case of structure formation, melting and freezing of clusters consisting of only a few particles and the influence of periodic external potentials provided by modulated light fields is investigated. In addition, configurations of particles with a mesoscopic "spin" will be presented, realized by colloidal spheres with permanent magnetic caps, which allow one to model the spin configurations of magnetic clusters. The transport investigations focus on phenomena in narrow channels and constrictions, similar to nano-wires and point contacts.

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Novel Mechanism of the Negative Expansion of Fullerite C_{60} Doped with Chemically Neutral Species

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Recent high-precision dilatometric measurements (cf. Dolbin et al. [1] and references therein) showed that the thermal expansion coefficient α of pure and doped fullerite C_{60} at low enough temperatures is negative. At higher temperatures, the thermal expansion of doped samples demonstrated smooth peaks. The mechanism suggested [2] to explain the negative expansivity effect is based on tunneling rotations of C_{60} molecules in irregular areas of the fullerite lattice (grain boundaries, dislocation cores, etc.). The sign of α is determined by the respective Grüneisen parameter, which for transitions between tunneling-split levels is negative. The other phenomenon, namely, the peaks in the α(T) dependence was ascribed [3] to the so called polyamorphic transitions between different orientational glassy states of C_{60}.

If chemically neutral species (rare gas atoms or simpler closed-shell molecules like N_2, CO, CO_2, etc.) are introduced as interstitials into fullerite C_{60}, they can be responsible for an additional negative contribution to the thermal expansivity. This effect is well known in the thermal expansion of rare gas solids containing substitution molecules (cf. [4] and references therein) was explained using the energy spectrum, calculated by Devonshire [5] for a linear molecule in a filed of octahedral symmetry. This model is basically appropriate for treating the respective contribution to α(T) of C_{60} doped with linear molecules, though accurate estimates were lacking. As shown recently [6] for the specific case of Xe, for which the spherical oscillator approximation is valid, atomic impurities can also contribute negatively to the thermal expansivity of doped C_{60} due to tunneling-split rotational levels of the vibrational states. For other rare gas impurities, especially the lighter ones, the effective crystal field is far from purely oscillatory. The relevant crystal field potentials and spectra for atomic and molecular dopant have been calculated (see poster "Dynamics of dopant particles in octahedral voids of fullerite C_{60}" [7]).

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Heat Transfer in Solid N-alkanes

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Normal alkanes C_nH_{2n+2} are a class of substances taking an intermediate, transitional position between simple molecular solids and long-chain polymers. The n-alkanes have a relatively simple composition and a molecular packing in the solid state: the axes of molecules are parallel the one of the other and nearly perpendicular to the lamella plane. Yet, despite this seeming simplicity, they show a wide variety of dynamical behavior both in the solid and liquid states. There is an interesting "odd-even" effect alternating the orthorhombic versus triclinic unit cells between the adjacent members of the series as well as the presence or absence of premelting cylindrical rotator phases. The melting point alternation is another well-known phenomenon in n-alkanes; that is, the even-numbered members of series melt at a relatively higher temperature than the odd-numbered members [1].

The short-chain ($n \leq 6$) n-alkanes are the least known members of the series. The crystal structure of ethane and propane is $P2_1/n$, and n-hexane is $P\bar{1}$ [1]. The triple points and entropy of melting of these substances $\Delta S_f/R$ are 90.3K and 0.77, 85.5K and 4.96, 177.8K and 8.85 correspondingly. To compare correctly experimental results of thermal conductivity with theory, it is necessary to perform experiments at a constant density to exclude the effect of thermal expansion. The measurements reported were carried out by a stationary method in a coaxial geometry high-pressure cell. The isochoric thermal conductivities of solid ethane (C_2H_6), propane (C_3H_8), and n-hexane (C_6H_{14}), have been investigated on samples of different densities. In all the cases the isochoric thermal conductivity exhibits dependences that are weaker than $\Lambda \propto 1/T$. As was shown earlier, the deviations of the isochoric thermal conductivity from the dependence $\Lambda \propto 1/T$ in the orientationaly - ordered phases of molecular crystals can be described using a model in which heat is transported by low-frequency phonons and by "diffusive" modes above the phonon mobility edge [2]:

$$\Lambda = \Lambda_{ph} + \Lambda_{dif} \qquad (1)$$

"Diffusive" refers to the modes whose mean free path is of the order of half wavelength $\alpha\lambda/2$, where $\alpha \approx 1$ [3]. We calculated appropriated contributions for ethane, propane, and n-hexane. The "diffusive" behavior of the vibrational modes begins manifest itself in ethane and propane above 50K, and in n-hexane above 110K. The "diffusive" contribution increases with temperature but it is smaller than phonon one even at premelting temperatures. This is in good agreement with the big thermal conductivity change at melting. The results obtained are compared with the thermal conductivities of other n-alkanes ranging from C_9H_{20} to $C_{19}H_{40}$ [4].

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A Quantum Theorem of Corresponding States Study of Small Quantum Fluid Clusters

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There is currently great interest in understanding superfluidity in small para-hydrogen (pH_2) clusters. Since at low temperatures pH_2 molecules are spin-less bosons Ginzburg and Sobyanin in 1972 predicted that pH_2 should be superfluid below about 6 K [1]. Superfluidity cannot be observed in the bulk since hydrogen freezes below the triple point at 13.8 K. Several Path Integral Monte Carlo (PIMC) calculations predict, however, that small pH_2 clusters ($N \leq 26$) are superfluid below about 2 K. [2] In contrast ^{4}He clusters of all sizes are predicted to be superfluid as demonstrated experimentally either indirectly for small clusters or directly for large clusters. To understand better the relation between pH_2 and ^{4}He clusters we have undertaken a Quantum Theorem of Corresponding States (QTCS) study of cold N = 13 and N = 26 quantum clusters. [3] According to QTCS the thermodynamic functions of a class of systems with a pair potential of the form $V(r) = \varepsilon V^{*}(r/r_0)$, when expressed in terms of the appropriate reduced dimensionless variables, will be the same for a given value of the de Boer parameter $\lambda^{*} = \lambdabar(\varepsilon)/r_0 = \hbar / r_0\sqrt{m\varepsilon}$, where $\lambdabar(\varepsilon)$ is an effective de Broglie wave length for relative motion with energy ε. Thus as $\lambdabar(\varepsilon)$ increases relative to the range of the potential r_0, which is proportional to the average distance between the particles, quantum delocalization becomes increasingly important. In addition to the reduced potential V^{*} and reduced distance, usually denoted by $x = r/r_0$, other important reduced quantities are the densities $\rho^{*} = \rho r_0^3$ and the various energies such as the total energy $E^{*} = E/\varepsilon$ and the temperature $T^{*} = T/\varepsilon$.

PIMC calculations of the energies, densities, radial pair distributions and pair distributions and superfluid fractions are reported at T = 0.5 K for a Lennard-Jones (12,6) potential using 6 different de Boer parameters including the accepted value for hydrogen and helium. The results indicate that the hydrogen clusters are on the borderline to being a non-superfluid solid but that the molecules are sufficiently delocalized to be superfluid. A general phase diagram for the total and kinetic energies of LJ (12,6) clusters encompassing all sizes form N = 2 to N = ∞ and for the entire range of de Boer parameters is presented. Finally the limiting de Boer parameters for quantum delocalization induced unbinding are estimated and the new results are found to agree with previous calculations for the bulk and smaller clusters.

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Regular-Chaotic Transitions in Quantum Dynamics of Nanosystems

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Unlike continuous spectra of macroscopic solids, the spectra of nanosystems are discrete. The discrete character of spectra results in the appearance of recurrence cycles, in which the population of the initially prepared state is partially revived. According to Poincare theorem, the period of recurrence cycles is determined by the mean inter-level spacing between neighboring levels.

A dynamical problem for an initial state coupled to a reservoir (a manifold of other states) has been analytically solved for various reservoir spectra, from regular to random one. It is demonstrated that a multi-component Loshmidt echo arises in each recurrence cycle. The number of components and the total width of the echo increase with increasing cycle number. At the certain critical cycle number, the components of neighboring cyc;les are overlapped and mixed. As a result, the initial state dynamics transforms from a regular to stochastic-like, in which an arbitrary small coarse graining (inherent to any real systems) leads to (i) the loss of one-to-one correspondence between the regular spectrum and irregular long-time evolution,
(ii) the loss of invariance with respect to time reversal.

When the spectrum is equidistant and coupling constants are the same for all reservoir states, the critical cycle number is $K_c = \pi^2 C^2 / \Omega^2$ (Ω is spacing, C is coupling constant). K_c decreases under equidistant spectrum deformations. Regular evolution disappears when the mean critical value of violations from mean spacing is achieved: $\langle \Omega_{n+1} - \Omega_n \rangle / \langle \Omega \rangle \geq K_c^{-1}$.

Reverse states are depleted synchronically in time leading to above described Loshmidt echo. Synchronization is held in initial recurrence cycles up to the critical cycle number. The reverse transitions from reservoir states to initial one leads to appearance of narrow double resonances at all reservoir state eigen-frequencies. These resonances are kept even in the stochastic-like region of the initial state evolution.

Two new phenomena described above – multicomponent Loshmidt echo and double resonances, as inherent specific feature of nanosystems, are responsible for a wide variety of evolution regimes (from exponential decay to irregular weakly damped oscillations) observed with the femtosecond spectroscopy techniques in various objects, common feature of which is the inter-level spacings of order 1-10 cm^{-1}.

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Nuclear Spin Ordering on the Surface of a ^{3}He Crystal: Magnetic Steps

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The growth rates of the basic, (110) and (100) facets on bcc ^{3}He crystals have been measured near the nuclear magnetic ordering transition at T_N=0.93 mK. In the ordered phase, we have observed several growth modes corresponding to different values of the step energy. We show that because of the quantum delocalization, the step induces a cluster of ferromagnetically ordered nuclear spins. The free energy of such a cluster is relatively large and depends on the orientation of the underlying antiferromagnetic domain. In the paramagnetic phase, the mobilities of the basic facets are greatly reduced because of the much slower spin diffusion in the bulk solid.

Phenomena on the Surface of Solid ^{4}He

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Recently we have observed [1] the so-called devil's staircase of high order facets on the surface of hcp ^{4}He crystals at 0.2 K. Such high roughening temperatures of high order facets could be associated with elementary kinks on the basal step, which would have correspondingly high excitation energy. As the free energy of the basal step is only 0.1 K, such kinks would provide a strong anisotropy of the basal step and, consequently, of the stiffness of vicinal surfaces, which was never observed before. With our interferometric technique we were able to measure the anisotropy of the stiffness of the basal step and of the azimuthal stiffness of vicinal surface and found it as high as 5-10 at low temperatures. We have measured also the temperature dependence of the anisotropy and found that the anisotropy disappears at 0.4-0.5 K.

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Crystal Shape and Crystal Growth of ^{3}He:
The Influence of Magnetic Order

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Experiments on crystal growth and crystal shape in ^{3}He at zero magnetic fields have revealed many new facets and strong anisotropy in the growth rates. One of the remarkable conclusions is the apparently dominating influence of the elastic interaction between the steps on the facets even for non-vicinal facets. Also unexpected was the apparent stiffness of the ^{3}He solid/liquid interface as compared to the situation in ^{4}He. It has been suggested that this is related to the magnetic interaction and ordering in the solid ^{3}He.

Solid ^{3}He orders magnetically into two different phases below the Néel transition depending on the magnetic field (*U2D2* or *low field phase* below 450 mT and *CNAF* or *high field phase* above 450 mT). This presents the unique possibility of investigating the influence of a magnetic field or magnetic order on the crystal growth properties. We have experimentally studied the shape and growth rate of solid ^{3}He in magnetic fields up to 9 T in our optical access cryostat with low temperature CCD and obtained clear images of the growth process.

We have performed measurements of the growth velocities and determined the step energies for different facets in both phases at B=0 T and B=2 T. It was found that the growth rate is much faster at B=2 T than at zero magnetic field. If we analyze the results in terms of a linear dependence of the facet growth velocity versus overpressure [1], we can determine the step energy for each facet type, at each value of the magnetic field (see figure below). We conclude that the ordering of the spins in the solid clearly affects the growth process of the crystals.

The Effect of ^{3}He Impurities on New Phase Nucleation Under Bcc-Hcp Phase Transition in Helium Solid

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Pure ^{4}He bcc crystals and 1% ^{3}He bcc solid mixture are studied by precise pressure measurement technique under constant overcooling ΔT. The lifetime τ of the metastable bcc phase was measured under different ΔT. The bcc-hcp phase transition is accompanied by both a sharp pressure decrease ΔP under constant volume condition (down to 1 bar) and a simultaneous appreciable heat release in the sample up to 25 mK. Decreasing of the overcooling leads to increasing the overcooled crystal lifetime τ from several seconds to several hours. The dependence of nucleation frequency J on overpressure ΔP for the bcc-hcp phase transition in ^{4}He demonstrates both homo- and heterogeneous nucleation mechanisms under different values of ΔP. Only heterogeneous nucleation is detected in 1% ^{3}He -^{4}He bcc mixture. A role of possible centers of nucleation including ^{3}He atoms is discussed.

Oscillation Spectra of a Crystal ^{4}He Facet and Its Destruction with Generating Crystallization Waves

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For rough ^{4}He crystal facets, crystallization waves are the well-known phenomenon. The same point for the smooth 4He crystal facets is less familiar. Here we study the spectrum of crystallization waves at the smooth crystal facets of a ^{4}He crystal. Besides the wavelength, the frequency of crystallization waves also depends both on the perturbation wave amplitude and on the number and arrangement of crystal facet steps per wave length. The smaller the wave amplitude and the more the number of facet steps, the larger the wave frequency. The continuous generation of crystallization waves results both in the destruction of crystal faceting and in the transition to the rough state of a crystal facet.

Probing the Phonon Spectra of Condensed ^{4}He with Atomic Impurities

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The phonon spectrum is an important characteristic of quantum fluids and solids and for such systems is mostly measured by neutron scattering. However, in conventional solids, optical (including infrared) spectroscopy of dopants is often used to investigate the lattice vibration spectrum. Optical and IR absorption spectroscopy has also been applied to the study of vibronic spectra of various molecules in quantum matrices, such as ^{4}He and ^{3}He droplets [1]. However, very little is known about the vibronic spectra of atoms and molecules in bulk condensed helium.

Here we present a systematic spectroscopic study of transition-metal (Au and Cu) atoms in normal fluid, superfluid and solid ^{4}He. Atoms implanted in the quantum matrix are laser-excited to high lying states, and the resulting fluorescence spectra are observed at different pressures and temperatures of the helium bulk.

Metal atoms in condensed helium reside in nanoscopic-size bubbles (topic reviewed in [2]). The metal atom to helium environment interaction results in modifications of the absorption and fluorescence spectra of the dopant's electronic transitions. We observe both outer shell and inner shell transitions.

Electronic transitions in the outer shell induce a sudden change of the bubble size and bubble interface oscillations, which can be understood as excitations of local or pseudo-local modes of the host matrix. The interaction leads to a strong homogeneous broadening and a blue shift of the atomic spectral lines. The fluorescence spectra of outer shell transitions depend strongly on He pressure – more specifically, the He density – in the three condensed phases, similarly to the well-understood spectra of alkali atoms [2].

The *d*-electrons in the inner shell are screened by the outer closed S-shell. Transitions of inner shell electrons therefore do not induce large changes of the bubble configuration, and the excitation of local modes is expected to be strongly suppressed. Nevertheless, we have observed a weak coupling of the *d*-electrons to matrix excitations (phonons). Fluorescence spectra of inner shell transitions have two common features – a sharp zero phonon line (ZPL) very close to the free-atomic transition frequency and a broad phonon wing (PW) on the red side of the ZPL. We speculate that the nature and shape of the ZPL and PW are universal and could thus be used to characterize excitations of the host matrix.

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Wigner Crystals Confined in Micrometer-Wide Channels

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Electrons floating on the surface of liquid helium form an ideal classical two-dimensional electron system with a density of 10^{12}-10^{13} m^{-2}. The ground state of this electron system is an electron crystal called Wigner crystal because of the predominance of the Coulomb interaction over the kinetic energy. In the Wigner crystal phase, the localized electrons are self-trapped in the commensurate deformation of the helium surface called dimple lattice. The appearance of the dimple lattice generates strong coupling between the Wigner crystal and helium surface, giving rise to a number of distinct phenomena in the transport properties of the Wigner crystal. Here we present the results of transport measurements of the Wigner crystal formed on superfluid ^{4}He and confined in quasi-one-dimensional channels 5, 8, and 15 μm in width, and ~900 μm in length.

The long channel geometry of our channels is suitable for observing clear nonlinear phenomena arising from the strong coupling between the Wigner crystal and helium surface. We observed that, in the Wigner crystal phase, the resistivity shows an increase with increasing excitation. At the same time, the velocity of the electrons saturates at the phase velocity of ripplons with the wavenumber which is equal to the first reciprocal lattice vector of the Wigner crystal. These are caused by the resonant scattering of ripplons by the Bragg-Cherenkov mechanism[1]; an electron traveling faster than the ripplon phase velocity radiates ripplons as in the case of the Cherenkov radiation, and ripplons emitted from different electrons interfere constructively if the wave number of the ripplons equals the reciprocal lattice vector of the Wigner crystal (the Bragg condition), resulting in the drastic increase of the scattering rate. At a high excitation, we observe a jump in the velocity to a very high value. This is attributed to the decoupling of the Wigner crystal from the dimple lattice. The magnitude of the driving field necessary to induce the decoupling indicates that the decoupling occurs from the dimple lattice which is dynamically deepened due to the Bragg-Cherenkov scattering[2].

The Bragg-Cherenkov scattering occurs only in the Wigner crystal phase, and therefore the Bragg-Cherenkov scattering provides useful information on the melting process of the Wigner crystal. We have investigated the melting process of the Wigner crystal confined in quasi-one-dimensional channels for three channel width (5, 8, and 15 μm), paying special attention to the Bragg-Cherenkov scattering. In two-dimensional system, the melting of the Wigner crystal is driven by the dislocation-mediated Kosterlitz-Thouless-Halperin-Nelson-Young mechanism[3]. In our quasi-one-dimensional channels, the properties of the melting should be strongly affected because the characteristic size of dislocations (~1 μm) is comparable to the channel width, and one-dimensional nature should appear. By changing the electron density systematically (10-60 electrons in width), we find that the BC scattering disappears at a higher temperature for fewer electrons in the confined direction, indicating that the crystal-like structure persists to a higher temperature for fewer electrons. We show that this behavior is understood by a model describing how the positional correlation is disordered by free dislocations in the quasi-one-dimensional geometry.

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Solvation of Impurities in Bulk Superfluid Helium

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Diffusion mediated clustering of atoms and molecules in superfluid helium may be significantly affected by the weak long-range interactions at low temperatures. When impurities are solvated in the liquid, the possible attractive van der Waals binding introduces strongly inhomogeneous helium solvent layers to form around them (i.e., the snowball structure). As two impurities approach each other in the liquid, the interaction between the solvent layers surrounding them causes deviation from the regular gas phase pair interaction where the overlap between the solvent layers introduces an energy barrier for impurity - impurity recombination. The present bosonic density functional theory calculations predict ca. 3.2 K recombination barrier for two solvated Ne atoms in the liquid. The effect of zero-point energy for light impurities is important and hence it must be included in the calculation. When many spherical impurities are present, this effect is expected to lead to a self-assembly process resulting in a quantum gel structure. In the case of non-spherical impurities, the anisotropic solvent layer structure is expected to lead to the self-assembly of 1D and 2D structures ("solvent layer guiding"). The present model also allows for the time-dependent treatment, which can be used to study impurity - impurity scattering in the liquid.

