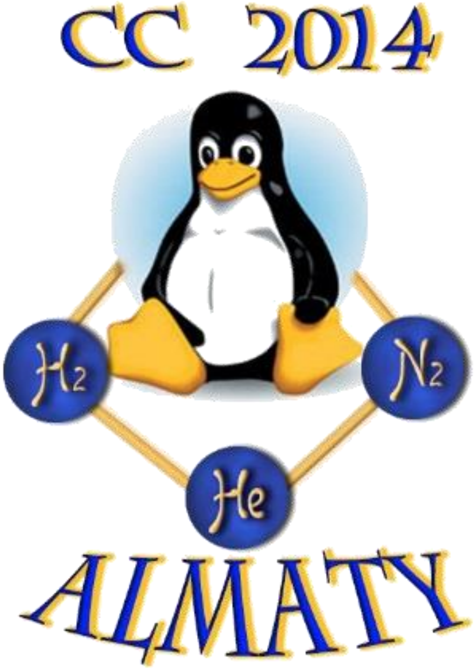
10th International Conference on Cryocrystals and Quantum Crystals

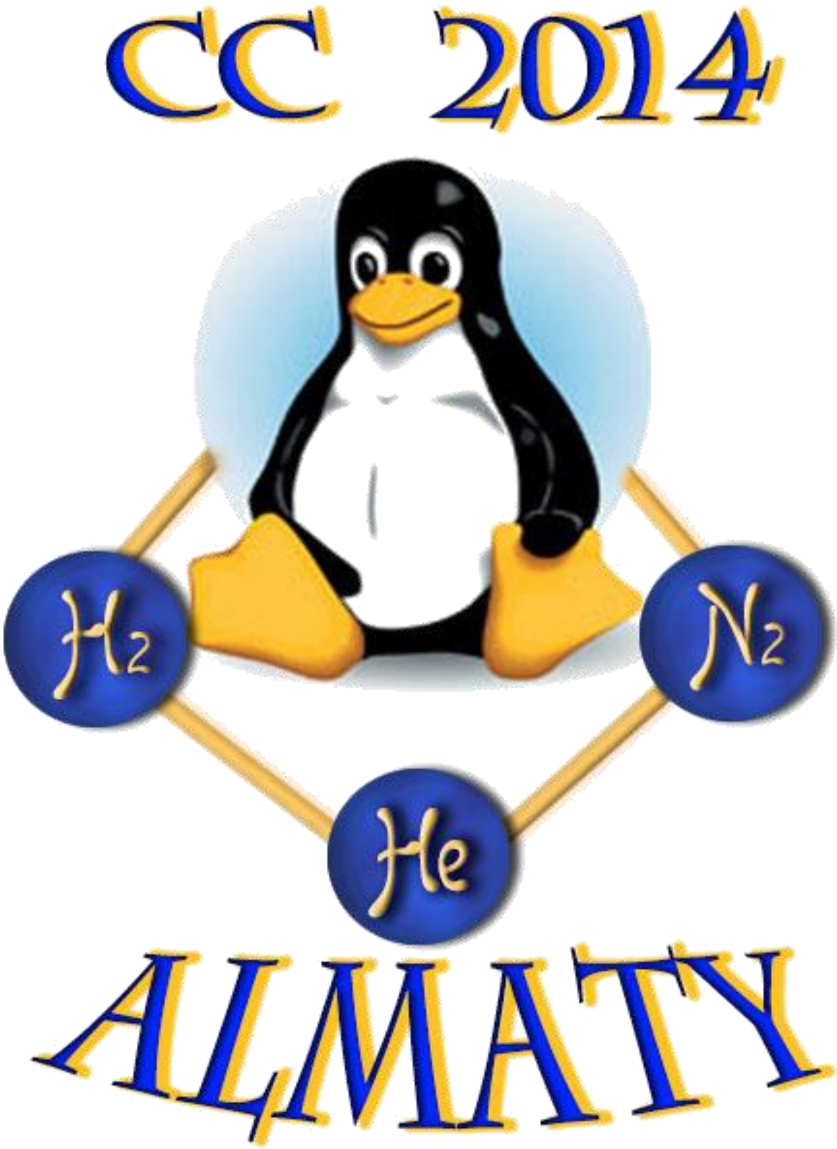


August 31-September 7

Programme & Abstracts

Almaty 2014

10th International Conference on Cryocrystals and Quantum Crystals



August 31-September 7

Programme & Abstracts

The organizers of the Conference would like to acknowledge the financial support of:

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10th International Conference on Cryocrystals and Quantum Crystals

August 31-September 7, Almaty, Kazakhstan

The 10th International Conference on Cryocrystals and Quantum Crystals (CC2014) is organized in Almaty (Kazakhstan) by Ministry of Science and Education of the Republic of Kazakhstan, National Academy of Science of the Republic of Kazakhstan, al-Farabi Kazakh National University, and Scientific Research Institute of Experimental and Theoretical Physics.

The Conference on Cryocrystals and Quantum Crystals (CC) dates back to 1979, when the first national USSR meeting dealing with cryocrystals and quantum crystals was organized in Viljandi, Estonia by V.G. Manzhelii (Verkin Institute for Low Temperature Physics and Engineering NASU) and A.F. Prikhot'ko (Institute of Physics NASU). The subsequent biannual meetings were held in Kharkov (Ukraine), Almaty (Kazakhstan), Donetsk (Ukraine) and Odessa (Ukraine).

The Almaty meeting of 1995 was organized by Kazakhstan National University as an international event. Since then the CC Conference had acquired international status becoming an important international forum for presenting new results on physics and chemistry of atomic and molecular solids. The great merit in achieving of this goal belongs to Prof. Vadim Manzhelii and Prof. Horst Meyer, the co-chairs of the first International CC-1995.

The next two CC conferences were held in Poland, in PolanicaZdrój (September 1997) and in SzklarskaPoręba (August 2000). The venues of the next CC conferences were Freising (Germany) in 2002, Wrocław (Poland) in 2004, Kharkov (Ukraine) in 2006, Wrocław (Poland) in 2008, Chernogolovka (Russia) in 2010. The ninth CC2012 conference was held in Odessa (Ukraine).

The scope of CC is wide, including, but not limited to:

Thermodynamic and mechanical properties of cryocrystals and quantum crystals
Order-disorderphenomena
Optical and neutron spectroscopy of cryocrystals
High-pressure studies of cryocrystals and quantum crystals
Charged species in cryocrystals and quantum crystals
Phenomena at the surface of quantum fluids and solids
Impurity-heliumcondensates
Matrixisolationincryocrystals
Ultrafastdynamicsincrystals
Crystalline and amorphous films, nanoscale systems
Supersolidstate
Newemergingmaterials
Technologicalapplicationsandinstrumentation

CC-2014 will be a forum where ideas on various aspects of the physical, chemical and technological properties of solidified gases and other relevant materials can be exchanged and where top experts in the field can meet.

A few Public Lectures are planned to be presented at CC2014. It is expected that majority of the attendees will arrive from outside the host country. In this regard, the Organize Committee

is planning to announce a competition among young scientists up to 28 years for conference participation grants (to be announced later).

During the preparatory stages of CC-2014, former and would-be CC participants voiced a suggestion to hold the CC-2014 conference as an event in commemoration of Prof. Vadim Manzhelii, who was the main force in the organization of all Cryocrystals meetings.

10th International Conference on Cryocrystals and Quantum Crystals

August 31-September7, Almaty, Kazakhstan

Organizers

Ministry of Science and Education of the Republic of Kazakhstan
National Academy of Science of the Republic of Kazakhstan
Al-Farabi Kazakh National University
Scientific Research Institute of Experimental and Theoretical Physics

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Dmitry SOKOLOV	Almaty, Kazakhstan

Conference Programme

August 31

6:00-22:00 Arrival of participants. **Registration**.
18:00 - 22:00 **TOGETHER** party.

September 1

8:00 - 9:00 Breakfast.
9:00 - 10:00 **OPENING CEREMONY Academician T. Kozhamkulov**

- ❖ Welcome speech. President of National Academy of Sciences RK, **Academician M. Zhurinov.**
- ❖ Welcome speech. Rector of Kazakh National University **Academician G. Mutanov.**
- ❖ Welcome speech. Chair of Program Committee **M. Strzhemechny.**
- ❖ Representation of the local committee. **A. Drobyshev.**

Morning Session 1, Chair: M. Strzhemechny.