Atomic and Molecular Spectra Emitted by Normal Liquid ^{4}He Excited by Corona Discharge

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Liquid ^{4}He under fixed temperature 4.2K and different pressures up to 8 MPa was excited by corona discharge both negative and positive polarity. Tungsten tips had radii r_p in the range 0.45-2μm. The electrode spacing was d=8 mm. The high voltage from a stabilized dc power supply was connected to the point electrode. Light emitted from the region close to the point electrode is collected on the entrance slit of a spectrograph (SpectraPro-300i, 300 mm focal length, aperture f/4.0), equipped with 3 gratings (150gr./mm and two of 1200gr./mm blazed at 750nm and 300nm respectively). The 2D-CCDTKB-UV/AR detector is located directly in the exit plane of the spectrograph. Its dimensions are 12.3x12.3mm with 512x512 pixels of 24x24μm for each pixel. In order to reduce the dark current, the detector was cooled to a temperature of 153K (dark current <1e/pixel/heure at 153K). In our conditions, the instrumental broadening measured by recording profiles of argon lines from a low pressure discharge lamp is $\Delta\lambda$=0.098nm for a 1200gr./mm grating.Emission HeI atomic lines and He_2 molecular bands are observed. Using a 1200gr./mm grating, spectra of higher resolution are obtained which show clearly atomic lines 706.8nm and 728.1nm and molecular bands 660nm and 640nm. The atomic lines spectra show (i) a distinct blue-shift with increasing pressure and (ii) line-broadening which becomes stronger with increasing pressure. The rotational structure of the band is resolved at the pressures (0.1 -0.2) MPa. The non-resolved profile of the band recorded at 0.6 MPa resembles the one from [1] where superfluid helium was bombarded with high energetic electrons. The shift of the Q-branch maximum at different pressures is studied. The shift measured is in a good agreement with experimental data [2] obtained in superfluid He II at 1.7K. The rotational structure of the singlet band $D^1\Sigma^+_u$ - $B^1\Sigma_g$ resolved for pressures < 0.2 MPa is similar to that observed in luminescence of liquid droplet excited by synchrotron radiation [3]. Rotational temperatures of 800 K were estimated showing that the excitations do not thermalise. Similar high rotational temperatures were observed for excimers ejected from photo excited ^{3}He and ^{4}He clusters and droplets [4, 5]. Furthermore, the populations derived from the P-branch intensities are larger than those from R-branch lines intensities. This fact can formally be interpreted by the existence of an additional source of radiation. The corona discharge on point anode (positive corona) was realized if a radius of the electrode was small enough, 0.45μm, and voltage was some larger than that in the case of the negative corona. The mobility of electrons and positive ions are close each other in LHe. Therefore, electric currents both negative and positive corona differ weakly. However the spectral analysis of the radiation from the positive corona shows qualitative differences of spectral features of these discharges. Both atomic lines and molecular bands were observed in the spectra of the positive corona in LHe at 4.2K under different applied pressures. The spectra observed in the positive corona have marked non-symmetric shape. The atomic spectra show an increased intensity of their long-length tails. Red satellites have been observed in the vicinity of both atomic and molecular lines. Comparison of intensities of R- and P-branches of the rotational structure of band $d^3\Sigma^+_u$ - $b^3\Pi_g$ shows increased intensity of the P-branch lines. This effect is more significant than in spectra of negative corona. The work was supported by RFBR NN 08-08-00694 and 09-08-01063.

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Propagation of Strongly Nonlinear Second Sound Waves In Anisotropic Phonon Systems

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It is at present, impossible to create in superfluid helium, a constant relative velocity, w, between the normal and superfluid which is close to the Landau critical velocity. However phonon pulses can be created, which are pulses of normal fluid moving through the stationary superfluid with a high relative velocity, without superfluidity breaking down. These pulses are $t_p = 10^{-5}$–10^{-7} s, long. In a recent paper [1] detailed measurements of the angular distributions of the energy in the phonon pulse were reported at zero pressure. The measurements were made at different distances from the heater, with various heater sizes and heater powers. The results showed a notable feature; the angular dependence of the energy flux of low energy phonons has a flat top, and concave steep sides. In [1] this kind of distribution was called a mesa shape. The dependences of the mesa height and width, on heater dimensions, distance to the detector and heater power, were measured [1]. Such phonon energy distributions cannot occur in the ballistic regime. In this case we would have cosine-like convex angular distribution, as it follows both from experiments at high enough pressure (above 19 bar) and from theoretical considerations (Lambert's law). At zero pressure we assume we have a hydrodynamic regime in the wings of the angular distribution, where the phonon density is sufficiently high, as well as in the centre of the pulse. We can use hydrodynamic description within a pulse comprised of low energy phonons due to the strong three-phonon scattering, which leads to a quasi equilibrium. Thus low energy phonon pulses can be defined in terms of a temperature T and a drift velocity w. Fast three phonon relaxation has been observed directly in the experiments with colliding phonon pulses [2]. Another feature of such phonon systems is that the energy density in the phonon pulse is much larger than the ambient phonon energy density in superfluid helium. Therefore the evolution of a strongly anisotropic phonon system must be essentially nonlinear. Nonlinear waves in superfluid helium, when w is small, have been studied for many years, but the analysis of nonlinear waves at arbitrary w has not been done until now. We present a theory for the formation of a mesa shaped phonon pulse, created by thermal pulse in superfluid helium. Starting from the hydrodynamic equations of superfluid helium, we obtain the system of nonlinear equations which describe the evolution of strongly anisotropic phonon systems created by thermal pulses in "superfluid vacuum" of helium. The family of exact solutions was found in an explicit analytical form. They are the simple waves of second sound for phonon systems. The relations between temperature T and components of the relative velocity **w** are studied for these waves. Using these exact solutions, we describe the longitudinal and transverse expansion of phonon pulses in superfluid helium at zero temperature. We find the expansion velocity of a phonon pulse into the "phonon vacuum", i.e. into superfluid helium with zero temperature. The theory developed allows us to qualitatively understand why the mesa width increases with decreasing the heater width [1]. A smaller heater width results in an earlier formation of the mesa, and this leads directly to an increase in the mesa width. This theory gives an explanation for the mesa width and height observed in the measured phonon angular distributions. Almost all dependencies of the mesa width and height on various parameters can be qualitatively understood.

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Radiation Effects in Atomic and Molecular Cryocrystals Probed by Optical and Current Spectroscopy

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Irradiation of materials by ionizing radiation is the generally recognized way of material properties change [1,2] and deep understanding of underlying radiation effects is not merely of fundamental interest but also an important prerequisite for many novel technological applications in material and surface sciences. Cryocrystals universally accepted as model insulating materials are perfectly suited for such a study. Despite the simplicity of these materials they show quite a rich branched relaxation pattern especially for doped cryocrystals e.g. [3]. Relaxation cascades involve a variety of neutral and charged particles – charge carriers (electrons and holes) trapped/self-trapped, ionic species formed by dopant, atoms and radicals. Processes of charge and mass transfer, as well as energy conversion in radiation-induced reactions form a basis of the relaxation scenario.

Here we present the short overview and our new results on radiation effects in atomic and molecular cryocrystals with a focus on the phenomena observed on completion of irradiation by an electron beam. Transformation of electronic states, defect formation, sputtering and appearance of new species on exposure time were monitored by emission spectroscopy. Electrons and neutral species formed were thermally or optically mobilized triggering relaxation cascades through recombination reactions. A set of relaxation emissions: emission of photons, exoelectrons and neutral particles was measured in time-correlated fashion.

It enabled us (i) to discriminate between reactions of charged and neutral species, (ii) to find nontrivial interconnection of atomic and electronic relaxation channels in doped rare-gas cryocrystals, (iii) to predict new relaxation channels triggered by radiative transitions, (iv) to detect anomalous low temperature post-desorption of “own” lattice atoms and to elucidate dominant processes underlying the phenomena in atomic and molecular cryocrystals.

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Structural Phase Transitions in Thin Films Glassy Condensates

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Experimental researches (using infrared spectrometry and thermodesorption) of structural-phase transitions in thin films of cryovacuum condensates were performed. Alongside with already known “glassformers” – water and ethanol – data for nitrous oxide cryocondensates are presented. The singularities observed at T≈38 K could be interpreted as indication to amorphous-crystal transition.

High Resolution EPR Spectroscopy of High-Spin Pyridylnitrene Molecules In Solid Argon

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The high-spin molecules represent a ferromagnetic electron spin cluster, being small enough for the exchange interaction between unpaired electrons to be dominant, enabling to define a total spin $S > ½$ in the ground electronic state. Such a type of molecules, so called "single molecular magnets" (SMM), attracted special attention aimed at the development of new magnetic materials. Important feature of such molecules is the internal magnetic anisotropy resulting in the splitting of $2S + 1$ magnetic sublevels even in the absence of an external magnetic field (zero field splitting, ZFS). The ZFS parameters are important characteristics of magnetic anisotropy; experimental measurements and theoretical predictions of ZFS parameters are the fundamental problems in design of the SMM's. Among all organic polyradicals, high-spin nitrenes have the largest ZFS parameters, exhibit the strongest ferromagnetic exchange interactions between unpaired electrons and are characterized by large energy gaps (~ 5-10 kcal/mol) between the ground high-spin and excited low-spin states. Therefore, such molecules are of considerable interest as the model systems for explorations of internal magnetic anisotropy in multi-spin molecular systems.

In this study the high resolution EPR spectra of quintet (S = 2) and septet (S =3) pyridyl-nitrenes isolated in solid argon matrix were recorded at 15 K. All EPR lines of the studied high-spin intermediates were unambiguously assigned based on the eigenfield calculations of the Zeeman energy levels and angular dependencies of resonance magnetic fields. Owing to high resolution of EPR spectra in solid argon matrix, the zero-field splitting parameters ($\boldsymbol{D}$ and $\boldsymbol{E}$) were determined with accuracy better than 10^{-3} cm^{-1}. These parameters provide correct information regarding the molecular angle and distance between two nitrene units. [1] Analysis of the magnetic parameters based on the DFT (B3LYP) calculated molecular geometry and spin populations on the nitrene groups shows that widely-used semi-empirical model of the fine-structure tensor [2] gives good prediction of the ZFS parameters for the quintet nitrenes as well as of the parameter $\boldsymbol{D_s}$ for the septet nitrenes, whereas the calculated parameter $\boldsymbol{E_s}$ in the chlorine-substituted septet trinitrene is on ~ 70 percent greater that that measured experimentally.

Theoretical DFT study of the ZFS parameters in experimentally well characterized nitrenes demonstrates that the most accurate predictions (within 10%) are achieved by using the pure BPE density functional in combination with the DZ basis sets. For high-spin nitrenes constituted from light atoms, major portion of the $\boldsymbol{D}$ parameter originates from the one-center spin-spin (SS) interactions, whereas the contribution of the spin-orbit interactions (SOC) to ZFS's is quite small (7-12 %). By contrast, for chlorine-substituted septet trinitrenes, the contribution of the SOC part is small only to $\boldsymbol{D}$ value but, in the case of $\boldsymbol{E}$ value, it is comparable in magnitude with the SS part and of opposing sign. Due to this partial cancellation of two different contributions, SS and SOC, the resulting values of $\boldsymbol{E}$ in heavy molecules of septet trinitrene are almost two times smaller than those predicted by analysis of the semi-empirical model [2]. This fact proves a validly of the semi-empirical consideration [2] for high-spin nitrenes with total spin S = 2 and 3, if their molecules are constructed from the first-row atoms and the contributions of the SOC term to the ZFS parameters are small. This work was supported by the Russian Foundation for Basic Research (Grant No. 07-03-00768) and the Russian Academy of Sciences (program № Okh-01).

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Electron Spin Resonance Studies of Hydrogen and Deuterium Atoms in Krypton-Helium Condensates

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Impurity-helium condensates containing krypton atoms along with atoms and molecules of hydrogen isotopes have been studied via continuous wave electron spin resonance (ESR) technique [1, 2]. Analysis of ESR spectra shows that most of the H and D atoms reside in molecular layers (H_2, D_2 or HD) formed on the surfaces of krypton nanoclusters. By changing the content of hydrogen isotopes injected into superfluid helium with the Kr-He gas mixture, we can alter the thickness of molecular hydrogen isotopes films formed on the surfaces of Kr nanoclusters. It was found that the Kr substrate influences the recombination rate of atoms stabilized in these molecular films. As a result of this influence, in thick H_2 films the recombination rate of H atoms is a little slower than that in bulk solid H_2 samples, but in thin films the recombination of stabilized H and D atoms was almost completely suppressed. The former effect allowed us to obtain very high average concentrations of stabilized H and D atoms, 10^{19} cm^{-3} and $3\cdot10^{19}$ cm^{-3}, respectively [3]. The results of studies of tunneling exchange chemical reactions of hydrogen isotopes on the surfaces of Kr nanoclusters also will be presented.

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Magnetic Resonance Studies of Atomic Hydrogen Stabilized in Solid H_2 at Temperatures below 1 K

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We present an experimental study of H atoms embedded in thin films of solid H_2 at temperatures below 1 K. H_2 films up to 50 nm thick were first grown as a result of slow recombination of atomic hydrogen gas on the sample cell walls. If the recombination occurred in three-body atomic collisions in the gas phase, small concentrations of atoms could be captured inside the films during the film deposition. As a second method of generating atomic populations inside the H_2 films, we used a direct dissociation by a low power rf discharge in the sample cell. With this latter method, we achieved record high atomic concentrations exceeding $3*10^{19}$ cm^{-3}. The samples were characterized by means of magnetic resonance: electron spin resonance (ESR) and electron-nuclear double resonance (ENDOR) a magnetic field of 4.6 T.

We observed density-dependent broadening and shifts of the ESR lines due to the dipolar interactions, and resolved these effects for like and unlike atoms. Relaxation of the relative hyperfine populations was measured as a function of temperature for H in H_2 films grown on different substrates. For H_2 films on Mylar substrates, the relative equilibrium populations of the two lowest hyperfine states of H were found to deviate substantially from the prediction of Boltzmann statistics.

We also found two narrow lines in the ENDOR spectra of H in H_2 films shifted to the red from the position for free atoms. This indicates two possible substitution positions of the atoms in H_2 matrices, both characterized by very homogeneous crystalline fields.

The Structure and Properties of Metallic Nanowires Formed in Quantized Vortices of Superfluid Helium

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Concentrating any nanoimpurities in the core of quantized vortices of superfluid helium causes a tremendous acceleration of particle coagulation. Practically whole condensation proceeds then in the vortices and, due to practically 1-D character of their structure, the primary products should be nanowires. This phenomenon we discovered earlier [1, 2] has been used for the production of metallic nanowires. The materials were sputtered by pulsed laser from the surface of targets submersed in liquid helium at T = 1.6 K. In accordance with the prediction formulated in [2] the long (up to 1 cm length) metallic nanowires grown in superfluid helium were attached by metallic bonds to the tips of electrodes to which the generating them vortices were pinned. This effect allows carrying out the electrical studies just at low temperature.

The nanowires made of ferromagnetic Nickel and superconductive Lead, Tin, Indium and Niobium were grown and investigated [3]. Electron microscopy of the filaments heated up to room temperature has shown that they represented the bundle of the nanowires connected by point contacts. The nanowires had the diameter of 5-7 nm and they consisted of conjunct monocrystals having regular structure. The bundles of nanowires just grown at T = 1.6K metallically closed two neighboring electrodes spaced by 3 mm and thus the electrical circuit. Being conductors of metallic type they demonstrated the strong size effect inherent for tiny nanowires, namely strong growth of specific resistivity and, for superconductors, the transformation and temperature shift of phase transition.

Due to their high length and small radius the bundles of nanowires demonstrated powerful field-induced electron emission at rather low voltage and represented such a way the prototype of effective cold cathodes.

The promises for using the developed experimental approach for basic and applied sciences will be outlined and discussed.

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Kinetic Model for Metal Atoms Coalescence in Superfluid Helium

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In accordance with experimental studies [1], metal atoms injected in superfluid helium are pinning to the vortices core and then form long wires of a nanometer width directed along the vortices. Because the quantized vortex is practically 1-D filament the approximation of a short-range interaction between superfluid helium and metal atoms is valid, and hence there are two extreme cases of atom pinning to a vortex- either atoms submersed in superfluid helium landed to immobile vortex as a result of their diffusion, or the moving chaotically vortices swept the liquid capturing suspended there immobile atoms. However the laser ablation being the common tools for atoms injection into HeII gives a lot of ions as well. They are easily pinned to vortices and alternative mechanism of more long-distance attraction of atoms to charged vortex may occur. Being captured by a vortex, the metal atoms are moving freely along the core up to collision and merging with other metal atoms or chains of atoms.

The atom affinity to vortex core is A_1 = 3-10 K and it is comparable with typical temperature of experiment, $T \approx 2K$, so the impurity atom density in a vortex is close to that in the rest volume of liquid. But the motion of atom along the vortex core is much faster than atom diffusion in a liquid; so meeting each other in the core the atoms form dimers with affinity $A_2 = 2A_1$ and then *n*-mers with affinity $A_n = nA_1$. It means that rather long chains will anchored to vortices and the rate of sedimentation gradually and very fast grows.

Within the framework of our model we assume a time of atom traveling to the nearest vortex and to the wire grown there to be enough large, and then the process of atom motion to be stationary. Indeed, one can divide a space in the Voronoy-Delone cells, so that metal atoms injected in a certain cell are captured by their own vortex. Each vortex is modeled by a cylinder of a radius r_o and we assume as the first approximation that the contact of each metal atom with a vortex leads to its attachment. The consecutive application of Voronoy-Delone method makes it possible to describe the self-accelerating character of metallic wire growth in superfluid helium.

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Impurity Gels Formed by D_2 and D_2O Clusters in Superfluid Helium: Usage of the Gel Samples in He-II for Production of Ultra Cold Neutrons

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High porous impurity-helium condensates (impurity gels) formed by deuterium, heavy water or oxygen clusters in He-II could be used for production and storage of UCN in superfluid He-II. The initial idea was based on a nonzero probability of inelastic scattering of cold neutrons on the gel backbone in He-II cooled down to a few mK. The next step looks as follows: whether the helium vessel of the UCN source on superfluid He-II cooled below 1K could be filled preliminary with the gel, and the gel sample density is sufficiently high, than the diffusive motion of the 0.9-nm neutrons through the gel should lead to a strong increase, in L/l_f times, of their effective propagation time in liquid helium and, hence, to a sharp increase of the *total* interaction cross-section of 0.9-nm neutrons with the sample consisting of the impurity nanoclusters near the same sizes soaked with He-II. Here L is characteristic dimensions of the vessel and l_f is the mean free path of neutrons scattered elastically on impurity clusters in the sample bulk. Under those conditions the idea of using impurity gel samples in He-II for production of UCN even at T <1K looks very attractive, and it could result in multiple reduction of the moderator dimensions in comparison with a moderator on pure HeII.