10:00 - 10:40 **G. Benedek, A. Kalinin, P. Nieto, and J. Peter Toennies**. Vacancy assisted flow of solid helium.
10:40 - 11:20 **O.W.B. Benningshof and R. Jochemsen**. Spin waves in the b-phase of superfluid Helium-3.
11:20 - 11:40 Coffee break.
11:40 - 12:20 **E. B. Gordon**. Thermal stability of metallic nanowires and microspheres.
12:20 - 13:00 **V.E. Bondybey, I.V. Khyzhniy, E.V. Savchenko**. Charge states and energy convertion in atomic and molecular cryocrystals.
13:00 - 14:00 Lunch.

Afternoon Session 2, Chair: L.P. Mezhov-Deglin.

15:20 - 16:00 **T. Takahasi, R. Nomura and Y. Okuda**. Equilibrium shape of ^{4}He crystal under zero gravity.
16:00 - 16:20 **Yu. A. Dmitriev**. Photoelectric emission from gas solids.

16:20 - 18:00 **Poster Session A. Chair: Yu. A. Freiman**

- **Yu. A. Dmitriev, V. D. Melnikov, K. G. Styrov, M. A. Tumanova.** Quantum rotor in solid gases: matrix effects on ERP.
- **M.S. Klochko, E.S. Syrkin, M.V. Voinova.** Effect of solidified rare gas adsorbed on the surface of a solid on the characteristics of the surface waves.
- **N.S. Mysko, V.V. Danchuk, A.A. Solodovnik.** Claster model of N_2 –Ar, CO –Arcryoalloys. Comparative analysis.
- **T. Romanova, P. Stachowiak, A. Jeżowski.** Heat transfer in Ar and N_2 doped solid CO.
- **Drobyshev, A. Aldiyarov, V. Kurnosov, E. Korshikov, D. Sokolov, E. Galitskaya.** Dynamic characteristics of the light emission, accompanying the cryocondensation of some gases.
- **S. Sheludiakov, J. Ahokas, J. Järvinen, D. Zvezdov, O. Vainio, L. Lehtonen, S. Vasiliev, S.Mao, V.V. Khmelenko, D.M.Lee.** Magnetic resonance study of atomic hydrogen stabilized at high densities in solid H_2 and D_2 matrices.
- **M. I. Bagatskii, M. S. Barabashko, V. V. Sumarokov.** Heat capacity of fullerite C_{60}.
- **O.O. Romantsova, A.I. Krivchikov.** Thermal conductivity of clathrate hydrates at low temperatures.

Dinner.

September 2

8:00 - 9:00 Breakfast.

Morning Session 3, Chair: R. Jochemsen.

9:00 - 9:40 **E. Gregoryanz**. Studies of oxygen and hydrogen at multi-megabar pressures.

9:40 - 10:20 **Y. Crespo, A. Laio, G. E. Santoro, M. Fabrizio, S. Scandolo, E. Tosatti**. Unconventional phase transitions on HD and O_2 cryocrystals.

10:20 - 10:40 **E.Yakub**. Melting of cryocrystals at high pressures. Computer simulation.

10:40 - 11:20 Coffee break.

11:20 - 12:00 **Yu.A. Freiman, A. Grechnev, S.M. Tretyak**. Quantum effects in elastic properties of solid hydrogen under pressure.

12:00 - 12:30 **R.T. Howie, I. B. Magdau, G.J. Ackland, E. Gregoryanz and A.F Goncharov**. Studies of H_2, HD and D_2at multi-megabar pressures.

12:30 - 13:00 **L.N. Yakub**. Phase diagram of polymerizing nitrogen –a theoretical prediction.

13:00 - 14:00	Lunch.
14:00 - 17:00	**Almaty sightseeing Visit to Kazakh National University Campus.**
18:00 - 19:30	Dinner.

September 3

8:00 - 9:00	Breakfast.
9:00 - 18:00	**Excursion to Alatauridge.** **Lunch at restaurant "Gate of Needles of Tuyuk-su"**
18:30 – 19:00	Dinner

September 4

8:00 – 9:00	Breakfast.

Morning Session 4, Chair: Y. Okuda.