Classical Capillary Turbulence on the Surface of Quantum Liquid He-II

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In this talk we present results of experimental study of capillary turbulence on the surface of superfluid ^{4}He at a temperature of T = 1.7 K. Motivation of this work was, first of all, the fact that capillary waves are an interesting object by itself - they are the only type of surface waves under microgravity conditions. Besides, capillary waves play an important role in the dynamics of sea surface (despite of the fact, that under normal gravity the wavelengths range of capillary waves on water surface is quite narrow: 0.5 mm < λ < 17 mm). For example, capillary waves are pumped by gravity waves and therefore they transport wave energy from bigger to small scales [1]. And secondly, capillary waves are an interesting model system to test the predictions of the wave turbulence theory [2].

In the work [3] the idea was proposed, that superfluid ^{4}He is the most suitable liquid for the study of capillary turbulence. It was assumed that in spite of surface tension coefficient for liquid helium is smaller than for water in two orders of magnitude [4], due to the absence of viscosity (superfluidity) the capillary wavelength range goes up to atomic scales, and the range of capillary wave vectors in turbulent distribution can reach five decades. Our previous experiments on He-II surface at T = 1.7 K [5] have shown that the temperature 1.7K isn't small enough for viscosity neglecting and capillary waves on He-II surface can be described well as capillary waves on the surface of classical liquid with very small, but finite viscosity. Inertial interval where Kolmogorov distribution can be observed (the range of capillary wave frequencies) reaches two decades (or even one decade for the wave vectors range). At high frequencies the turbulent cascade is cut off by viscous damping.

In our recent measurements [6], it was shown that superfluid helium is excellent liquid to study influence of the discreteness of the wave spectrum, caused by finite size of the experimental cell where capillary turbulence was studied. Experiments were performed in the cylindrical cell of inner diameter D = 30 mm and depth 4 mm. We observed for the first time wave energy accumulation at high frequencies – a local maximum in the turbulent spectrum - when the He-II surface was pumped by low-frequency harmonic force. In this report we suggest a qualitative model of this phenomenon in the frames of weak wave turbulence approach that takes into account discreteness of the eigenfrequencies spectrum of surface oscillations in the cylindrical resonator. Formation of the local maximum can be explained by a detuning effect of nonlinear harmonic frequencies and eigenfrequencies of surface oscillations in the cell. As we know, this experimental result is one of the first observations of discrete turbulence in laboratory conditions in the system of capillary waves excited in a container.

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Quantum Turbulence in Superfluid Helium at T ≥ 0

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The experimental investigation of behaviour of vibrating bodies gives us important information about formation, behaviour and decay of vortex system. This is very important at extremely low temperatures, when possibility of used thermal, optical and other experimental methods is hampered. In our experiments we investigate behaviour of vibrating grid and tuning forks in a wide temperature range down to fridge base temperature T>10 mK. Experimental setup allowed us to study properties of grid and forks irrespectively and mutual influence one device on another, for example, one fork on another.

The experimental results of stationary response of grid as well as forks on excitation, influence one fork response on amplitude of vibration of another fork and free decay of grid vibrations indicate that there are three different regime of body motion in superfluid helium and two critical velocities.

There is no formation of vortexes by vibrating body at low velocity of its motion. The motion is laminar and its velocity is proportional to excitation (force). The exceeding of grid or fork vibrations of first critical velocity leads to formation of vortexes and, for example, loss of energy at free decay of grid vibrations. The mechanism of this vortex formation may be“vortex evaporation” at process of pinned vortexes banding and reconnection [1]. At this regime the detector fork begins to feel a vibration of generator fork, grid changes its rate of energy loss at free decay vibrations.

The enhancement of second critical velocity establishes a turbulent state in liquid. The turbulent creation exhibits as a change of dependence of velocity of motion from value of applied force, like in normal fluid, and drastically quick loss of energy of free decay vibration. The first critical velocity is equal to some mm/s, while the second critical velocity has value of one order higher ~ 15 cm/s for grid and tuning forks.

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Vortex Fluid Relaxation Model for Torsional Oscillation Responses Of Solid ^{4}He

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A phenomenological model is developed to explain new sets of detailed torsion oscillator data for hcp ^{4}He. The model is based on Anderson's idea of a vortex fluid (vortex tangle) in solid ^{4}He. Utilizing a well-studied treatment of dynamics of quantized vortices we describe how the "superfluid component" is involved in rotation (torsion oscillations) via a polarized vortices tangle.

The polarization in the tangle appears both due to alignment of the remnant or thermal vortices and due to penetration of additional vortices into the volume. Both are supposed to occur in a relaxation manner and the inverse full relaxation time τ^{-1} is the sum of them. One of them is found to change linearly with respect to the rim velocity Vac. The developed approach explains behavior of both NLRS and Q^{-1} seen in the experiment. We reproduce not only the unique Vac dependence, but also obtain new information about the vortices tangle, namely a divergence in τ^{-1} as extrapolated to T~30 mK.

Charged Impurity Clusters in Liquid Helium

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The prospects of experimental investigation of charged clusters in liquid helium are argued. The potential of interaction of the negative ions electron bubbles) and inert clusters consisted of atoms or molecules Ne, Ar, Xe, H_2, N_2 is defined. Small clusters levitate above the negative ion at a distance of 13-16 A. The scaling laws for the properties of charged inert clusters are revealed and proved. The number of their quantum states and quantum levels is defined. The measurement of the charged clusters' mobility may be used as a new method to investigate the properties of nanoparticles immersed into liquid He.

Negative Ions in Liquid Helium

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Structure and mobility of positive and negative ions in liquid ^{4}He are analyzed. The possibility of the formation of clusters or bubbles around impurity ions of both signs is discussed. It is demonstrated that complexes formed around negative metal and halogen ions in superfluid helium investigated by Kasimov *et al.* [1] have qualitatively different structures, although the measured values of the mobility were similar. In the case of Ba^- and Ga^- ions, which have low electron affinities, bubbles are formed around the ions; these bubbles are similar to the electron bubbles but have a slightly smaller radius. In the case of Cl^-, F^-, and I^- ions, which have high electron affinities, clusters are formed near the ion; these clusters are similar to the well-studied clusters at the He^+ ion.

The nature of so called “fast” and “exotic” negative ions [2-5] observed in superfluid helium, whose mobilities exceed several times the mobility of the electron bubbles, is discussed. Still, their mobilities are several orders of magnitude less than the mobility of free electrons. Both kinds of high mobility ions are observed when a gas discharge above the liquid surface is the source of ionization. Only “fast” ions are observed when the ionization is produced by α- or β-radiation.

In the further discussion we assume that the “fast” ions are negative ions of helium excimer molecules localized in bubbles. In the gas discharge experiments, the excimer molecules diffuse from the surface into the bulk of the liquid. The lifetime of these ions ($\sim 10^{-4}$ s) is much less than their drift time. As a hypothesis we assume that after escaping from the ion with energy of about 19 eV, the electron is termalized during approximately 1 ps [6] and then captured by an excimer molecule. The transport proceeds by jumps from one excimer molecule to another. We suggest that the average time between two successive captures of the electron is very small in comparison with the lifetime of the excimer ions. Thus we can consider that the electrons are localized inside excimer ion bubbles practically all the time. The size of the excimer ion is smaller the size of an electron bubble leading to a higher mobility.

The “exotic” ions are stable negative impurity ions, which are always present in small amounts in gas discharge plasma. Around ions, formed from impurities with a relatively small electron affinity, bubbles are created and on the contrary around ions with a high electron affinity clusters are created. For example, the bubble radius around the negative ion of the oxygen molecule in liquid ^{4}He at $T = 1$ K is equal about 6 Å and its mobility practically coincides with the mobility of the fastest “exotic” ion.

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Critical Types of Electron Mobility in Cryogenic Matter

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The term “critical” applied to electron mobility describes the electron behavior in transition domains where electrons change their status, i.e. can transform from the free to localized states and vice versa. Actually, such domains are realized in the following situations:

1) Sharp reduction of electron mobility in cryogenic media with positive scattering length when free electron can transform to the bubble state.
2) Strong peak in electron mobility in media with negative scattering length in the density range corresponding to electron delocalization.
3) 2D electron transition from the free state to 2D-bubble structures at sufficiently high helium vapor density.

In all the above cases our treatment of effective conductivity considers the competing contributions of currents carried by two types of electron states: free electrons and charged structures formed by localized electrons. Results of calculations are compared with available experimental data and alternative models commonly used to explain the observed jumps in conductivity.

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Low Temperature Heat Capacity of Fullerite C_{60} Doped with CD_4

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It has been revealed in the dilatometric [1], NMR [2], and neutron diffraction [3] studies, that deuteromethane impurity changes essentially properties of fullerite C_{60}. The heat capacity of fullerite C_{60} containing 39.8 mol % of CD_4 was investigated in the temperature range 1.2 – 280 K. It was revealed experimentally that the interstitial impurity CD_4 leads to qualitative and quantitative changes of the heat capacity of fullerite C_{60}. The heat capacity of solution C_{sol} (T) is greater that the heat capacity of fullerite. The orientation phase transition in fullerite at T = 260 K is diffused by impurity CD_4 on temperature area 235-260 K. At helium temperatures the curve C_{sol}(T) shows a minimum. The heat capacity of solution exceeds a heat capacity of fullerite in 10 times at $T < 2$ K.

The analysis of experimental results at low temperatures was performed within the framework of model, where the contribution caused by movement of molecules CD_4 in octahedral interstitial space of fullerite C_{60} is occurred along with the lattice and tunnel contributions C_{60} in C_{sol}(T). It was shown, that the low temperature feature on curve C_{sol}(T) is connected with tunnel rotary movement of molecules CD_4. Strong influence of impurity molecules CD_4 on tunnel rotation of molecules C_{60} was detected.

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Dynamics of Dopant Particles in Octahedral Voids of Fullerite C_{60}

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Considered is an atomic impurity placed inside an octahedral void of the face-centered cubic lattice of fullerite C_{60}. Even though the surrounding molecules are shifted due to the presence of the dopant particle, the symmetry of the resulting crystal field felt by the dopant remains predominantly cubic.

We used the dopant-carbon interaction potential in the Lennard-Jones form [1]. To obtain the interaction between a dopant atom and the sphere-like C_{60} molecule with continuously distributed carbon atoms, we integrated over the said sphere of radius r_0.

We summed up over the six C_{60} molecules that make up the octahedral void cage to obtain the crystal field energy, the position of the dopant particle being shifted to a general point R within the void.

Our computations for Xe, Kr, Ar, Ne and He showed that even the shape of the $V_0(R)$ potential depends essentially on the rare gas species. The $V_0(R)$ potential for the heavier rare gases as Xe and Kr very close to the harmonic oscillator well. The lighter species He and Ne do not have a minimum at center of the void.

The general conclusion that can be drawn is that all rare gas species, even the bulky xenon, have negative energies inside the octahedral cavity, i.e., from thermodynamic consideration they must tend to penetrate into the fullerite lattice, which might be kinetically precluded by a rather high energy barrier between voids and between voids and the outside.

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Quantum Effects in Radial Thermal Expansion of Single-Walled Carbon Nanotube Bundles Doped with Helium

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The coefficients of radial thermal expansion α_r of bundles of closed single-walled carbon nanotubes (c-SWNT) and the effect of gas (Xe, H_2 and N_2) impurities on α_r have been investigated at low temperatures ($T > 2$ K). In the case of pure SWNT bundles [1] the α_r-values are negative in the interval 2—5 K and positive at $T > 5$ K. The gas impurities decrease the negative contribution and the temperature region where it is dominant. They also enhance greatly the positive contribution to α_r. According to theory [2], the quasi-twodimensionality of CNT walls causes negative Grüneisen coefficients and hence negative α_r at the lowest temperatures. Gas sorption suppresses the twodimensionality of SWNT bundles and decreases the negative contribution to α_r [3—5].

In this study the temperature dependence $\alpha_r(T)$ of c-SWNT bundles saturated with He to the molar concentration 9.38% was measured in the interval 2.1—9.5 K using the dilatometric method. Negative α_r was observed in the interval 2.1—3.7 K and was several times higher than the corresponding values for pure SWNT bundles [1]. The excess decreased with the lowering He concentration. According to the results in [3—5], the absorbed gas is expected to decrease the negative contribution to α_r or at least to keep it from exceeding the negative contribution to α_r for pure CNT bundles. The observed opposite effect can be due to possible tunneling of the He atoms between their different positions in the SWNT bundle system, which must lead to negative thermal expansion [6].

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Simulation of Long-Wave Phonon Scattering at Geometric Imperfections In Nanowires by the FDTD Method

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Today’s semiconductor devices have a tendency to shrink in size because of the appearance of advanced technologies that permit to control, with almost atomic precision, the geometry of a sample like, for example, a suspended silicon nanowire of less than 40 nm in cross-section. Recently developed experimental techniques make it possible to measure the thermal properties of nanostructures, while new numerical methods allow appropriate interpretation of their transport characteristics. As a building block of low-dimensional micro/nanodevices, nanowires have received considerable attention in recent years owing to their unique thermal, electrical, and optical properties. In this work we use the finite-difference-time-domain (FDTD) method to simulate phonon scattering in a nanowire of complicated geometry.

The FDTD method developed in the 1970s in geophysics to describe the propagation of seismic waves is now widely used for simulation of the propagation of both electromagnetic [1] and elastic [2] waves in inhomogeneous solids. Its advantage over other techniques is that it may be used to study the wave propagation in samples of complicated geometry with inhomogeneous composition. Within the framework of this method one can model an elementary act of scattering of an elastic wave (phonon) by an arbitrarily complex defect. In the present work the scattering of long-wave phonons in nanowires is studied at branch points of the main waveguide. We consider phonons from the low-frequency spectral region characterized by two acoustic branches corresponding to bending vibrations and compression waves. The phonon reflection (transmission) coefficient is analyzed as a function of the frequency, polarization, and geometric parameters of the defect.

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Dense Dusty Plasma Structures in Cryogenic DC Glow Discharges

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The problem “Cryogenic dusty plasma” is a gas discharge dusty system formed at very low (cryogenic) temperatures of gas. Experiments conduct with liquid nitrogen and liquid helium which cool dc glow discharges. A decrease in the neutral gas temperature in gas-discharge plasma to several Kelvins causes a decrease in the ionic Debye radius, and this may result in weaker repulsive interaction of dust particles. In this case, micron-sized dust particles may approach one another closer and thus form dense dust structures. The method of cooling to a temperature of several Kelvins or milli-Kelvins was traditionally employed for increasing the non-ideality of plasma and plasma-like media. This is how one manages to obtain ionic crystal structures in cryogenic gas discharges and under conditions of laser cooling of atomic ions in non-neutral plasma in Penning traps, in Paul RF traps, and in storage rings, as well as a 2D electron crystal structure on the surface of liquid helium. Uniqueness of the present researches is caused by the fact that cryogenic dust plasma allows to combine two approaches at research of fundamental questions of physics of strongly coupled systems – a method of deep cooling and a method of interaction potential energy increase, realized in case of dusty plasma. Thus an actual problem is a development of the diagnostic approaches providing direct measurements of quantitative characteristics of dusty plasma structures at cryogenic temperatures.

In the work the results of experimental investigations of structural and dynamic properties of dense dusty plasma structures in dc glow discharge at cryogenic temperatures are presented. For this purpose the novel optical helium cryostat was designed and created. The cylindrical glass gas-discharge tube was placed inside the cryostat and plasma was generated after tube cooling. The diagnostic complex for visualization and registration of dusty plasma structures in the discharge inside the cryostat was developed. Structural and dynamic characteristics of the cryogenic dust structures were measured. As it was shown in the experiments, the deep cooling of discharge tube walls leads to dramatic change of dusty plasma properties. In particular, sufficient increase of dust particle kinetic temperature (by about an order) and dust density (by several orders) due to cooling from 77 to 4.2 K was observed. These phenomena were reproduced in the experiments with various initial conditions: dust particles of different material and sizes (mono- and polydisperse μm-particles), different buffer gases (He, Ne) and gas mixtures (He-Kr).

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Orientational Order Parameter in CO_2 – Kr Solution

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The problem of the orientational order in mixed cryocrystals consisting of two components, one of which is a linear molecule and the other is a rare gas atom, still remains an important issue for random systems. Usually, orientational order is quantitatively described by the orientational order parameter (OOP), which in a solid made up of linear is determined as

$$\eta = \left\langle P_2(\cos\theta) \right\rangle$$

where $P_2\ (x)$ is the Legendre polynomial and θ is the angle the molecule in a specific sublattice of an orientationally ordered structure makes with the axis of the preferable orientation of this molecule. The resonance methods, which are traditionally used to determine $\boldsymbol{\eta}$, fail for mixed systems and, actually, the only constructive option is to utilize diffraction data for that purpose. In paper [1] devoted to OPP reconstruction in mixed systems was outlined the general approach for a specific case of Ar-CO_2 cryoalloys. This approach has been developed to a quite high precision for diatomics and then successfully applied for the reconstruction of $\boldsymbol{\eta}$ in α-N_2 powder x-ray diffraction measurements [2] and in the orientationally ordered almost pure para-deuterium [3] from the old neutron diffraction data of Yarnell *et al* [4]. Then the method of reconstruction of absolute orientational order parameter values has been modified for the case of the triatomic CO_2 cryocrystal [5]. It is shown that, because of the comparatively large length of the CO_2 molecule, a consistent description of the orientational subsystem can be obtained only if an orientational order parameter of a higher (fourth) rank, $\boldsymbol{\eta}4$ is taken into consideration together with the standard (rank-2) order parameter $\boldsymbol{\eta}2$. Both orientational order parameters $\boldsymbol{\eta}2$ and $\boldsymbol{\eta}4$ in pure CO_2 have been reconstructed for temperatures from 6 to 70 K.

We present (OPP) method's applications to the CO_2 – Kr binary solid solutions. Concentration dependence both orientational order parameters $\boldsymbol{\eta}2$ and $\boldsymbol{\eta}4$ in CO_2 – Kr solutions have been reconstructed for the temperature 30 K, in all range of mutual component's solubility. Conceptually new techniques of solubility and solution morphology analysis, based on OPP method have been applied to the CO_2 – Kr cryoalloys.

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The Low Frequency Internal Friction (LFIF) and Phase Transition of Solid Oxygen

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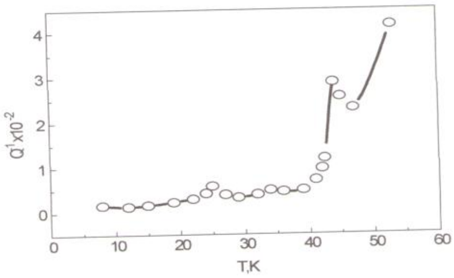
Solid oxygen is one of the most peculiar crystal of the group of the diatomic molecular crystals. The peculiarity is largely due to the fact that the O_2 molecule in its electronic ground state has a spin S=1. As a result, solid oxygen combines the properties of a molecular crystal and a magnetic material.

The equilibrium vapor pressure oxygen exists in three crystalline modifications. Low-temperature monoclinic α-phase is long-range orientational order and quasi-two-dimensional antiferromagnetic molecules order [1,2]. After phase transition at the T=23.88K Rhombohedral β-modification solid oxygen (23.88K≤T≤43.78K) is paramagnetic with long-range orientation molecular order [1-3] (α→β transition not concerning orientational structure). In high-temperature cubic γ-phase are two orientationally disordering molecules and six molecules they do plane rotation [2]. Note, β→γ transition is very radical in contrast to α→β transition. Near β→γ transition a change of both coordination and orientation crystal structure occurs.



Unique data for temperature dependence of LFIF $Q^{-1}(T)$ for crystalline oxygen in temperature range 7-52 K were obtained on free specimens exfoliated from container wall (see fig.). Near temperatures of αβ and βγ phase transitions there are peaks of LFIF, greatly differs one from another to the power of relaxation($\Delta_{\alpha\beta}\approx 1.10^{-2}$ and $\Delta_{\beta\gamma}\approx 4.10^{-2}$), that corresponds to above thermodynamic features of these phase transitions.

The IF measuring is conducted by methods of inverse torsion pendulum under deformation amplitude 10^{-4}-10^{-5} using original setup for study of non-elastic properties of solidified gases [4,5]. An experimental error of LFIF measuring does not exceed 5%.

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***Ab Initio* Calculation of Three-Body Interaction in Cryocrystals under Pressure**

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The short-range three-body forces obliged to ceiling of electronic shells of atoms of crystals of cryocrystals (rare-gas solids – RGS) are explored. It was before [1,2] pointed out that the requirement of orthogonality of waves functions of electrons of neighboring atoms of crystal results in appearance of elements in potential energy, three nearest atoms depending on co-ordinates l, l', l''.

$$W_3 = -\sum_{ll'l''} S^2 \;\; \mathbf{r}^{ll''} \;\; f\left(\left|\mathbf{r}^{l'} - \frac{1}{2}\mathbf{r}^{ll''}\right|\right), \;\; f \;\; |\mathbf{r}_2| \;\; = S(\mathbf{r}_2)/|\mathbf{r}_2|, \quad \mathbf{r}_2 = \frac{a\sqrt{6}}{2}, \qquad (1)$$

where $S = S_{zz}^{ll'}$ is integral of covering of waves functions of electrons of the isolated atoms φ_z^l and $\varphi_z^{l'}$. Three-body energy (1) gives in equalization of motion for displacements of atoms the elements of two types. First from them has that dependence on k, what given by pair interaction. It will result in some additions δH and δG to the power parameters H and G. Besides it three-body interaction results in appearance of element with new dependence on k, which is characterized by a parameter V_0.

$$V_0 = 128\frac{a^3}{e^2}\left[S(\mathbf{r})\frac{a}{\mathbf{r}}\frac{dS(r)}{dr}\right]_{r=a\sqrt{2}}\left[\frac{a}{R}\frac{df(\frac{R}{2})}{dR}\right]_{R=a\sqrt{6}} \quad . \qquad (2)$$

For RGS cohesive energy taking into account three-body interaction looks like:

$E_{coh} = -\frac{C}{2}\sum_{l'}\frac{1}{|r^{ll'}|^6} + \frac{12}{2}W_2 \;\; a\sqrt{2} \;\; + W_3 \;\; a\sqrt{2}, a\sqrt{6}$, where C is constant of Van-der-Vaals.

In the Birch elastic module $\mathcal{B}_{11}$ new elements of three-body interaction will not give, and in the $\mathcal{B}_{12}$ and $\mathcal{B}_{44}$ holdings from the examined three-body forces will be equal on a size, but with opposite signs.

$$\mathcal{B}_{44} = \frac{e^2}{2a^4}\left[\frac{V_0}{2} + H + \frac{G}{2} - 0.26247D\right], \;\; \mathcal{B}_{12} = \frac{e^2}{2a^4}\left[-\frac{V_0}{2} - H + \frac{G}{2} - 0.86472D\right], \qquad (3)$$

where $H = H_0 + \delta H$ and $G = G_0 + \delta G.$ H_0 and G_0 are parameters which take into account pair interaction only. Then deviation from Cauchy relation δ taking into account equation of the state will be

$$\delta = \mathcal{B}_{12} - \mathcal{B}_{44} - 2p = \frac{e^2}{2a^4} \;\; 2\delta H - V_0 - 4R_t \;\; . \qquad (4)$$

The conducted calculations with the use of Rutan functions [3] allows us to describe the deposit of three-body interaction in the elastic constant and equation of the state in the wide interval of pressures. The consent of our calculation and experiments [4,5] are good.

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The Phonon Spectrum of Graphite and Stability Conditions In Quasi-Two-Dimensional Structures

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The phonon spectrum of graphite is analyzed in detail at the microscopic level and the partial contributions from the displacement of atoms in and perpendicular to the plane of the layers to the phonon density of states are calculated. The main distinctive features of the phonon spectrum of graphite are determined; they are due to the quasi-two-dimensional character of phonon propagation as is characteristic for graphite.

The model has been proposed for the crystal lattice of graphite that not only completely reflects all distinguishing features of the phonon spectrum graphite but also makes it possible to calculate quantitatively, to a high degree of accuracy, the vibrational characteristics of this compound. All force constants appearing in this model have been determined from the experimental data on inelastic neutron and soft x-ray scattering as well as from measurements of the sound velocities. It was shown that the weak interlayer van der Waals interaction can be described by the Lennard-Jones potential and the parameters of this potential were found. The phonon density of states of graphite and the spectral densities corresponding to the displacements of the atoms of different sublattices of graphite along the directions of the weak bond and in the plane of the layers were calculated on the basis of this model. It was shown that these densities exhibit two-dimensional behavior at frequencies above the van Hove frequencies, which correspond for each polarization to a transition from closed to open isofrequency surfaces along the *c* axis. In this frequency range the vibrations polarized in and perpendicular to the plane of the layers do not, for all practical purpose, interact with one another and can be studied independently.

It was shown that for the frequency corresponding to the *K* point in the first Brillouin zone of graphite the component of the phonon density of states of graphite that is due to vibrations polarized along the *c* axis.

The calculations for the spectral densities in our proposed model is much better correspond with known experimental data [1,2] than in the well-known models from [3]. Because graphite is a strongly anisotropic crystal with a weak interlayer interaction then it should be substantially manifest the role of bending vibrations. The reasons for the appearance of flexural rigidity of layers in strongly anisotropic layered crystals are investigated. Structures consisting of loosely bound monatomic layers (specifically, graphite) as well as formed loosely bound structural elements each consisting of several monolayers which are coupled much more strongly with one another (for example, in dichalcogenide transition metals) are examined. The effect of the flexural rigidity on the phonon spectra of these compounds—quasi-flexural bending of the dispersion curves of phonon modes polarized in a direction normal to the layers—and the particularities appearing in the phonon densities of states as a result of quasi-flexural vibrational branches crossing low-frequency optical modes are analyzed.

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Thermal Inactivation of Excitonically-Induced Defect Formation in Solid Xe and Kr

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Rare-gas cryocrystals (solid Xe, Kr, Ar and Ne) are widely used as the model systems in fundamental investigations and as the working media of particle detectors and positron moderators. Selective excitation of excitons in rare-gas cryocrystals by photons with energies $h\nu < E_g$ results in accumulation of Frenkel-pairs by intrinsic excited-state mechanism of defect formation via self-trapping of excitons [1]. Recently the simple kinetic model was proposed, which allows fitting the experimental dose dependences of "defect" luminescence subbands and obtaining the particular kinetic parameters [2]. Application of this model provided a way of qualitative and quantitative analysis of rare-gas cryocrystals, which is indispensable at any attempt of comparison of luminescence spectra from different samples. At the same time it is well known that there is a strong thermal quenching of the defect formation processes, which was initially explained by temperature dependence of lifetime of emitting states [3]. In the same temperature range the electron traps become active and charge recombination processes result in rich spectra of thermo luminescence [4].

In the present study we apply the Eyring's transition state concept to the processes of thermal activation-inactivation of exciton trapping states resulting in luminescence spectra evolution under selective synchrotron irradiation. The experiments were carried out at the SUPERLUMI-station at HASYLAB, DESY, Hamburg [5]. The selective photon excitation of solid Xe and Kr samples was performed with spectral resolution $\Delta\lambda = 0.2$ nm. The VUV-luminescence analysis was performed with $\Delta\lambda = 2$ nm, Pouey high-flux monochromator equipped with a multisphere plate detector. The dose dependences of luminescence of molecular-type self-trapped excitons at different temperatures under irradiation by photons with energies $E < E_g$ were measured. These curves are saturated at long time of irradiation therefore we used the slopes of the initial linear parts of the dose curves at $t = 0$ as the defect formation rates w. Following Eyring assumption we can fit the temperature dependence of the defect formation rate as

$$w(T) = \beta \cdot T \cdot \exp(-E/kT) \cdot (1 + \exp(\Delta S/k) \cdot \exp(\Delta H/kT))^{-1},$$

where k – the Boltzmann's constant, E – Arrhenius activation energy, β – scaling factor. The values of activation energy E and enthalpy of inactivation ΔH was determined from the upper and lower tangents of the $w(T)$ in the coordinates $(\ln[w(T)])$ vs. (T^{-1}). The value of entropy of inactivation ΔS was obtained from the equilibration condition $d(\ln[w(T_{\max})])/dT = 0$. At high $1/T$ the temperature dependence of the defect formation rate tends to $\ln(w(T)) = (-E/k)(T^{-1})$. At high temperatures $(T^{-1} \rightarrow 0)$ the temperature dependence tends to $\ln(w(T)) = [-(\Delta H - E)/k](T^{-1})$. The value of entropy of inactivation ΔS may be obtained from the equilibration condition $d(\ln[w(T_{\max})])/dT = 0$, which can be expressed in the form $(E + kT_{\max}) \cdot (\Delta H - E - kT) = \exp(-\Delta H/kT) \cdot \exp(\Delta S/k)$, where $T_{\max}$ – the of the maximum of $w(T)$. The best fit of the data for solid Xe was obtained with $T_{\max} = 30$ K, $E = 2.8$ meV, $\Delta H = 28$ meV, $\Delta S = 0.8$ meV$\cdot$K^{-1} For solid Kr correspondent values are $T_{\max} = 27$ K, $E = 4$ meV, $\Delta H = 30$ meV, $\Delta S = 1$ meV$\cdot$K^{-1}.

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Cellular Nanostructure of Methane Hydrate

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Methane hydrate has a large practical importance today as it is non-conventional energy source. In the nature it exists in the form of natural pools at the sea bottom. Methane hydrate fields had been recovered at various regions of the Earth. Moreover, gas hydrates are formed in the gas pipelines when the wet gas is transported at temperatures near zero Celsius. It is quite necessary to know thermodynamical conditions of the transition of methane-water system to crystal hydrate both during methane capturing from the hydrate fields and for development of methods against forming of gas hydrate plugs in the gas pipelines. This problem is not studied well as it is shown here.

In the present work we study experimentally a phase transition of the methane-water system to the crystalline state under temperature lowering. A new intermediate state of this system is recovered, and thermodynamic conditions of the system forming are determined. It was found that a viscosity of the intermediate phase varies from water viscosity to crystalline hydrate one according to gas pressure [1-4].

To describe the process of creation of the methane hydrate intermediate state and explain its observed properties we propose a model of methane hydrate creation as thin films of crystalline hydrate, which form a cellular structure with water filling the cells. Creation of such cellular structure is governed by competition between the volume (difference of chemical potentials, specific energy of elastic deformation) and surface energies.

The intermediate phase of methane hydrate is a fine-dispersed two-phase mixture of water and crystalline hydrate, which is ordered as cellular nanostructure with cell size about 10^{-5} cm. After isothermal soaking such a structure has filled the whole volume of our experimental chamber. Theoretical estimations of wall thickness of the cells give the value about 10^{-7} cm at temperature +1 °C. At temperatures higher than 0 °C the crystalline methane hydrate is formed at pressure higher than 6 MPa.

The obtained results may be useful for: i) development of chemical methods based on formation and decomposition of gas hydrates; ii) designing of methods for prevention of the hydrate plugs in gas pipelines; iii) transport of natural gas; iv) development of methods of methane capturing from methane hydrate fields.

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Cell Model of Hydrogen Liquid at Megabar Pressures

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We present a model of a quantum conductive fluid which forms as molecular crystal hydrogen is subjected to melting at megabar pressures. This model is founded on cell approach that takes the contribution of localized state into consideration. The model predictions are in agreement with the recent experimental observations of anomalies in this melting process. Besides they indicate that the fluid produced by the melting process may exist in a metastable state with a density ~2.3 g/cc. The issue of hydrogen state at megabar pressures is one of the great problems in condensed matter physics, astrophysics, also important the general understanding of the behavior of matter at extreme conditions. At low temperatures and pressures, hydrogen is a molecular solid or fluid. At high pressures above 100 GPa, hydrogen is supposed to undergo a transition to a highly conducting state. This fact has been verified theoretically and experimentally, with noteworthy development including measurements of melting temperature at extremely high pressures (~ 300-400 GPa) obtained in diamond anvil cells [1, 2], and a calculation by Scandolo [3], an analysis of the melting line by Bonev et al. [4] predicted a peak at 80 GPa and 900 K. Furthermore, at higher temperatures they found a transition from H_2 to nonmolecular hydrogen, with a negative slope.. Below 100 GPa it has a normal behavior – a melting temperature is monotonically increasing with pressure and the phase transition takes place: molecular solid (MS) –molecular liduid (ML). However, above 100 GPa the melting temperature reached a peak and began to decrease. Extrapolation of this melt line to even higher pressures and lower temperatures implies that at a pressure greater than 400 GPa hydrogen might be a liquid at T = 0 K. The existence of a peak in the melting line will show a possible new pathway to metallic hydrogen and the importance of extending calculations and experiments to higher pressures and lower temperatures. The present knowledge of the liquid phase state, in which MS undergoes at pressure above 100 GPa, is inconclusive.

Here we show that at pressures (100 – 600) GPa, when average distances between protons (ions) become comparable with the internuclear distances in molecule H_2 (molecular ion H_2^+), the MS state is thermodynamically not the most advantageous. A more disordered state, namely quantum conducting liquid (QCL), can compete with it. It is suggested that every ion is localized in the Wigner – Seitz cells, the charge of which is screening completely. There is a domain in the center of this cell, where own electron of hydrogen atom is localized for the most part (a virtual atomic – like structure (VA). The probability density of this electron is distributed non-uniformly over the cell and describe by the wave function of the hydrogen ground state. Since classically accessible spheres of such electrons of neighboring atoms overlap, screening leads to admixing of free – like (FL) electron states, which are on the cell periphery mainly and distributed uniformly. We calculate the cell energy taking into account the kinetic energy of LE and DE electrons, the interaction of these electrons with the central ion, electron-electron and exchange interactions. We can neglect the thermal contribution of the electrons in thermodynamic functions in comparison with the proton contribution. The latter is calculated in the hard sphere approach. The hard sphere diameter is found as an average size of the cell.

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Thermal Conductivity of Molecular Crystals of Monoatomic Alcohols: From Methanol to Butanol

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Primary monoatomic alcohols are organic compounds whose molecules have one hydroxyl OH-group at the end. In the condensed phase monoatomic alcohols are considered as associated objects with medium-strength hydrogen bonds. H-bound chains are important for the formation of the crystalline structure of alcohols.

Normally, the thermal conductivity $\kappa(T)$ of dielectric crystals consisting of molecules with orientational degrees of freedom in orientationally-ordered phases at temperature above the phonon maximum decreases exponentially with rising temperature. On a further rise of temperature $\kappa(T)$ obeys $1/T$ law [1, 2]. However, on deviation of $\kappa(T)$ from this law was observed in the row of simple alcohols [3] and the reason for this behavior is obscure. The goal of this study is to investigate phonon scattering in H-bound molecular crystals with orientational degrees of freedom.

The thermal conductivity $\kappa(T)$ of some simple alcohols (methyl, hydrogenated and fully-deuterated ethyl, 1-propyl and 1-butyl) in thermodynamically-equilibrium phases at the equilibrium vapor pressure at $T = 2$ K-T_m was measured and analyzed. The investigated phases correspond to crystals with complete orientational ordering. It is shown that above the maximum thermal conductivity the dependence $\kappa(T)$ deviates with increasing temperature from the expected law $1/T$, which is dictated by the anharmonic interactions of acoustic excitations. The deviation is caused by the fact that the total thermal conductivity $\kappa(T)$ contains, in addition to the contribution $\kappa_I(T)$ of propagating phonons, another contribution $\kappa_{II}(T)$ made by short-living phonons: $\kappa(T) = \kappa_I(T) + \kappa_{II}(T)$. Above $T = 40$ K $\kappa_I(T)$ obeys the $1/T$ law and $\kappa_{II}(T)$ is practically independent of temperature. The contribution $\kappa_I(T)$ is described well by the Debye – Peierls model allowing for the phonon-phonon Umklapp processes and phonon scattering at dislocations. On the contrary, the contribution $\kappa_{II}(T)$ is an indication of the influence of high-energy excitations which are thermally activated above 40 K (Cahill-Pohl model [4]). It is shown that the force of phonon-phonon scattering reduces in inverse proportion to the mass of the molecule as the molecular mass of a monoatomic alcohol increases.

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Thermal Expansion Effect on Phonon Localization in Simple Molecular Crystals

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Our investigations of isochoric thermal conductivity in simple molecular crystals have revealed a considerable dependence of this kinetic coefficient on heat transfer by nonpropagating (localized) phonon modes occupying part of phonon spectrum [1-3]. The reason is that the thermal conductivity approaches to its lower limit $\Lambda_{\min}$. In this case, the mean free path of thermal phonon becomes comparable to the lattice parameter and, as consequence; part of thermal energy diffuses between neighboring molecules vibrating with random phases. In simple molecular crystals, thermal conductivity approaches to its lower limit quite closely due to the additional phonon scattering caused by the collective rotational molecular motions.

The thermal conductivity in orientationally-ordered and orientationally-disordered phases of simple molecular crystals are analyzed within the Debye model, under supposition that the phonon mean free path is approximately equal to one half of the wavelength. A quantitative description is given under assumption that the heat is transferred by phonons and “diffusive” modes, and taking into account translation-rotation coupling. The calculations were carried out for the isochoric and isobaric cases, which allowed the influence of thermal expansion on phonon localization to be determined. Based on studies results it is concluded that the thermal expansion brings about an increase of phonon localization temperature. Also from this analysis, it was found that the transition from strongly to weakly hindered rotation of molecules is accompanied by a decrease in the portion of thermal energy that transferred by “diffusive’ modes.

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Isochoric Thermal Conductivity of Isobutane

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There has been considerable interest in the structure, dynamics and thermal properties of the saturated hydrocarbons. In particular they are convenient objects for study of influence of rotational degrees of freedom of molecules and their symmetry on the behavior of the thermal conductivity of crystals. Depending on the material and temperature, the form of orientational motion in this materials changes over a wide range, i.e., from librations at small angles to a retarded or practically free rotation. Crystals consisting of high-symmetry molecules form high-temperature “plastic” or orientationally disordered phases, in which the rotational motion of molecules resembles their motion in the liquid state. In crystals consisting of molecules of a lower symmetry the long-range orientational order is preserved, as a rule, up to the melting point. To compare correctly experimental results of thermal conductivity with theory at high temperatures, it is necessary to perform experiments at a constant density to exclude the effect of thermal expansion.