9:00 - 9:40	**J.Schou, B.Thestrup.** Enhanced desorption from solid deuterium driven by charging with keV electrons.
9:40 - 10:20	**M. A. Ramos, T. Pérez-Castañeda, R. J. Jiménez-Riobóo, C. Rodríguez-Tinoco, J. Rodríguez-Viejo.** Do tunneling states and boson peak persist or disappear in extremely stabilized glasses.
10:20 - 10:40	Coffee break.
10:40 - 11:20	**S. Bonev.** Elements at high pressure revisited.
11:20 - 12:00	**M. Frost, R. Howie, J.Gollmart, P.Dalladay-Simpson, E.Gregoryanz.** High-pressure stability of oxygen clathrate.
12:00 - 12:40	**L. Khriachtchev.** Matrix-isolation studies of non-covalent interactions: More sophisticated approaches.
12:40 - 13:00	**A. Gospodarev, E.V. Manzhelii, K.A. Minakova, E.S. Syrkin, S.B. Feodosyev**. Phonon spectrum and vibrational characteristics of linear nanostructures in solid matrices
13:00 - 14:00	Lunch.

Afternoon Session 5, Chair: A. Jeżowski.

15:40 - 16:20	**M.A. Strzhemechny, P.V. Zinoviev, and V.N. Zoryansky.** Exciton transport and orientational glassification point in doped C_{60} .
16:20 - 16:40	**V. B. Efimov, A. V. Lokhov, L. P. Mezhov-Deglin, C. Dewhurst, V. V. Nesvizhevskyi, and G. V. Kolmakov.**Nanocluster Impurity Gels in Superfluid HeII.
16:40 - 17:20	**V.Shikin**. Multiply charged clusters in condensed matter.
17:20 - 17:40	**E. Salamatov, A. Taranovand E. Khazanov**. Phononic band gap structures based on compacted nanoceramics.
17:40 - 18:00	**M.S. Klochko and M.A. Strzhemechny.**Low-temperature

thermodynamics of xenon doped fullerite C_{60} .

18:00 – 19:00 Dinner.

September 5

8:00 - 9:00 Breakfast.

Morning Session 6, Chair: A.A. Levchenko.

9:00 - 9:40 **L.VAbdurakhimov,M.YuBrazhnikov, G.V Kolmakov, A.ALevchenko, I.ARemizov.** Turbulence on the surface of cryogenic liquids in restricted geometry of experimental cell.

9:40 - 10:20 **V. B. Efimov, A. V. Lokhov, L. P. Mezhov-Deglin, C. Dewhurst, V. V. Nesvizhevskyi, and G. V. Kolmakov.** Dynamic of ethanol phase transition in solid state.

10:20 - 10:40 Coffee break.

10:40 - 11:10 **A.A. Pelmenev, R.E. Boltnev, I.B. Bykhalo, I.N. Krushinskaya.** Application of impedance spectroscopy for studying of charged nanoclusters in impurity-helium condensates.

11:10 - 11:40 **P. Dalladay-Simpson, R. T. Howie, E. Gregoryanz.** Melting of Hydrogen at Multi-Mbar Pressures.

11:40 - 12:10 **S. K. Nemirovskii**. Energy spectrum of the quantum vortices configurations.

12.10-12.40 **Ya.Yu. Fysun, A.P. Birchenko, N.P. Mikhin.** NMR research of confined diffusion in liquid inclusions in hcp He^3- He^4 matrix

13:00 - 14:00 Lunch.

16:00 - 18:30 **Poster session B,Chair: V.B. Shikin.**

- **R. Nikonkov, P. Stachowiak, A. Jeżowski.** Thermal properties of simple Van der Waals crystal-based nanocomposite materials.
- **T.D. Shestova, V.P. Zhelezny.** Investigation of the surface properties of complex thermodynamic systems and cryogenic liquids.
- **N.A. Shimchuk, V.P. Zhelezny.** Investigation of Al_2 O_3 nanoparticle influence on caloric properties of isopropanol.
- **P. Stachowiak , A. Jeżowski, R. Nikonkov, T. Romanova.** Investigations of thermal properties of simple van der vaals crystal based nanocomposites.
- **V.V.Danchuk, N.S.Mysko, A.A.Solodovnik, M.A. Strzhemechny.** Theed study of Ar – Kr equimolar alloy morphology.
- **A.J. Tychengulova, A.U., Aldiyarov, A.S. Drobyshev.** Molecular dynamics simulation of thermodynamic and transport properties of h-bonded low-temperature substances.
- **I. V. Sharapova, V. E. Syvokon.** The Dynamic Transition In A Wigner Crystal Over Liquid Helium.
- **D.N. Borisenko, P.M.Walmsley, A.I. Golov, N.N.Kolesnikov, Yu.V. Kotov, A.A. Levchenko, M.J. Fear.** Field-emission source of

chagesbased on nanotubes for low temperature experiments.