The peculiar feature of hydrocarbons is an existence of isomers. There are no systematic investigations of the thermal conductivity in series of solid isomers. Here we presented the study of the isochoric thermal conductivity of solid isobutane. Iso-C_4H_{10} was studied for samples of different densities in temperature interval from 60 K to the onset of melting. Solid isobutane exists only in the one crystalline phase and melts at 113,74K with entropy of melting $\Delta S_f/R = 4.8$, whereas the criteria of “plastic” state is $\Delta S_f/R = 2,5$ [1,2]. In all the cases the isochoric thermal conductivity exhibits dependences that are weaker than $\Lambda \propto 1/T$. The results obtained are compared with those for other representatives of saturated hydrocarbons. The experimental data are discussed within a model in which the heat is transported by low-frequency phonons and by «diffusive» modes above the phonon mobility edge.

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Thermal Conductivity of Solid Cyclohexane

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The thermal properties of simple molecular crystals are determined by the combined translational and orientational motion of molecules in the lattice sites. The orientational motion can be either oscillatory or rotational depending on the relation between the central and noncentral forces and temperature. Except for rare cases (quantum crystals), the motion of molecules at rather low temperatures is essentially oscillatory: at $T = 0$ the molecules execute zero orientational vibrations about equilibrium directions. As the temperature rises, the root-mean-square amplitudes of the librations increase, and the molecules can pass from one orientation to another. In some cases this may lead to a phase transition because the long-range orientational order disappears. By choosing crystals with different parameters of molecular interaction and varying the temperature, it is possible to change the degree of orientational disorder and study the effect of the molecule rotation upon the thermal properties, e.g. thermal conductivity of the material.

For a correct comparison with theory, the thermal conductivity must be measured at constant density to preclude the thermal expansion effect. In regard to the cyclic molecules the isochoric thermal conductivity was measured only for the benzene [1-2]. Here we presented similar studies for the cyclohexane-C_6H_{12}. Cyclohexane has a phase transition at 186.1K and melts at 279.8K [3]. High temperature phase (I) is plastic with entropy of melting $\Delta S_m/R=1.14$. X-Ray data shows HCP structure *Fm3m* with Z=4 [4]. Phase transition (II↔I) at 186.1K is isothermal with the large entropy change $\Delta S_f/R=4.33$. Phase (II) is monoclinic ***C2/****C* with Z=4 [4]. The Debye temperature is 50K in the phase (I) and 71K in the phase (II) [5]. At heating from 155 up to 180K the second NMR momentum decreases sharply from $26G^2$ down to $6G^2$, what shows on appearance of molecular reorientations about the tree fold axes [6]. In the high temperature phase (I) molecules have significant orientational freedom, that intermolecular contribution to the second NMR momentum becomes neglible small. Thermal conductivity of solid cyclohexane has been studied in the temperature interval 80-280K at atmospheric pressure and at constant volume for samples of different densities in the orientationally-disordered phase (I). The thermal conductivity measured at atmospheric pressure changes as $\Lambda_P \propto T^{-1.15}$ in the orientationally-ordered phase (II) and as $\Lambda_P \propto T^{-0.31}$ in the disordered phase (I). The isochoric thermal conductivity changes as $\Lambda_V \propto T^{-0.8}$ in the low temperature phase (II) and increases with temperature growth in the “plastic” phase (I). The experimental data are discussed in the approximation of the corresponding relaxation times within a model in which the heat is transported by low-frequency phonons and by «diffusive» modes above the phonon mobility edge [7].

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A Simple Low Temperature Adiabatic Calorimeter-Inset for Small Samples

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A vacuum adiabatic calorimeter-inset has been home-made for calorimetric studies of small samples (with diameter ≤10 mm, ~ 1 cm^3 by volume) of carbon nanomaterials in the temperature range from 1 K to 300 K. Design of the inset makes possible: a) a mounting of an under study sample during short time (it is important for investigation of both heat capacity of pure nanomaterials and effects are caused by doping of gases); b) the doping of a sample by gases directly in the calorimeter-inset; c) cooling of sample to helium temperatures during short time. The calorimeter-inset can be inserted into a helium reservoir of transport helium Dewar or a helium cryostat.

The calorimeter cell (the calorimeter with a thermal shield), a low temperature helium chamber, an adsorb pump, tubes and wires are placed inside the vacuum cylindrical inset. The calorimeter mass is equal to about 0.8 g. It is surrounded by a thermal shield. The calorimeter cell is suspended from the low temperature chamber. Liquid helium – 4 can be condensed into the chamber. The adsorb pump is filled by absorbent carbon “SKN-1K”. The adsorb pump is cooled with supply of helium from outside helium volume. Temperature of the low temperature chamber can be decreased down to about 1 K by pumping of helium vapour by the adsorb pump. The personal computer controls the calorimetric experiment.

Heat capacity of the fullerit C_{60} sample has been measured in the temperature range from 1 to 30 K. The fullerit sample is 99.99 % pure. The sample mass is equal to about 0.6 g. Apiezon N grease is used for good thermal contact between the sample and the calorimeter. The heat capacity of an empty calorimeter has measured in a separate experiment. The obtained results of studies of heat capacity of fullerit are compared with literary data [1, 2].

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Low Temperature Specific Heat Capacity of Fullerit C_{60}

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A number of low temperature anomalies have been revealed in thermal expansion studies of fullerit doped with gases [1] (and references in it) recently. Low temperature heat capacity of these objects has not enough been studied.

Present work marked the beginning of a program of systematic research of influence of gaseous atomic and molecular admixture on low temperature heat capacity of carbon nanomaterial, fullerit in particular. There are disparities between literary data of low temperature heat capacity of fullerit C_{60} [2, 3]. For example, differences of the values of the linear contribution to heat capacity are more than 20 times [3]. So, reliable data of low temperature heat capacity of fullerit C_{60} (which can be used as a basic for separation of admixture effects) are absent practically.

The heat capacity of the sample of fullerite C_{60} has been measured over the temperature range 1 - 30 K in the home-made adiabatic calorimeter [4]. The fullerite sample is 99.99% pure. Its mass is equal to about 0.6 g. The analysis of temperature dependence of heat capacity of fullerite is made. The parameters of its temperature curve are defined. The linear contribution to the total heat capacity of fullerite is observed below about 3 K. Nature of the linear contribution is discussed. A comparison between the results of this work and literary data [2, 3] is considered.

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Metastable Defect Structure in Orientational Ordered Crystal of Ethanol

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Alcohols are compounds containing one or several hydroxyl groups (OH). Primary alcohols based on $H(CH_2)_nOH$ molecules (n is the number of carbon atoms in the alcohol molecule) are the simplest associative molecular systems suitable for investigation of physical phenomena in molecular crystals at low temperature. Thermodynamically-equilibrium solid phase of these molecular substances has a crystalline structure with a long-range orientational ordering. The properties of ethanol attract special interest in the homologous series of simple monatomic solids. Ethanol (CH_3CH_2OH) can have three metastable long-lived phases under equilibrium vapor pressure — a structural glass, an orientationally disordered crystal with static disorder (orientational glass), a crystal with dynamic orientational disorder (rotator phase) and an orientationally ordered crystal, which is the only stable thermodynamically equilibrium phase [1, 2].

Here the temperature dependences of the thermal conductivity measured on polycrystalline samples of protonated and deuterated ethanol are described. The samples were obtained through an irreversible solid-state first-order transition from the rotator phase. The thermal conductivity of solid alcohols C_2H_5OH and C_2D_5OD at the equilibrium vapor pressure was measured in the interval from 2 K to 155 K using the method of steady-state linear heat flow [3]. The structure of C_2D_5OD in orientationally-ordered phase was specified by the neutron-scattering technique and the X-ray structural analysis.

The temperature dependences of the thermal conductivity of both protonated and deuterated alcohols in the orientationally-ordered phase are similar to those typically observed in dielectric orientationally-ordered crystals. A significant annealing effect is observed in the thermal conductivity $\kappa(T)$ of the protonated alcohol. The curve $\kappa(T)$ varies systematically as the annealing temperature increases from 102 to 156 K. The thermal conductivity curves have been analyzed with the Debye model. It is shown that only the orientationally-ordered phase of protonated ethyl alcohol has an appreciable number of metastable orientational point defects, and their content decreases as the sample is heating in temperature range from 102 to 156 K. The metastable defects are attributed to the presence of the metastable monoclinic crystalline phase of protonated ethyl alcohol [4].

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Investigation of Conversion of Methane Molecular Spins in CD4-Kr Solid Solution

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The spin conversion of methane molecules in pure deuterated methane crystal and CD4--Kr solid solution for a vast concentration of krypton was investigated in the temperature range 1.5--10K. The experiment was performed by use of a steady-state heat flow experimental setup for determination of the thermal conductivity, utilized in an unconventional way. The obtained results were discussed in the frame of the spin conversion model taking into account direct one-phonon processes and indirect librationally-activated processes.

Observation of the Nonequilibrium Superfluid Phase into Solid Helium within Aerogel

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The results of the fresh neutron scattering study of solid helium in silica Aerogel is discussed. Recently [1] we have discover the existence of superfliud phase in the solid helium at the temperature lower than 0.6K under pressure 53.5 bar in spite of the ^{4}He phase diagram indicated that helium should be solid at this thermodynamic conditions. Present work is a continuation of abovementioned study, the main goal of which is the checking of the phenomena found out, and the determination of the general parameters of the new superfliud phase.

The sample represented the thin-walled copper container with the silica Aerogel inserted inside which has been fully filled by the liquid helium. The solid helium has been received with use of a method of blocking capillary. The presence of a solid phase and the value of pressure in the sample were determined by the positions of Bragg peaks of the solid helium. The analysis of the experimental data gives the temperature of the solid helium-superfluid helium transition T_S=1.3 K. The parameters of the superfluid phase excitations (life-time, intensity, and energy) have the temperature dependences similar to the bulk helium ones. Superfluid phase exists within the experimental temperature range from 0.05K up to T_S, is nonequilibrium, and is anneal at T_S.

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The Free Energy, Pressure Change, and Twin Boundaries in Solid Helium at the bcc-hcp Phase Transition

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In solid ^{4}He the phase transition (PT) bcc-hcp has martensitic-like features. The overcooling below the phase equilibrium line bcc→hcp was found in the optic and pressure experiments [1,2]. The experiments [2] indicated asymmetry of this PT: the reverse PT hcp→bcc is fixed in just in the phase equilibrium line. This asymmetry up to the present has been left unexplained. In solid helium the phase transition, the bcc-hcp coherent phase boundary (PB) and tween boundary (TB) were investigated theoretically in the fraims of one order parameter (OP) model [3,4]. These works applayed ideas of the coherent lattice transformations at martensitic PT in metals. The two OPs theory [5] was developed on the base of the Burgers mechanism. However these theories do not take into account volume change. The Kaschenko wave theory of the bcc-hcp martensitic transition [6] takes into account the volume change of the phases. A martensitic bcc-hcp PB satisfies [3-6] the Burgers and Nishiyama orientation relationships $(110)_{bcc} \| (001)_{hcp}$; $[111]_{bcc} \| [\bar{2}110]_{hcp}$.

We propose the three OP theory that combines Sanati [5] and Kaschenko [6] treatments that allows to take into account the changes in volume and pressure. The free energy depends on folloing three order parameters: the relative atomic plane displacement ξ along $[110]_{bcc}$, the stretching strain along $[110]_{bcc}$, and the compressive strain along $[100]_{bcc}$. We consecutively exclude the strain order parameters. With this purpose, in the space of the OPs we find the crossection (or trajectory) with minimal energy. Each excluded OP is found as function of the remainder ones. As the result, we have a variation problem for the last remainder order parameter ξ. After solution of the variation problem, other order parameters can be restored consecutively. So we reduce the three OPs free energy to the effective form in terms of one OP. The restored strains give volume change at constant pressure or pressure change at constant volume.

We introduce a thermodynamic parameter that characterizes the deviation from the phase equilibrium. The parameter describes the fine structure of a 180^o boundary and its split into two phase boundaries. The twin boundaries are nuclei of the original phase. On this basis we explain the bcc-hcp phase transition asymmetry and pressure change, found in solid ^{4}He experiments. The asymmetry in the bcc-hcp PT experiments in solid ^{4}He is explained as follows. At the direct PT the bcc then hcp crystals are formed at cooling from liquid. This is threshold nucleation with overcooling etc. At the reverse PT the topological defects in the hcp crystal, namely twin boundaries, split into pairs of the phase boundaries and form the bcc nucleous before the PT point.

The new experimental scheme is proposed to inverse the asymmetry of the bcc-hcp PT in solid ^{4}He. It is necessary to change the order of the obtained solid phases. At the direct PT the hcp phase must be initially obtained. The bcc phase must be the second (with threshold and so on). At the reverse PT, splitting of the twin boundaries must provide the hcp nucleation without threshold.

To explane the pressure relaxation in the ^{4}He hcp phase at ciclic annealing we need to introduce additional straine and its interaction with other OPs in the tween boundary.

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Vacancy Destabilization of hcp Solid Helium

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We analyze the problem of bcc phase existence in solid helium using identification of contributions of phonons and vacancies to thermodynamic properties. Phonons are considered within the classical Debye theory and vacancies are treated as wide-band quasi-particles according to Hetherington's approach [1]. The analysis of Debye temperature, Θ_D, and vacancy activation energy, Q_V, was performed in wide molar volume range for hcp ^{4}He and bcc ^{3}He [2]. Using dependence $Q_V(V_m)$ [2], we estimate vacancy concentration, x_v, on the bcc-hcp pressure-temperature line for the both helium isotopes. It results in the same dependence of $x_v(V_m)$ for ^{3}He and ^{4}He under condition of V_m increasing by 10% in ^{3}He. It means that in high temperature range, where vacancy contribution is essential, the hcp lattice is destabilized by high value of x_v. We establish that wide-band vacancies destabilize the hcp lattice and tend it to the hcp-bcc phase transition under raising their concentration with temperature near the melting curve for both helium isotopes. The criterion for hcp phase destabilization is found.

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Polarization Bremsstrahlung from Xenon Atoms and Clusters

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It was established that in the process of scattering of a charged particle by a target the bremsstrahlung (BS) is formed in two essentially different ways [1]. The first mechanism had been studied rather thoroughly earlier and implies *ordinary (static) bremsstrahlung* (OBS) resulting from breaking of a charged particle in the static field of the target accompanied by emission of photons. According to the other mechanism that was found later, the continuous spectrum photons are emitted not by the scattered particle, but by the target atoms as a result of their dynamic polarization in an alternating field of the incident particle. The bremsstrahlung formed in the latter way was given the name of *polarization bremsstrahlung* (PBS). OBS and PBS spectra do not only differ in the mechanisms of their formation (in particular, the PBS does not need any deceleration of the electron), but also have different dependences on frequency, radiation angle, mass and energy of the incident particle [1]. It should also be noted that the OBS is formed at small aiming distances from the target, while the PBS at greater ones.

In this work for the first time the results of experiments on PBS which arises from scattering of 0.7 keV electrons by gaseous and solid xenon are presented. The measurements were made in the photon energy range 80-180 eV. The concentration and size of clusters in the jet target was changed by varying temperature and pressure at the entrance to the supersonic nozzle. Gas and cluster supersonic jets were used as the targets [2], in the latter case the number of atoms in a cluster was varied from several tens to $8.5 \cdot 10^3$ at/cl. It was found that the PBS maximum shifts towards lower photon energies and narrows upon a passage from the gaseous target to the cluster one. The strongest narrowing was observed upon an increase in atom number for clusters having more than 500 atoms (up to almost 30% for $\langle N \rangle = 8.5 \cdot 10^3$ at/cl, cluster diameter being ~100 Å).

To describe the measured PBS spectra we performed model calculations of PBS cross section for an emitting center placed in a rarefied gas or in a solid state environment of Xe atoms. The environment was considered as a medium having a certain dielectric permeability [3,4]. For the solid state case, an additional calculation of PBS spectra was made to take account of the retardation effect that takes place in interaction of a damped oscillator with the surrounding atoms. The calculations describe well the measured PBS spectra and reproduce the spectral changes observed upon transition from gas to cluster targets.

Cooperative effects in a solid to have a strong impact on the PBS spectrum are found.

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The Amount of Non-Classical Rotational Inertia in Solid ^{4}He as a Function of the Crystal Quality

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We report measurements of the non-classical rotational inertia fraction in solid ^{4}He for crystals grown in an annular cell under different conditions. In our experiments the quality of the sample was characterized by measuring the thermal conductivity below 250 mK, where it is controlled by phonon scattering off dislocations and grain boundaries. Samples with the phonon mean free path in the range from 0.5 to 1annular spacing have been studied so far.

Investigation of Thermodynamic Properties of Deformed ^{4}He In the Supersolid Region

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A new series of experiments has been performed to find out the conditions for the formation of a glass phase in solid ^{4}He in the region where an anomalous behavior attributed to the supersolid effect was observed previously. A special two chamber cell was used to deform the sample in situ. The contribution of the glass phase was identified by analyzing the measured temperature dependence of the sample pressure under different experimental conditions. It is found that the contribution of the glass phase increased sharply after deformation of the sample and practically disappears after its annealing

Concentration Dependence of Fluctuation Effects in Solid ^{3}He-^{4}He Mixtures

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Experimental study of fluctuation effects in solid ^{3}He-^{4}He mixtures are carried out by high-precision pressure measurements at pre-separation region. The pressure was measured during the step-like cooling of the samples. At low temperatures total pressure of the system observed as the superposition of phonon and fluctuation contribution. The experimental dependences were compared with the theory. Phonon contribution is described in terms of Debye model, and the fluctuation contribution determined by correlation effects in the impurity subsystem. Due to fluctuations in local concentration the nuclei of a new phase grow as compact clusters containing hundreds of atoms. This effect implies an increase in pressure far from the phase transition onset. The fluctuation contribution exceeds the phonon contribution in concentrated solid ^{3}He-^{4}He mixtures, but it is not detected in week mixtures obviously due to the smallness of the effect. The concentration dependences of fluctuation pressure and nucleus size were obtained for the first time.

Oscillation Spectroscopy of Nanosized Structures of Indium In Cryomatrices of Condensed Gases. Methods, Installation, Results

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Influence of nanosized structures of indium on vibrational spectrums of nitrogen, oxygen and water matrixes was researched. Researched samples were formed during joint sputtering of metal vapors with matrix gases under different temperatures, pressures and concentration proportions.

Influence of Water and Ethanol Cryocondensate Film’s Thickness On Structural-Phase Transitions in the Range of Temperatures 12-160К

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Results of experimental researches of influence of water and ethanol cryocondensate film’s thickness on infrared spectrum of samples and also on thermostimulated transitions in the range of temperatures 12-160 К are presented. Film’s thickness varied from 0.5 to 30 mcm. Discovered size features are connected with presence of intermolecular long-ranged hydrogen ties in researched substances.

Dynamical Transitions in Cryocondensates Of Ethanol Close to Glass-Transition Temperature

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Experimental researches of structural-phase transitions in thin films of cryocondensates of ethanol close to glass-transition temperature T_g=97 K were done. Time-dependent relaxation processes under fixed temperatures ingenuously close to glass-transition temperature were studied. Characteristics of transitions amorphous (structureless)-glass (Am-G), glass- supercooled liquid (G-SCL), supercooled liquid – plastic crystal (SCL-PC), plastic crystal - orientational glass (PC- OG) and plastic crystal - monoclinic crystal (PC-MC) were defined simultaneously using infrared spectrometry and thermodesorption methods.