- **A.A.Levchenko, D.A.Khramov, V.B. Shikin, A.M. Likhter V.A. Gryasnova.** Penetration of charges through the surface of water.
- **I. V. Sharapova, V. E. Syvokon.** The dynamic transition in a wigner crystal over liquid helium.

19:00 - 22:00 **Conference Dinner.**

September 6

8:00 - 9:00 Breakfast.

Morning Session 7, Chair: M. Ramos.

9:00 - 9:40 **D.Szewczyk, A.Jeżowski.** Glassy crystals of adamantane derivatives induced by thermal treatment.

9:40 - 10:20 **A.Drobyshev, A.Aldiyarov, V.Kurnosov, K.Katpayeva, E.Korshikov, D.Sokolov, A.Shinbayeva, A.Timchenko.** Physical modeling of the formation of clathrate hydrates of methane.

10:20 - 10:40 Coffee break.

10:40 - 11:10 **A.Drobyshev, A.Aldiyarov, Zh.Nurkeyev, T.Duysebaev.**Thermally stimulated transformations in thin films of cryovacuum condensates of methane.

11:10 - 11:50 **A. I. Krivchikov, G. A. Vdovychenko, O. A. Korolyuk and O.O. Romantsova.** Thermal conductivity of molecular solids: regularities and singularities.

11.50-12.30 **A. Drobyshev, A. Aldiyarov, K. Katpayeva, E. Korshikov, V. Kurnosov, D. Sokolov, A. Timchenko.** Relaxation processes in a week solution of cryocondensed water, heavy water and ethanol with nitrogen and argon.

13:00 - 14:00 Lunch.

16:00 - 18:00 **Poster session C, Chair: A. Aldiyarov.**

- **Luiza P. Kondaurova.** Numerical Study on the Free Decay of Vortex Tangle at Zero Temperature in Superfluid Helium.
- **I.Chikina,V.Shikin.** Thermal effects induced by development of screening in electrolytes.
- **Shinbayeva, A. Drobyshev, N. Drobyshev, A. Kubetaeva.** The standardization and certification procedures of cryogenic equipment in Kazakhstan.
- **D.A. Gordon, G.A. Estrina, A.I. Bol’shakov, A.I. Mikhailov.** Oligomerization of methylacrylate and methylmethacrylate under the influence of molecular chlorine at low temperature.
- **O. Churiukova, A. Jeżowski, P. Stachowiak, J. Mucha, P. Perlin, T. Suski.** Thermal conductivity of donor-doped gan investigations with 3-ω and stationary methods.

- **I.Chikina, V.Shikin.** Dilute solutions of weak electrolytes.
- **T. Romanova, P. Stachowiak, A. Jezowski.** Heat transfer in Ar and N_2 doped solid CO.
- **A. N. Ogurtsov, O. N. Bliznjuk, N. Yu. Masalitina.** Energy loss and inelastic scattering of photoelectrons in N_2 doped solid Kr.
- **A.V. Dolbin, V.B. Esel'son, V.G. Gavrilko, V.G. Manzhelii, N.A.Vinnikov, R.M. Basnukaeva, I.I. Yaskovets, B. A. Danilchenko, I. Yu. Uvarova.** Quantum effects in the kinetics of He_3, He_4, H_2 and D_2 sorption by bundles of single-walled carbon nanotubes.
- **I.N. Krushinskaya, R.E. Boltnev, I.B. Bykhalo, A.A. Pelmenev V.V. Khmelenko, and D.M. Lee.** Optical spectroscopy and current detection during warm-up and destruction of impurity-helium condensates**.**
- **V.A. Konstantinov, V.V. Sagan, V.P. Revyakin and A.V. Karachevtseva.** Pseudo-rotational motion of cyclic molecules and thermal conductivity of tetrahydrofuran.
- **Z.V. Kalmykova, M. K. Makova, L.P. Mezhov-Deglin, A.N. Lanin, I.V. Petrusenko, V. V. Shafranov.** Portable devices for cryogenic surgery and therapy.

18:00 - 19:00	Dinner.
19:00 - 21:00	**Concert**.

September 7

8:00 - 9:00	Breakfast.
10:00 - 11:30	**Conference Closing**.
13:00 - 18:00	**Barbeque.**
18:00	**Departure of participants.**
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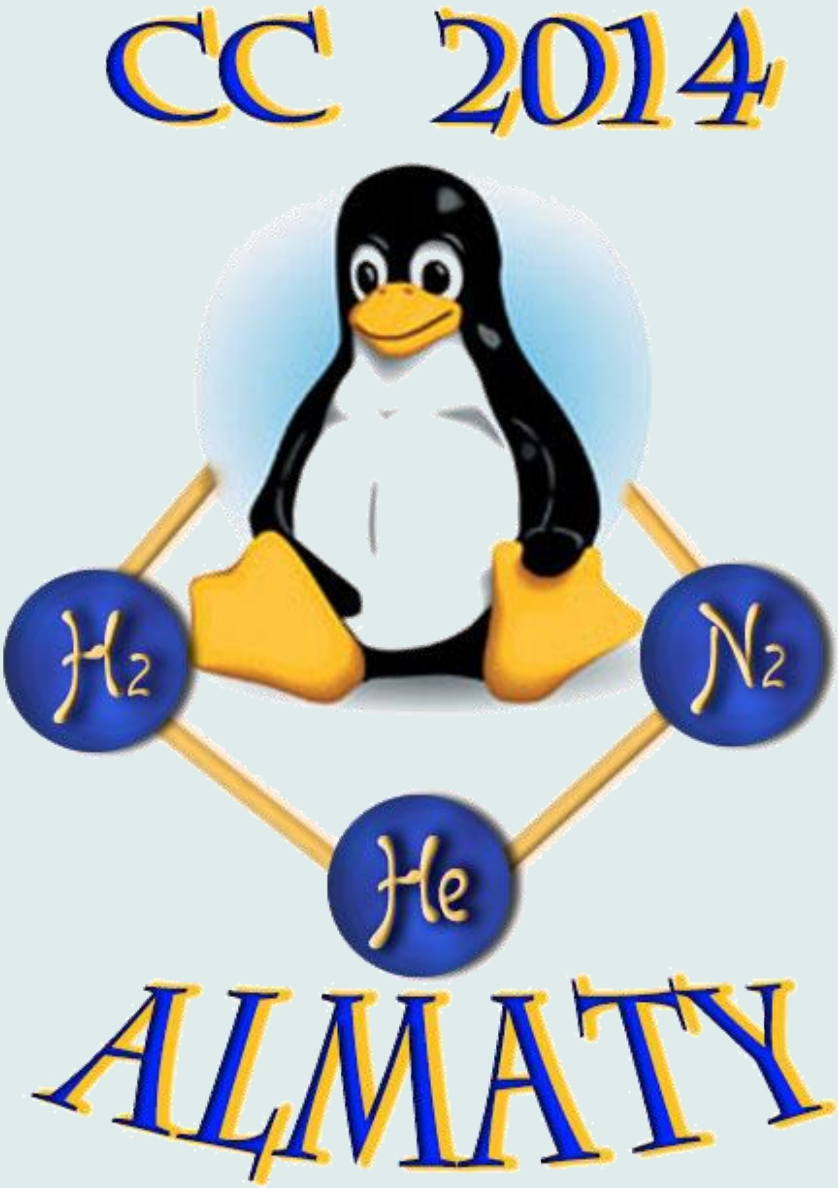

Invited lectures

I - 1

VACANCY ASSISTED FLOW OF SOLID HELIUM

Giorgio Benedek[1], Anton Kalinin[2], Pablo Nieto[3], and J. Peter Toennies [4]

[1]Dipartimento di ScienzadeiMateriali, Università di Milano-Bicocca, Via R. Cozzi 53, 20125 Milano, Italy.(Giorgio.Benedek@unimib.it) [2]Institut für Kernphysik, J.W. Goethe-Universität, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany. (Kalinin@atom.uni-frankfurt.de) [3]Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin. (pnieto@physiktu-berlin.de) [4]Max Planck Institut für Dynamik und Selbstorganisation, Am Fassberg 17, 37077 Göttingen, Germany (jtoenni@gwdg.de)