Infrared Spectrometry of Structural-Phase Transitions In Two-Layer (Crystal-Amorphous) Films of Ethanol Cryocondensates

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haracteristics of transitions amorphous (structureless)-glass (Am-G), glass- supercooled liquid (G-SCL), supercooled liquid – plastic crystal (SCL-PC), plastic crystal - orientational glass (PC- OG) and plastic crystal - monoclinic crystal (PC-MC) for two-layer films of ethanol cryocondensates were defined using infrared spectrometry and thermodesorption methods. Crystalline sublayer generated during condensation in the range of monoclinic crystal existence's temperatures. Further, bottom layer was cooled until T=12 K, and a film of solid ethanol in amorphous phase condensed.

Low-Temperature Post-Desorption from Solid Nitrogen

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A sequence of relaxation processes occur in solid insulators after excitation by some kind of ionizing radiation. A number of radiation induced defects (defects of structure, electrons and holes self-trapped/trapped in the lattice, molecule fragments) take part in these processes. For understanding of the radiation effects one has to follow different channels of relaxation processes. Different types of materials were investigated by various methods [1]. Thermally stimulated luminescence (TSL) based on measurements of total and spectrally-resolved yields of recombination emissions is the most popular method. However its use is limited in solids consisting of neutral and charged subsystems because in both of them radiative recombination can take place. In this case an interpretation of TSL measurements is complicated because one cannot distinguish these emissions. The most effective approach to investigation of relaxation processes is a combination of TSL and current spectroscopy methods, e.g. thermally stimulated exoelectron emission (TSEE). As TSL and TSEE methods are very sensitive to a sample prehistory it is very important to take both characteristics from the same sample at the same time. Our group has developed an experimental setup for simultaneous monitoring of several channels of relaxation in pre-irradiated cryogenic solids: concurrent measuring of the TSL yield, TSEE yield and the yield of sputtered atoms [2]. The TSL of solid nitrogen subjected to an electron bombardment was detected already at the beginning of matrix isolation studies [3], however its mechanism is still under discussion. We present the study of relaxation processes in solid nitrogen performed by the set of activation spectroscopy methods in combination with luminescence analysis. The yield of TSEE from solid nitrogen was measured for the first time.

The samples were grown from the gas phase by condensation on a cooled metal substrate. The substrate was grounded. The quality of our samples was controlled spectroscopically. Then they were exposed to an electron beam (500 eV). The energy transfer processes, defect energy levels and relaxation processes were probed by TSEE and TSL measurements.

We have found a correlation of TSL, TSEE and desorption yields from solid nitrogen previously subjected to an electron beam. This suggests an interconnection between electron-hole recombination and low-temperature desorption processes. Possible mechanisms of TSL and thermally stimulated desorption are discussed.

Charged Centers and Their Relaxation in Pre-Irradiated by an Electron Beam Solid Kr

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The role of charged centers attracts particular attention because of their role in different electronically induced phenomena like defect formation, diffusion and desorption of neutral and charged particles from material surfaces. The recent study of atomic and electronic relaxation processes in atomic cryocrystals revealed an anomalous low temperature “post-desorption” (ALTpD) from pre-irradiated Ne and Ar solids [1,2] at $T \ll T_{sb}$ (T_{sb} is the sublimation temperature). The basic mechanism of the ALTpD suggested is related to – the “cavity ejection” (CE) mechanism for atomic cryocrystals with negative electron affinity E_a (Ne and Ar) In order to exclude the contribution from the cavity ejection mechanism to “post-desorption” we focused on the study of this phenomenon in solid Kr characterized by positive E_a.

The experiments were performed employing cathode luminescence (CL) method in combination with correlated in real time measurements of thermally stimulated luminescence (TSL), thermally stimulated exoelectron emission (TSEE) and detection of the “post-desorption” yield by pressure measuring. Two heating modes were used: linear and step-wise heating. Strong influence of the grain size on charge accumulation was revealed and the role of surface-related traps was ascertained. The study enabled us to identify electronically induced defects similar to those detected in pre-irradiated solid Xe [2]. Activation energy of these defects was estimated by a set of activation spectroscopy methods. Analysis of the yields correlation enabled us to verify a two-stage mechanism of the ALTpD: (i) thermally assisted release of electrons from their traps followed by (ii) the intrinsic charge recombination reaction: $Kr_2^+ + e \rightarrow Kr_2^*$. The second stage of the ALTpD in solid Kr was found to be caused by the Kr_2^* “excimer dissociation” via radiative transition to a repulsive part of the ground state potential curve – the process which resulted in appearance of “hot” atoms capable to desorb the energy..

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Charged Molecular Centers in Pure Kr and Mixed Kr-Ar Clusters

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Excited charged and neutral molecules are the main radiative centers in the VUV spectral range in cryocrystals and cryoclusters of rare gases. Neutral molecular centers of R_2^* type arising from localization of excitons and electron-hole recombination are typical of bulk cryocrystals. Charged molecular centers of $(R_2^+)^*$ type were first found upon excitation of rare gas clusters (see Ref. [1] and references therein): when an electron-hole pair is formed in a cluster, the electron is more likely to leave the cluster preventing thus the electron-hole recombination. Emission from such centers was also found in bulk Xe-Ne cryoalloys, in which Xe atoms form small clusters in the Ne matrix [2]. Here we study the formation of excited charged molecules in free pure Kr and mixed Kr-Ar nanoclusters produced by gas condensation in a supersonic jet. The obtained free solid-state clusters with the temperature of 60 K were excited by a beam of 1 keV-electrons. The emission spectrum was registered in the photon energy range 7-10 eV where the molecular bands Kr_2^* (8.4 eV) и $(Kr_2^+)^*$ (7.8 eV) are located. In pure Kr clusters the intensity ratio of the bands was found to be close to 1 for clusters containing over 2000 atoms, which was reported earlier in Ref. [1]. At the same time, addition of even a small amount of Ar to clusters having more than 1000 atoms (Ar being dissolved in Kr) causes a substantial (more than two times) growth of the charged molecule band. This suggests that addition of Ar favors emission of electrons out of the cluster upon its excitation. The obtained results are of interest from the viewpoint of creation and investigation of ionized cluster beams [3].

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Quasi-Particles Spectra in Graphite Compounds with Metallic Intercalated Layers

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Phonon spectra of graphite starting with consideration of bigraphene, are analyzed at the microscopic level. Partial contributions to the phonon density of states of the atomic displacements along the directions of strong and weak coupling (along the layers and perpendicular to them) are calculated. Characteristic features of the vibrational spectra of these structures are analyzed. High accuracy of the description of the phonon spectra of the compounds is confirmed by the practically complete coincidence of our calculations with the data of neutron diffraction, acoustic and optical experiments. For each of the examined compounds to calculate the temperature dependence of the mean-square displacements of bulk samples and nanofilms along different crystallographic directions, which allow us to estimate the stability of graphite nanofilms.

It is shown that the spectral density of phonons polarized along c axis has in graphite the V-type singularity analogous to so-called Dirac singularity typical for the grapheme electron density states [1,2]. We study the appearance of quasilocalized states which increase number of quasiparticles near this singularity by using as examples the phonon spectra of graphite intercalated by metals and electron spectra of grapheme containing vacancies. It is proved that in the electron spectrum of grapheme with isolated vacancy the quasilocalized states exist only for atoms from sublattice not containing this defect.

Our calculations make it possible to forecast the general properties of graphite phonon and electron spectra in the case of intercalation of graphite by different metals.

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Ergodic Instability in Amorphous Solids

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Broadly speaking, there is no conceptual gap between amorphous states in supercooled liquids, glass-forming polymers, orientational glasses, and metallic glasses. Indeed, near the glass transformation temperature T_g detected by differential scanning calorimetry, the primary relaxation dynamics of glass-like clusters is universal [1] and as a consequence the two-level tunneling cluster states can be observed via the configurational entropy in all glass formers [2]. The structural transformation, which occurs under cooling rates preventing formation of the long-rage crystalline order, is essentially a crossover from the high-temperature thermally equilibrated ergodic state to low-temperature non-ergodic glassy states, characteristic of amorphous solids. Researchers have long searched for any signature of the underlying "true" ergodic-non-ergodic transition emerging at a certain ergodic-instability temperature T_e designated by a critical temperature at which the certain physical characteristics exposes a divergent behavior. A traditional approach is to map the order-disorder thermodynamic transitions onto the geometric, cluster percolation picture [1].

Relaxation timescale for glass-forming materials was analyzed within a self-consistent thermodynamic cluster description combined with the cluster percolation concept. Using of the ergodic hypothesis, its violation was found near crossover from the Gaussian to non-Gaussian (Poisson) cluster-volume fluctuations, with the help of Stauffer scaling form known for the finite-size fractal cluster distribution. The crossover of the compact-structure “ergodic” clusters to hole-like glassy nanoclusters treated at mesoscopic scale of consideration is attributed to their critical-size thermal fluctuations. For the special case of organic molecular supercooled liquids, the ergodic-non-ergodic phase diagram was predicted [3] in terms of the ergodic-phase instability temperature T_e, as a function of the glass fragility parameter. In the present study, the method communicated in Ref. 3 is extended over inorganic liquids and amorphous solids. Equation for T_e is re-analyzed in the model-independent form that provided the ergodic instability boundary in different glass forming materials. This boundary now is tested by recent experimental data obtained for glass-forming polymers and metal alloys. In all cases the temperature of ergodic instability is located below and close to the glass transformation temperature. The distance between the two characteristic temperatures decreases when the glass material fragility grows.

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Condensed Phases of Hard Core Bosons on a Square Lattice

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A hard-core boson (HCB) model on a square lattice is known to exemplify liquid, solid and superfluid phases. Up to now finite temperature phase diagrams for classical and quantum square lattice HCB models have been investigated for the most part numerically. Analytically the diagrams were built mainly within mean field approximation (MFA), which in essence implies that the Ising model was treated, so that the hopping term in the HCB Hamiltonian was completely neglected.

It is important to elucidate using analytical methods how the hopping modifies the properties of the HCB system as compared with those found within MFA. For this, using two-time Green-function formalism with the decoupling on the first step (random phase approximation) we build finite temperature phase diagrams and calculate thermodynamic functions for a quantum square lattice hard-core boson model with nearest neighbor (nn) and next nearest neighbor (nnn) interactions [1]. The nn interaction is assumed to be repulsive while nnn interaction is considered to be either attractive or moderately repulsive, so that the collinear or other complicated phases do not appear.

The behavior of the system has been investigated at different magnitudes of hopping t and ratio between the nn and nnn interactions. It turned out that for HCB model with only nn interaction even arbitrary small hopping leads to the appearance of the first order phase transitions in the low temperature region, whereas within MFA only continuous phase transitions are possible in this case. The RPA analysis shows a significant distinction in the behavior of the HCB model at high and small hopping. Namely, at small hopping with decrease in temperature neither solid nor liquid can exist as stable homogeneous phases, so that below a definite temperature the system is necessarily separated into two-phase mixture. In this respect the system with small t displays behavior similar to that found for the Ising model. In the case of high enough hopping the properties of the system are quite different. Due to the high kinetic energy there exists a density region where a stable homogeneous liquid phase occurs up to zero temperature. Furthermore, if the nnn interaction is repulsive then the density region of absolute instability at zero temperature extends till some density, above which a homogeneous solid phase can exist up to zero temperature at least as metastable.

Our investigations indicated conclusively the possibility of reentrant phase transitions in a square lattice HCB with nn and nnn interactions. In particular, we confirm the corresponding numerical results [2,3] found for HCB with only nn interaction.

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Two-Dimensional Hard Core Bosons at Zero Temperature: Superfluid Density and Spin Wave Dispersion

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Two-dimensional hard core boson (HCB) model exemplifies different phases such as liquid, superfluid, solid, and supersolid characterized by coexistence of both diagonal and off-diagonal long-range order.

Ground state properties of the HCB model with nearest-neighbor (nn) repulsion, V_1, and next-nearest-neighbor (nnn), V_2, interaction (repulsive or attractive) on a square and triangular lattices are investigated by mapping onto a quantum magnet spin—1/2 model. Using the nonlinear spin-wave approximation we find the ground state energy, the particle density ρ, and the superfluid density ρ_s as functions of the chemical potential. We also calculate excitation spectra $\omega(\mathbf{k})$. The spin-wave dispersion curves of HCB on both types of lattices at various values of ρ, V_1, and V_2, are presented along different directions in the Brillouin zone. For both types of lattices the spectrum is gapless at $\mathbf{k} = 0$. We obtain corrections to the spin wave velocity due to the spin wave interaction. The behavior of the excitation spectrum in special points on the boundary of the first Brillouin zone is analyzed with the aim to determine the parameters ρ, V_1, and V_2 at which $\omega(\mathbf{k})$ in these points becomes unstable and turns to zero. Vanishing $\omega(\mathbf{k})$ implies the possibility of a phase transition into a new phase.

At particle densities not too different from half-filling for a square lattice a roton minimum develops in the dispersion curve at the antiferromagnetic wave vector $\mathbf{k} = (\pi,\pi)$. The minimum becomes more pronounced with increase in nnn attraction, in complete accord with the fact that nnn attraction stabilizes the Neel order. Account for nonlinear corrections deepens noticeably the roton minimum, which means that at fixed attractive V_2 this minimum collapses to zero at smaller values of V_1 than the linear spin-wave theory predicts. If V_2 is repulsive, in the curve $\omega(\mathbf{k})$ there appear another minimum at the wave vector $\mathbf{k} = (\pi,0)$. This minimum deepens with increase in nnn repulsion. Such a behavior is quite expectable since the nnn repulsion gives rise to the formation of the striped phase.

In the case of triangular lattice at ρ close to half-filling the excitation spectrum has well-defined roton minima at the point $\mathbf{k} = (4\pi/3,0)$ and equivalent boundary points of the Brillouin zone. Account for the nonlinear spin-wave corrections for a triangular lattice in distinction to a square lattice shallows the roton minima making them less pronounced. Increase in attractive nnn interaction leads to a decrease in the roton gap. On the contrary, the nnn repulsion removes the roton minimum changing it into a maximum.

The case of half-filling, when the expressions for $\omega(\mathbf{k})$, ρ, and ρ_s simplify essentially, is investigated in details. In literature the HCB at $\rho=1/2$ has been extensively studied for the most part numerically. Despite of its simplicity, this special case is of particular interest, for it clearly demonstrates the significant difference in the behavior of HCB on square and triangular lattices. Indeed, at $\rho=1/2$ on a square lattice the transition from the superfluid is possible only into solid phases, whereas on a triangular lattice the superfluid always changes by supersolid.

We compared our analytical results on excitation spectra, particle density and superfluid density with numerical simulation data [1-3] and obtained a good agreement.

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Two Dimensional Hard Core Bosons in the Random Phase Approximation

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A hard-core boson (HCB) model is appropriate for the description of quantum condensed systems, such as atomic and molecular monolayers on substrates, particles trapped in optical lattices. It is also used in helium physics, supersolid phenomena, and superconductivity. The HCB Hamiltonian is naturally mapped into an anisotropic spin-1/2 XXZ model in a magnetic field, whose properties are in itself of great interest.

Using random phase approximation we calculate thermodynamic functions of a square lattice hard core boson model with nearest (nn) V_1 and next nearest neighbors V_2 (nnn) interactions in terms of equivalent to it an anisotropic spin-1/2 XXZ model in a magnetic field [1]. Contrary to the mean field approximation, the present method takes consistently into account the hopping term in the HCB Hamiltonian giving rise to the nontrivial dispersion of elementary excitations.

The system undergoes liquid-solid phase transitions that can be either of the first or second order. Depending on the hopping value t and ratio $\alpha = V_1 / V_2$ between nn and nnn interactions the system displays two types of critical behavior. The line of the first order transitions terminates in a bicritical endpoint inside the solid phase or ends in a tricritical point continuously giving way to the second order phase transition line. The connection of the hopping and the ratio α with criticality of the system is investigated. We have built the α $-1/\Delta$ ($\Delta = V_1/2t$) diagram, the locus of critical points where bi- and tricritical regimes change each other. It turned out that over the interval $1/(1+\alpha) < \Delta < \Delta_0 > 1.38$ only the tricritical regime is possible. At fixed $\Delta > \Delta_0$ two points α_{c1} and α_{c2} appear in the α $-1/\Delta$ plane, so that inside and outside the interval $\alpha_{c1} < \alpha < \alpha_{c2}$ the system displays the bi- and tricritical behavior, respectively. If Δ tends to infinity then $\alpha_{c1} \rightarrow 0$ and $\alpha_{c2} \rightarrow 0.6$ in full agreement with the well-known MFA results.

Thermodynamic properties of the system under study are investigated. For the anisotropic 1/2-spin XXZ model in a magnetic field we have derived the exact expression connecting the internal energy with the transverse Green function. The heat capacity C and magnetic susceptibility χ are calculated. As one would expect, the dependences $C(T)$ and $\chi(T)$ exhibit λ-point kind irregularities at the corresponding phase transition temperatures. In the paramagnetic phase a temperature run of the susceptibility depends significantly on whether the magnetic field h is lower or higher than the critical value h_c which is a function of both α and Δ. The quantity h_c is the critical field that determines the phase transition between spin-flop and paramagnetic states at zero temperature.

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Behavior of Structural Characteristics of CO_2 Solids With Atomic Impurities

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Solid alloys of cryocrystals consisting of “long” linear molecules and rare gas atoms are convenient objects to investigate random systems, the problems of orientational glass states, phase transitions related with changing the orientational order/disorder in the lattice [1]. Structural investigations and analysis of such molecular solids make it possible to obtain the important information for theory of the formation of solutions, data about the character of phase diagrams [2-4]. The peculiarity of classical cryosolid such as CO_2 is the absence of transition from highly oriented ordered phase to orientationally disordered one with raising the temperature. A strong anisotropic interaction between particles prevents the rotation of molecules and may be changed by the introduction of spherically symmetric inert gas atoms in the lattice of molecular crystal. The orientational behavior of molecules in mixtures is studied using a concentration-dependent intensity of diffraction peaks. Additional important information can be obtained from an analysis of the dependence of lattice parameter on the composition. There is the correlation between a degree of long range orientational order in the matrix and the character of the concentration dependence of the lattice parameter of the solution. We present the detailed study of the lattice parameters of the binary cryoalloys carbon dioxide – rare gas.

Investigations were carried out by transmission high – energy electron diffraction (THEED) technique using a special helium cryostat. The samples were prepared *in situ* by depositing room-temperature gas mixtures of known composition onto a substrate at various temperatures. The composition of the investigated binary alloys was varied from 0 to 1. Measurements were made at temperature from 6 K to the sublimation temperature of pure rare gas. The relative error of precise measurement of the lattice parameter was usually about 0.1 %.

The crystallographic structure and the range of solubility of the CO_2 – rare gas alloys have been determined. Solid solutions are practically not formed from the rare gas side. The solubility of Kr and Ar in CO_2 matrix doesn’t exceed 38 and 30 mol.% respectively. The structure of solid solutions belongs to the ordered state *Pa3* symmetry. A characteristic feature of solid solutions is the nonmonotonic dependence of the lattice parameter on composition. For CO_2 – Kr system the graph can be divided into different regions, including an interval, where a curve has a minimum. In solutions enriched by Ar atoms the dependence is shaped unusually as a curve with a maximum. The anomalous behavior is explained within a cluster approach, which accounts three mechanism of interaction of rare gas clusters with their CO_2 environment. Variations in the morphology due to the possible lack of homogeneity of the solutions are discussed.

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Phase Transition Line of Solid Molecular Nitrogen into *CG*-Polymeric Phase

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Two equations of state for solid nitrogen – one for the high-pressure molecular phase [1], and second one developed earlier [2] for the polymeric *cubique gauche* crystalline phase, based on Monte Carlo simulations [3], and *ab initio* calculations of energy differences of two crystalline structures have been employed to predict the coexistence line of these two phases in *P*-*T*-diagram and calculate phase transition parameters: latent heat, volume and entropy gaps. In contrast to the transition into layered A7-structure [1], the transition into spatial-polymerized *CG*-structure is typical entropic transition with negative slope of *P*(*T*)-curve and almost constant entropy gap. At low temperatures the predicted *P*(*T*)-curve is in a good agreement with the recent experimental data [4] and at elevated temperatures tends to the vicinity of the pressure maximum on the melting line, observed in recent experiments [4,5].

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Similarity of the Boson Peak in Disordered Systems to the Acoustic van Hove Singularities in Regular Crystals

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The present report has clarified at the microscopic level the reasons for the appearance of characteristic differences of the phonon spectrum of solids from the Debye spectrum in the low-frequency region. It can be concluded that the nature of the Ioffe–Regel' features and disordered systems is similar to the nature of the formation of the first van Hove singularity in structures with crystalline regularity in the arrangement of the atoms. The Ioffe–Regel' feature, defined as the boundary between rapidly propagating phonons ("propagons") and slower phonons ("diffusons") [1], corresponds to the wavelength of rapidly propagating phonons for which these phonons start to feel the defect structure. The frequency of the first van Hove singularity corresponds to the wavelength of fast acoustic phonons starting at which the propagation of these phonons changes qualitatively—the discreteness of the crystal lattice starts to affect the propagation. The average velocity and the average wavelength of acoustic phonons change abruptly. Consequently, the first van Hove singularity also separates fast acoustic phonons with a nearly acoustic dispersion law (the same "propagons") from much slower phonons ("diffusons") whose dispersion law is different from the acoustic dispersion law. The presence of different kinds of defects in a crystal can result in additional retardation of fast acoustic phonons, which under certain conditions can also be manifested as a jump in the frequency dependence of their group velocity. The conditions reduce to the formation of quasilocalized states in the phonon spectrum, i.e. very slowly propagating phonons localized near any defect. These states can not only give rise to low-frequency maxima in the "propagon" frequency range of the initial idea of crystal but they can also serve as scattering centers for fast acoustic phonons corresponding to the vibrations of atoms of the main lattice. It was shown that defect clusters which are at least two interatomic distances in size can serve as effective scattering centers. Consequently, we calculated the parameter, which can be taken as the disorder parameter, becomes comparable to the wavelength (Ioffe–Regel' limit [2,3]).

The phonon enrichment of the low-frequency region of a quasicontinuous spectrum causes the density of states to deviate appreciably from the Debye form. It was shown that this deviation, often manifested as peaks in the ratio of the phonon density of states to the squared frequency (so called "boson peaks" or "boson maxima"), is due to the additional dispersion of sound waves. Nonetheless, the low temperature specific heat and the temperature dependence, expressed through it, of the Debye temperature are informative characteristics of this redistribution of phonons over the spectrum.

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D_2 Dissociation in Xe Matrix under Electron Beam Irradiation

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In the sequence of rare gas (Rg) cryocrystals, only in Ne the energy of electron-hole pare suffices to bring about dissociation of a D_2 molecule in well-known way of its ionization and formation of RgD^+ centers. In Kr, and much less in Xe (the forbidden gap E_g=9,3 eV), the standard scheme of dissociation by recombination of electron with ion RgD^+ is doubtful. The nontrivial question arises of whether or not the dissociation process of D_2 in Xe matrix can be efficient on condition that matrix electron subsystem undergoes the excitation.

In the present work, the experimental study of formation processes of $(Xe_2D)^*$ complexes is carried out in solid binary mixtures Xe-D_2 under their irradiation by monochromatic electron beam with energy 1 KeV, when the processes of the matrix electron excitations creation are prevailing. The measurements were performed at T=4,2 K using the method of VUV and UV luminescence spectroscopy, with D_2 concentrations ranging from 10 to 10^{-2} %. Among all the observed spectra the most intensive is the band "*M*" at 7,03 eV, which corresponds to the well-known radiation of self-trapped two-center states of Xe_2^* in xenon matrix. Also, we have observed the band "*XD*" with maximum at 4,8 eV, which have been identified as the radiation from impurity centers $(Xe_2D)^*$ [1]. The intensity of this band serves as a measure of the efficiency of D_2 molecule dissociation. The band "*XD*" considerably increases its intensity when impurity concentration in the solution increases, though not exceeding 30% of the intensity of the "*M*" band.

Hence, it is for the first time discovered that in solid mixtures subject to electron beam radiation there occur the transport of matrix electron excitations to the impurity D_2. The excitation trapping by the local center results in dissociation of molecular deuterium. D atoms diffusion all over the lattice at small concentration of the impurities results in separation of the dissociation products and accumulation of one-atom impurity centers within the matrix. Then, under conditions of competition with excitation self-trapping process they become excited, which manifests itself in the form of radiation of excited molecular exciplexes $(Xe_2D)^*$.

For rather low concentration of D_2, c=0,1%, we have investigated the process of the band *XD* "build-up" at the initial period of irradiation. It is found that characteristic time of the molecule D_2 dissociation in Xe matrix amounts to 5 seconds.

At given excitation conditions, we have also performed control measurements of spectra of pure solid deuterium, solid mixtures Kr-D_2, and triple mixtures Kr-Xe-D_2. In deuterium radiation spectrum there were found no indications of dissociation of D_2 molecules in the crystal bulk. The luminescence spectrum of solid mixtures Kr-D_2 turned out to be completely equivalent to the spectrum of nominally pure krypton up to the concentration of D_2 amounts to 25%. The addition only of Xe impurity leads to the occurrence in Kr-Xe-D_2 crystal of radiation bands of centers $(Kr_2D)^*$ and $(Xe_2D)^*$, whose intensity depends substantially on the irradiation dose. This fact suggests that Xe excitation stimulates in a specific way the reaction of molecule D_2 dissociation.

The mechanism of the molecule D_2 dissociation in the xenon matrix is discussed. It is shown that creation of $(XeD_2)^*$ intermediate states in the localization process of matrix excitons at the impurity molecule can facilitate this phenomenon.

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Oxygen-Helium Condensates as Optimal Medium for Very Cold Neutron Reflectors

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Discovery of efficient reflection of very cold neutrons (VCN) from powders of diamond nanoparticles [1] suggests that oxygen-helium condensates may be among the best materials for reflectors of VCN. An extremely intense scattering of VCN observed from thin powder samples was in good agreement with the theoretical model of independent nanoparticles at rest [2]. The model predicts that nanoparticle powders can be efficient reflectors of VCN with energies up to 10^{-4} eV. This value of the energy and the reflection probability far exceed values for the best available supermirrors, although the reflection for nanoparticles is not specular. Nanostructured materials provide a sufficiently large cross-section of coherent interaction and inhomogeneity of the moderator density on a spatial scale approximately corresponding to the neutron wavelength [3]. For this purpose such materials have to meet certain requirements: ultrafine size of the building blocks (~nm), high porosity and rigidity of the inner structure. A large number of neutron–nanoparticle collisions needed for VCN reflection (they scatter in forward direction preferably) restricts the choice to low absorbing materials with a high effective Fermi potential.

Impurity-helium condensates (IHCs) are formed in superfluid HeII upon condensation of a helium gas jet containing ~ 1 % of admixtures (molecular and/or atomic hydrogen, nitrogen or oxygen, and/or atoms of neon, argon, krypton). This technique was invented in Chernogolovka to stabilize and study free radicals in superfluid helium in the 70’s [4]. As the jet traverses through the cold gas above the liquid level, impurity nanoclusters are formed. The ensemble of clusters penetrates through the superfluid surface and forms a gel-like substance. Each cluster is surrounded by a thin layer of solid helium. The clusters aggregate to form long interconnected strands with the pores between the strands containing liquid helium. From X-ray [5,6] and ultrasound [7,8] investigations the linear dimensions of the clusters were ~5–6 nm and the pore diameters ranged from 1 nm to 860 nm. Impurity atom densities as low as of ~10^{20} cm^{-3} could be detected. Impurities heavier than molecular deuterium form semirigid porous structures in HeII [8]. IHCs made of molecular oxygen meet all the requirements to serve as a medium for reflectors of VCN. The temperature range of the IHC stability (below 4.2 K) eliminates the problem of upscattering VCN.

The feasibility of efficiently reflecting VCN from powders of nanoparticles bridges the energy gap between efficient reactor reflectors for thermal and cold neutrons and the effective Fermi potential for ultracold neutrons (UCN). This phenomenon has a number of applications, including storage of VCN in closed traps, reflectors for VCN and UCN sources, the more efficient guiding of VCN and, probably, of even faster neutrons.

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Ions in Impurity-Helium Condensates

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Impurity-helium condensates consisting of impurity (H_2, D_2, or N_2 molecules, atoms of neon, argon or krypton) nanoclusters can be used to store and study very high concentrations of radicals [1,2]. Nevertheless, experimental conditions optimal for creation and storage of high concentrations of radicals are quite different from those needed to obtain and stabilize ions in impurity nanoclusters. We will report on first observations of molecular nitrogen ions in impurity-helium condensates.

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Hindered Rotation of Impurity Molecules In Ordered and Disordered Matrices

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The paper extends findings on EPR of matrix isolated methyl, CH_3, radicals to a temperature region above 4.2 K. It was shown earlier that, at temperatures below 4.2K, the spectra reveal noticeable anisotropy of both the hyperfine interaction of the unpaired electron with the molecule protons and the g-tensor [1, 2, 3]. The extent of the anisotropy was different in different solid gas matrices and varied from unobservable in n-H_2 to emerging through splitting of the hf-lines in CO matrix. It was supposed that molecular matrices with orientation ordering, like CO, fix the C_3 axis of the CH_3 radical, while enabling fast torsional tunneling rotation. In matrices with no orientational ordering, Ne, Ar, Kr, the axis is allowed to perform fast tunneling hopping between different preferable positions which leads to the much less pronounced anisotropy appearing only in the difference in the linewidths and amplitudes of the hf-components.

This model of the CH_3 rotation in solid gas matrices is now verified and discussed in greater detail using experimental results in higher temperature range from 6 K to 40 K and other matrices with orientation ordering, CO_2, N_2, N_2O. Also we obtained much narrower lines for CH_3 in p-H_2 compared to n-H_2 and verified an assumption [1] that the radical is free to rotate in solid H_2. It is shown, also, that molecular matrices with orientational order and disorder result in different temperature dependencies of the line shape of the radical EPR spectrum: the sample temperature rising largely reduces the anisotropy in a non-ordered molecular solid while remaining it nearly intact in an ordered molecular solid.

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Equation of State for Compressed Inert Gases

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The equation of state for solid inert gases valid at high pressure is of importance for modeling the general problem of matter transformation at ultrahigh densities. The main interest here is the transition of the solid from perfect insulator to highly conductive metal. That is why the common way of investigation there is the observation of electrical conductivity sporadically appeared at some temperature and pressure applied to a sample. Meanwhile provided some amount of excess electrons were introduced into a solid the study of the electrical properties, first of all the charge mobility, should be carried out a long before the dielectric-metal transition occurrence. The experimental approach to such a study is the electrical discharge organization inside condensed inert gases [1, 2]. The very possibility of a discharge realization as well as the peculiarities of metal made of compressed inert gas, such as its conductivity, are strongly dependent from free electron transport properties and their density at high pressure. With this goal we composed the state equation for compressed heavy inert gases at wide range of its pressure up to the pressures close to these corresponding to metallization. The dielectric-metal transition experimentally observed already in xenon at ultrahigh pressure has been described as intersection of electron terms for an atomic ion and atom located in a compressed inert gas, and the main contribution to this term behavior is due to an exchange interaction of an ion with surrounding atoms [3]. Therefore the upper limit of our approach validity is the pressure when the system of repelling atoms is a dielectric with "forbidden band" not less then $1eV$.

We suggest that a pairwise interaction can perfectly describe a system of repelling atoms with completed electron shells. Indeed, this interaction result from exchange by valence electrons which belong to different atomic cores, and this exchange interaction potential is determined by regions of electrons when they are located in a vicinity of the axis joined atomic centers. Basing on this reasoning we used experimental interaction potential between inert gas atoms in a gas to describe a condensed atom system at high pressure. We consider the interaction potential of a test atom with surrounding atoms as the sum of pair interaction potentials of this atom with nearest neighbors. The equations of state for Ar, Kr and Xe were found such a way and then the dependences of "forbidden band" on pressure were calculated for all three heavy gases up to the pressures close to these where metallization takes place.

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High Efficient Field-Induced Electron Emission from the Bundles of Nanowires Grown in Superfluid Helium

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Cold cathodes based on field-induced electron emission from metallic nanowires and carbon nanotubes are now widely studied. The arrays of needles usually give at arbitrary low temperature the electron current about tens of nanoA under reasonably low applied voltage. The common methods of producing tiny nanowires and nanotubes as a rule restricted their length by 1 – 2 mkm, whereas the bundles of nanowires being by 3 orders of magnitude longer can be produced by laser sputtering of metal in superfluid helium [1]. That was the reason to reveal the ability of so produced nanowires to emit electrons. The bundle was found to be fixed at the top of the needle-like electrode, where the generated nanowire quantized vortex was pinned, thus the electrical measurements could be performed just in liquid helium.

Electron microscopy study performed at room temperature have shown that for all investigated metals, such as Ni, Pb, Sn, and In, the nanowires had the diameter of 5-7 nm and they consisted of conjunct single crystals having regular structure.

The dependence of emission current I on voltage U was typical for cold cathode, namely sharp growth of I at small U was followed by $I \sim U^2$ dependence. No temperature influence on I value was observed at the 1.6 – 4.2 K range, even when superconducting wire passed to its normal state. For small voltage $I(U)$ dependence was well described by Fowler-Nordheim formula and it was characteristic for every metal, whereas at high U it better fitted to classical $I \sim U^2$ dependence.

The most interesting result was the huge value of electron emission; for all metals the electron current at U = 100V was as much as tens of μA or at 3 orders of magnitude more than for conventional cold cathodes. The problem is only how to fix the nanowires at the tip enough tightly to use the array as effective cold cathode.

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Infrared Light Interaction with Impurity Gels in Superfluid Helium

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Atoms and molecules of majority of matters introduced in helium format clusters with attractive impurity core covered by helium atoms. The quick cooling of these clusters into superfluid helium formats a distinctive soft matter – impurity-helium gel, the clusters of which conglutinate into nanoparticles. The possibility of using of these gel of nanoparticles as a moderator for thermolization of ultracold neutrons depends from mass of these nanoparticles and from mutual interaction of clusters compounding these nanoparticles. The purpose of the next experiments was to try to estimate an applicability of these gels as a neutron moderator.

Our previous investigation of neutron scattering by deuterium and heavy water gels indicated that a deuterium gel has a very wide set of sizes of particles from nm up to mkm. Concentration of lowest particles may be increased by heating of the helium soaking the gel to normal state. Gauge of heavy water gel particles is limited by sizes from nm up to ~10 nm. Hereby, the size of quasiparticles of deuterium consist gels makes these materials promising as a neutron moderator.

In the last set of experiments we try to understand a nature of intermolecular interaction in water gel in superfluid helium. The primary results of measurements of adsorption of infrared light indicated that the characteristic peaks for gel is different from a water or a simple ice. It may imply that water molecular in helium surrounding have a different interaction. We are planning to report results of these experiments.

X-ray Studies of Impurity-Helium Condensates

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Impurity-helium condensates are nanostructured materials produced by injection of a helium gas jet containing a dilute amount of another chemical species into superfluid helium. They consist of a highly-porous assembly of impurity nanoclusters suspended inside liquid helium. These complex materials hold potential for various applications, as well as serve as an intriguing system for fundamental studies. Examples include cluster physics, properties of helium in a confining medium, free-radical chemistry, energy storage, and production of cold neutrons. Structure of the impurity network in impurity-helium condensates is of key importance for studies of these materials. Herein, we present x-ray diffraction studies of several noble-gas and molecular-gas based condensates, and discuss the obtained structures of the impurity nanoclusters forming the backbone of these materials.

Nanocluster Condensates in He-II as a Tool for Production of Ultra-Cold Neutrons: Experiment and Numerical Simulation

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Ultra-cold neutrons (UCN, $E<10^{-7}$ eV) provide an excellent tool for high-sensitive experiments in condensed matter physics, search for non-zero neutron electric dipole moment, gravitational studies, *etc*. Recently we elaborate new idea based on the use of impurity-helium nanocluster condensates (quantum gel) in superfluid helium He-II as a new tool for production of UCN at high densities. The reason for significant interplay between nanocluster condensate with slow neutrons is, on one hand, in an approximate equality of wavelength of the last and characteristic size of inhomogeneities in gels and, on another hand, relatively high cross-section of neutrons scattering on a backbone of the condensate.

As it was reported earlier, see e.g. [1,2], cold neutrons (CN, 10^{-4} eV $<E<10^{-2}$ eV) are scattered effectively on macroscopic samples of gels made of heavy water in superfluid He-II at $T\sim$ 1.6 K. In particular, strong changes in angular distribution of neutrons scattered on D_2O sample of size 2.8 cm with variation in the neutron energy was observed: At low energies $E<0.5$ K neutrons show isotropic s-scattering, whereas the increase of neutron energy up to 5 K results in the transition to strongly anisotropic scattering where ~90% of neutron beam is scattered into the angle $\leq 8^{o}$. It was also shown that the characteristic dimensions of impurity clusters are $3<d<150$ nm for as-prepared deuterium gel sample and $d<15$ nm for heavy-water gel samples.

To understand better the effect of gel structure on neutron scattering, we perform numerical modeling of gel formation processes in a cold gas flow and in a cell filled with He-II. It is shown that finite size of the cell (and, hence, geometry of the gas flow inside) affects strongly the resulting gel structure. The density correlation function for the gel is computed numerically basing on the results of modeling. We also propose a model suitable for description of neutrons propagation through the gel sample. According to the model, at low gel densities (i.e. when the effective mean free path of neutron, l_f, is of the order of, or larger than the sample size L) neutrons of wavelength ~9 A propagate nearly ballistically through a D_2O or D_2 gel, therefore having only a few scattering events in the sample bulk, whereas at high gel densities ($l_f << L$) neutrons diffuse through the gel sample. This diffusive motion of neutrons in the gel leads to strong increase, in L/l_f times, of effective propagation time and, hence, to sharp increase of the total interaction cross-section of neutrons with the sample. Results of the analysis are discussed in view of production of high-intensive UCN beams.

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On the Role of Distortion in the HCP vs FCC Competition In Rare Gas Solids

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As a prototype of initial or intermediate structure somewhere in between HCP and FCC lattices we consider a very distorted BCC crystal. We showed previously [1,2] that small BCC crystallites may freely relax towards the HCP structure under the applied Lennard-Jones [1] and Aziz [2] potentials. In some particular distortion cases an increasing contribution of the FCC phase was found [2]. In the presented work we calculate first the bulk phase diagrams for heavier rare gas solids in the quasiharmonic approximation applying the Aziz potentials and confirm that in line with the previously found prevalence of HCP over FCC the former structure (HCP) is still dominant in the bulk over the wide *P-T* ranges analyzed. The situation is different for small clusters where owing to the specific surface energetics the structures with five-fold symmetry comprising FCC fragments are dominant [3-5]. As a second step we consider a free relaxation of differently distorted BCC clusters, and show that two types of an initial distortion and its degree is a driving force for the HCP vs FCC final realizations. Possible energetic links between the initial and final structures are shown and analyzed.

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Conductivity and Critical Field of the 2D-Electron Crystal at the Dynamic Phase Transition

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The complex conductivity of 2D electron crystals (with surface charge density 2.3×10^8-12.6×10^8 cm^{-2}) over liquid helium is studied experimentally depending on driving electric field. The measurements are carried out at the temperature T ~ 100 mK essentially lower than melting temperature. The complicated behavior of both conductivity components and their sharp change are observed at some critical value of electric field. The value of critical electric field of dynamic non-equilibrium phase transition is estimated within a simple model. Analysis of obtained results indicates a possibility of dynamic melting of 2D electron crystal by electric field in nonlinear regime.

Laser Ablation of Boron in Bulk Superfluid Helium

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Laser ablation of solid boron target embedded in bulk superfluid 4He at 1.5 K was used to generate boron atoms in the liquid. Within ca. 100 microseconds these atoms are thermalized and become partially solvated. The excitation spectrum of the 2P state boron atoms were recorded by the laser induced fluorescence technique (2S <- 2P transition) by monitoring the atomic emission line near 250 nm. The excitation spectrum shows two sets of broad asymmetric lines around 238 nm and 230 nm. The preliminary interpretation of the two sets of bands assigns them to boron atoms in the bulk (230 nm) and in dense gas bubbles (238 nm). The 230 nm band shows similar features that have been observed for boron atoms trapped in solid argon but is less blueshifted. The strong blueshift suggests a non-spherical ground state solvation structure, which is a result of the dynamic Jahn-Teller effect.

Rotational Spectroscopy of Doped Small Helium Clusters

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Spectroscopy of atomic and molecular clusters is a perfect tool to understand how properties of matter evolve from the molecular size scale to the bulk phase. Much progress, both in experiment and theory, has been made in recent years for the helium nanodroplets (10^3-10^4 He atoms) [1, 2] and smaller clusters (< 100 He atoms) [3, 4]. It was found for small clusters of the type He_N–molecule, that the cluster rotational constant, *B* (proportional to the inverse moment of inertia), decreases initially classically with the number of helium atoms *N*, but then starts to increase at a certain critical *N* value. This 'turnaround' in *B* value is the result of a decoupling of helium density from the rotational motion of the dopant molecule and the critical *N* value depends on this molecule.

We have recently shown that such non-classical behaviour can occur in clusters with as few as four helium atoms, as in the case of He_N–CO [5]. High resolution microwave and millimeter-wave spectra of He_N–CO clusters with *N* up to 10, produced in a molecular expansion, were observed. The moment inertia of cluster and frequency shift of fundamental vibration of CO in dependence on the number of helium atoms were determined and compared with those from quantum Monte-Carlo calculations and used to further interpret recent infrared measurements of CO in helium nanodroplets [6].

To provide a deeper insight into the observed effects our experimental investigations are currently directed to clusters involving fermionic particles, i.e., $^3\mathrm{He}_N$–CO.

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Viscous Decay of Capillary Turbulence on the Surface of Liquid Hydrogen

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Relatively low viscosity of liquid hydrogen and high nonlinear coefficient of wave interaction allow to observe the turbulent cascade of capillary waves in a frequency range of about two orders of width. The power injected at low frequencies into the wave system is transferred to a higher frequencies due to nonlinear wave interaction. At high frequencies viscous losses dominates over nonlinear energy transfer and the turbulence decays. In our experiments waves on the surface of liquid hydrogen were driven by random force at frequencies about 100 Hz. The spectrum of pair correlation function of the surface oscillations clearly demonstrated two domains: the inertial range with Zakharov-Kolmogorov power-law dependency for the spectrum of the oscillations, and the dissipation region, where the spectrum can be approximated by exponential decay $I_\omega \sim \exp(-\omega/\omega_d)$. The boundary frequency ω_b between these domains is directly proportional to the characteristic frequency of the exponential decay ω_d and depends on the amplitude of the driving force as $\omega_b \sim A^{0.9\pm0.1}$. The exponential dependency in dissipation domain is in a quality agreement with "quasy-Planck" distribution [1] predicted with assumption that waves in the dissipation region interact mainly with each other than with waves from the inertial range.

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Decay of Second Sound Turbulence in He-II

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One of the most intriguing problems of nonlinear wave dynamics is the question of how the transition occurs from linear wave propagation via nonlinear wave interactions to the formation of a turbulent cascade. Experiments with very nonlinear second sound (temperature) waves allow us to measure their shape precisely and to study in detail the dynamics of the formation and decay of the turbulent cascades.

We have used a high *Q* cylindrical resonator to study the decay of turbulent cascades of second sound acoustic energy. The high quality of the resonator allowed us to create high intensity standing waves at resonance with only a low energy flux into the system.

The experiments were carried out at relatively low resonance mode numbers to prevent the formation of an inverse cascade. After switching off the pumping of energy into the system we monitored the decay of the direct turbulent cascade.

We found that, during the decay, the fundamental harmonic at the driving frequency had an amplitude larger than the amplitudes of high-frequency harmonics. The higher harmonics decreased fast, at first, simultaneously exhibiting clear evidence of amplitude oscillations. The total decay took place at a rate that was an order of magnitude slower, corresponding by order of magnitude to the *Q* factor of the resonator at low excitation. As we know, these experiments allowed first time to estimate a time of nonlinear energy transformation at turbulent processes.

Discrete Turbulent Cascade in the Dissipative Region on the Surface Of Liquid Helium and Hydrogen

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We performed experimental investigations of the relaxation of turbulent cascade on the surface of liquid helium and hydrogen in the dissipative interval. In our experiments capillary waves at the charged surface were excited by harmonic electrical force and were detected from the variation with time of the total power of a light beam reflected from the surface.

On the surface of liquid helium and hydrogen Kolmogorov cascade is formed in a range from low frequency ω_p, where the surface is excited to high frequency ω_b, where viscous dissipation takes place. For harmonic excitation the steady-state distribution of the energy of surface waves in the inertial range is described well by power law function [1] of frequency in terms of the pair correlation function in the Fourier representation $I_\omega = \langle|\eta_\omega|^2\rangle$ of an elevation of the surface from the equilibrium state $\eta(r, t)$. Structure functions $S_q(\tau)= \langle(\eta(t+\tau)-\eta(t))^q\rangle$ also demonstrate the power dependence.

At high frequencies on the surface of liquid hydrogen and helium turbulent cascade decays within narrow frequency interval due to viscous damping: the power distribution in the inertial interval is replaced by a steep decrease in the damping range. The frequency dependence of correlation function I_ω in the dissipative range can be approximated by power law function. It should be noted that in the case of noisy force excitation of the surface the decay of correlation function at high frequencies is described by exponential dependence [2]. Such behavior of the cascades at $\omega > \omega_b$ can be connected with influence of discreteness of turbulent distribution on transfer of energy towards high frequencies.

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Structure Functions of Capillary Wave Turbulence on the Surface of He-II

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We present new experimental result of investigation of the capillary wave turbulence on the surface of superfluid ^{4}He at the temperature of T=1.7 K. The experiments were carried out in an optical cell placed in helium cryostat. Helium was condensed into a cup 30 mm in diameter and 4 mm in height. The free surface of liquid was positively charged by means of the radioactive source irradiating β-electrons. Oscillations on the surface were excited by applying AC electric field perpendicular to the surface. Two types of excitation were used: monochromatic pumping at resonance frequency or noisy pumping at broad-band frequency range. Waves on the surface of the liquid were registered by measurements of power of the laser beam P(t) reflected from the surface. In our experiments wave elevation of the surface η(t) was proportional to the time variation of the laser beam power P(t), η(t) ~ P(t).

From obtained experimental results η(t) we calculated spectrum of the wave elevations $<\eta^2(\omega)>$ and the wave elevation structure functions (SFs) of the order from one to six

$$S_q(\tau)= <(\eta(t+\tau)-\eta(t))^q>$$

Here q is the order of SFs (q=1,2, …, 6), and the angle brackets denote averaging over t. At high level of the pumping amplitude, formation of a turbulence cascade in system of capillary waves was observed in the inertial interval with the width of approximately one decade. Power spectrum $<\eta^2(\omega)>$ was described in the frequency inertial interval by a power law function in according with our previous experiments. In the reported work it was found, that in the τ-scale range, corresponding to the inertial interval, SFs also varied as power law function $S_\tau(q)\sim\tau^{f(q)}$. The exponent index function f(q) can be represented by linear function f(q)=0.6*q and f(q)=0.9*q for case of monochromatic and noisy pumping respectively.

Numerical Simulation of Vortex Tangle without Mutual Friction in Superfluid Helium

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The experiments indicate that superfluid turbulence at very low temperatures decays in time. We study the dynamics of quantized vortex loops initially confined inside a small region. In absence of friction a vortex lines move according to the Biot-Savart law. The numerical simulation is performed with using of localized induction approximation. An algorithm, which is based on consideration of crossing lines, is used for vortex reconnection processes. The calculations are carried out in an infinite volume. Since using model is incompressible the transformation of kinetic energy into sound can not be studied. We have performed numerical experiments to determine the influence of different factors on decay of an inhomogeneous vortex tangle: an diffusion (large vortex loops break up to smaller ones which go away from initial volume), fluctuating of length owing to reconnection processes, the eliminations of small vortices below the space resolution, the insertion and removing of points to supply numerical algorithm stability. The obtained numerical results demonstrate that a packet of quantized vorticity, initially localized in small region, evaporates and diffuses away as a gas of small vortex loops. The time evolution of vortex line density satisfactory agrees with the ones, obtained from solution of diffusion equation. The above rest factors do not influence appreciably on decay inhomogeneous turbulence. The spatial density of vortex lines, the number of reconnections (the quantities of reconnections leading to breakdown of vortex loops and to fusion of sloops), the average vortex loop length the distribution of loops in their length, the average intervortex distance are calculated at each time**.**

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Diffusion Transport of Negative Ions Through Interface between Cryogenic Liquids

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A theory of electron bubble transport through the interface between cryogenic liquids is developed based on a new approach to calculating the potential of interaction of a bubble with the interface. The theory is in good agreement with experiments on the electric field dependence of the potential barrier near the interface between liquid 4He, 3He, and vacuum, as well as at the interface between 3He and 4He saturated solutions. It is found that the interaction potential dependence on the distance between the electron bubble and the interface is isotopically invariant to three versions of such an interface. The dependence of the lifetime of negative ions in 4He and 3He on the temperature and electric field has been determined using the Kramers theory.

Dynamical Phenomena with Participation Of Charged Clusters in Cryogenic Matter

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Discussed in the paper are resonance phenomena in electrolytes related to possible relative motion of the charged core and hydrate (solvate) shell of individual clusters. The resonances are shown to contain important information on the internal structure of clusters. Special attention is paid to the process of formation of the cluster associated mass in the solvent. It shown also that finite solvent viscosity does not suppress completely the structure resonance.

Surface Electrons' Current along a He-Film Covered Metal Rod

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We use the cylindrical- instead of conventional flat-geometry to study the electron transport on the super-fluid helium film formed on a vertical metallic needle. The bottom part of the needle is immersed into the bulk liquid helium and connected to the positively biased electrode. Thermo-emitter produced electrons are gathered on the helium film and drift to the needle's tip which serves as a collector (drain) because the tunnel barrier here is low. The resulting source-to-drain current can be controlled with a gate - an additional ring-electrode placed in the middle plane of the needle. This arrangement somehow resembles “the helium FET” from [1] but is simpler and has the natural reduced geometry. In addition, the possibility to control source-to-drain current with an axial magnetic field extends the capabilities of studying the high-density electron conductivity phenomena.

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A Possible Crystal–Glass Transition in a 2D Surface Electron System

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A new phase transition in the electron solid over superfluid liquid helium surface is observed. The solid is studied at temperature T = 100 mK, which is lower considerably than the equilibrium melting temperature. The real and imaginary components of the complex inverse conductivity of the electron layer are measured at frequency f = 1 MHz. The real component is found to undergo a sharp increase when the holding electric field is decreasing. Probably such a behavior indicates the transition in a new state. The new state can be destroyed by high driving electric field. It is supposed that the new state is a 2D electron glass.

Open Questions in Metallisation and Superconductivity of Silane

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There is a considerable interest in producing metallic, and possibly superconducting, states of hydrogen at multimegabar pressures; the pressures that are thought to be needed for metallization (>400 GPa) are however currently not achievable with static compression techniques. It has been recently suggested that hydrogen-rich compounds such as CH_4, SiH_4, and GeH_4 with hydrogen being "chemically pre-compressed" will require pressures far less than expected for pure hydrogen at equivalent densities to enter metallic states [1,2]. As is the case for pure hydrogen, these compounds are considered to be good candidates for high temperature superconductors in their dense metallic forms. For silane (SiH_4), however, there is a disagreement between different theoretical studies with metallization pressure ranging from above 91 GPa [2] to as high as 220-250 GPa [3,4].

Although the ambient pressure crystal structure of silane (with freezing temperature of 88 K) was unknown until two years ago [5], there were several experimental reports on its high-pressure behaviour. A study [6] claimed a discovery of metallization and superconductivity of silane at pressures above 50 GPa and reported a hexagonal close-packed (hcp) structure for the metallic phase of silane. On further compression above 110 GPa this phase is found to partially transform to a molecular insulating phase with a positive volume change of ~25% which co-existed with the metallic hcp phase up to 190 GPa [6] – an observation that contradicts thermodynamic rules (i.e. Le Chatelier's principle). Subsequent *ab initio* calculations [4,7] showed that the proposed metallic hcp structure is mechanically unstable suggesting a possible partial dissociation and a phase of a different composition. These discrepancies between various theoretical studies as well as experimental work prompted us to further investigate the crystal structure of silane at high pressures.

Using raman and x-ray diffraction techniques we found [8] that at ~50 GPa silane amorphises and partially decomposes into pure Si and hydrogen, where released hydrogen readily reacts with the surrounding metals in the diamond anvil cell chamber forming metal hydrides. We find a formation of Re hydride after decomposition of silane and reaction of hydrogen with the Re gasket. We also identify the recently reported metallic hcp phase of silane [6] as PtH [9], that forms upon the decomposition of silane and reaction of released hydrogen with platinum metal that is present in the sample chamber. We conclude that the synthesised PtH was mistaken for the metallic phase of silane in [6]. The amorphous silane is found to re-crystallize into an insulating polymeric structure on further pressure increase above 90 GPa.

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Low Melting Point in Compressed Alkali Metals: Electronic Origin

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Unusually low melting temperature of light alkali metal Na was found recently at pressures exceeding 1 Mbar [1]. The measurements revealed an increase of the melting line to 1000 K below 30 GPa and then a sharp decline to 300 K at 118 GPa. Negative melting curves have been reported in some elements and molecular solids implying a common physical origin in this behavior of materials under strong compression. The stability of the complex crystal structures in alkali metals that follow the bcc and fcc has recently been analyzed within a Hume-Rothery model [2]. It appears that the structural distortions from bcc give rise to new diffraction planes forming a Brillouin zone (BZ) boundary close to the Fermi surface (FS); a pseudogap can then open at these BZ planes and reduce the overall band-structure (electronic) energy. Even in bcc and fcc phases the increase of FS-BZ interactions under compression can result in a special feature of the melting curve that liquid state becomes more dense than solid state due to different contribution of the electronic energy. In the case of alkali metals we should consider the increased role of the core electrons becoming more appreciable with decreased volume and possible increase of the valence electrons as in solid [3] as well in liquid states.

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On Quantum Effects in Dense Lithium

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Surprisingly little is know about the behavior of dense lithium, the first and lightest metal in the periodic table. Using combined powder and single-crystal high-pressure diffraction techniques we mapped out the lithium phase diagram up to 150 GPa in a wide temperature range between 70 and 300 K.

Our measurement reveal a minimum on the melting curve with unprecedented drop of temperature making lithium an elemental metal with the lowest melting point. We also find several low symmetry phases forming at high pressure   previously unobserved in other elements. We will discuss the differences in the phase diagrams of Na and Li and will show that significant increase of quantum effects in Li on compression are responsible for them.

Classical Deformation Explains the Properties of Solid/Fluid He

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P.L Kapitza strictly confirmed the absolute principal role of slit hard walls (the so-called confinement effect) for the superfluid flow (and extremely high thermal conductivity, TC) in numerous experiments on ^{4}HeII phase [1a]. Then Landau referred to the identical effect in water [1b]. Since that times much attention was paid to the same properties of various materials under work-hardening (WH), in micro- and nanoscale geometries [2-4, etc.]. Confinement of matter flow changes its structural, hydrodynamical (the viscosity η(300K) of glycerin is 10^4 times smaller in nanoporous silica gel than in its bulk counterpart [4]), thermal, chemical, diffusion, crystallization, condensation properties, etc. [2-3]. For example, the identical thermo-mechani-cal effect in water [2] and liquid He, where two phase states (water and ice, liquid He and HeII) differ in their density and rigidity-WH; the work [5] confirms the close relationship between microhardness and TC. The same WH effects have been discovered for phase transitions (PT) in crystals, glasses, liquids, gels, biological tissues (BT), polymers, plasma, gases, Bose-Einstein condensates (BEC), etc. under different tests, where the WH- local rigidity was due to high density ρ_d of dislocation-like defects, lines, cells, etc.[6-8] and the η was determined by the reversed value of WH coefficient $\theta=d\tau/d\varepsilon$ [6]. This universal effect determines cancer cells development in BT, superconductivity of metals and ceramics [8] and supersolidity in He to be highly dependent on WH- to start with increasing local Young modulus of matter and then even its decrease due to cross-slip dislocation-like defects [9,10] in smaller pore-slit sizes, at higher loading rates and lower temperatures, impurity contamination and state in the matter, irradiation and pressure, higher ρ_d, aging in BT [6-7], etc. [3,4,6-8]. The identical conditions are present in the so-called superfluidity and supersolidity of ^{4}He and BEC, cancer cells [9], superconductors [10], etc. and determine their domed dependences on interior and external actions. The energy spectrum for thermal excitations in liquid ^{4}He-II, where the energy is plotted as a function of momentum ($T_\lambda > T > T=1.1K$) [11], designates the atomic-scaled drag of He atom to move in the superfluid ^{4}He-II as a function of its displacement under external slow neutron particle. This deformation upper yield point (the so-called “roton-hollow” part of the curve) is typical for many WH stress-strain curves in comparison with softening of the smooth and lower flow stress curves at higher temperatures (liquid ^{4}He at 4.2K). Strict analysis of the data on crystallization waves in solid He [12], the above data, the key role of deformation localization in the pairing of electrons at low temperatures [8] and the scaling of flow and fracture stresses in crystals from atomic to global scale lengths from solid helium up to diamond and hard ceramics, metallic glasses, etc. [13] confirm the identical mechanisms of wave plastic deformation at PT [14].

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