The idea that solid helium might become a supersolid goes back to Andreev and Lifshiz [1]. The 2004 observation of supersolidity in torsional oscillator experiments by E. Kim and M. Chan [2] started an extensive worldwide series of related investigations. Since the report by

D. Y. Kim and M. Chan in 2012 [3] that their effect was spurious, interest in the phenomenon has largely subsided. In 2001 Galli andReatto predicted that another type of supersolidity might occur at temperatures close to the lambda line provided that the concentration of vacancies is sufficiently large.[4] This has inspired our experiments which take advantage of the geyser effect [5] in which vacancy diffusion from the vacuum side of a flow system leads to a sudden collapse of the solid. The resulting flow through a 0.1 mm dia 14 mm long capillary is monitored by pressure sensors up- and downstream of the capillary at temperatures between 1.64 to 2.66 K and pressures up to 102 bar. After the initial sharp geyser pressure pulse, three different capillary flow regimes are observed as the upstream pressure decrease: (1) an oscillatory (minigeyser) regime. (2) a constant flow regime with a linearly decreasing pressure gradient, and (3) a non-resistant regime. The comparative analysis of the three regimes indicates that the flow of solid ^{4}He is driven by a coherent counterflow of excess vacancies, which are injected at the solid/liquid interface near the micrometric orifice exposed to vacuum. In the constant flow regime the velocity of about 20 cm/s, which is independent of the pressure gradient, is interpreted as evidence for a new phase of solid helium induced by non-equilibrium vacancies, in agreement with recent theories.

References: [1] Andreev, A.F.&Lifshitz, I.M. Quantum theory of defects in crystals, *Sov. Phys. JETP USSR***29**, 1107- & (1969). [2] Kim, E. & Chan, M. H. W. Observation of superflow in solid helium, *Science***305**, 1941-1944 (2004). [3] Kim, D. Y. & Chan, M. H. W. Absence of supersolidity in solid helium in porous vycor glass. *Phys. Rev. Lett.* **109**, 155301-155301 (2012). [4] Galli, D.E. &Reatto, L. Vacancies in solid He-4 and Bose Einstein condensation. *J. Low. Temp. Phys.* **124**, 197-207 (2001). [5] Benedek, G., Dalfovo, F., Grisenti, R. E., Käsz, M. & Toennies, J. P. Oscillations in the expansion of solid He-4 into vacuum. *Phys. Rev. Lett.* **95**, 095301 (2005).

I - 2

SPIN WAVES IN THE B-PHASE OF SUPERFLUID HELIUM-3

O.W.B. Benningshof and R. Jochemsen

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We describe experiments on superfluid 3He in a cylinder of 1 mm in diameter. This geometry causes the preferred orientation of the $\hat{n}$-vector in the superfluid B-phase to be locally different, resulting in a curved configuration across the sample. Exclusive to our experiment is the observation that we succeeded in obtaining a texture which is meta-stable and unchanged in our pressure and temperature ranges, most likely because the experiment is performed at low pressures and low magnetic fields. As this texture can be considered as a potential for spin waves, we had the unique opportunity to study spin waves for several pressures in exactly the same texture. Our geometry causes this texture potential to be nearly quadratic, allowing an analytic solution of the theory which can be compared to our experimental results. As predicted we find the intensities of all spin wave modes more or less equal. Increasing the pressure shows a gradual increase in the number of spin wave modes in our cell.

Finally we were able to cause a transition from the metastable to the predicted stable texture, concluding unexpectedly that the meta-stable texture is realized if the growing (or cooling) speed is sufficiently slow.

I - 3

THERMAL STABILITY OF METALLIC NANOWIRES AND MICROSPHERES

Eugene B. Gordon

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Quantized vortices in superfluid helium are the perfect one-dimensional template, imposing growing the product of condensation of any impurities suspended in HeII only along the core of the vortex. Nevertheless, we have demonstrated that it is impossible in the case of metal to prepare the chain of single atoms or molecules. Even in HeII possessing a uniquely high thermal conductivity the collision of small metal particles leads to their self-melting, which resulted in a spherical shape of product cluster. And only starting from their certain size the metal clusters begin to coalesce into a nanowire. The thickness of these nanowires depends on the thermo-physical properties of the metal and varies from 8 nm for the low-melting indium to 3 nm for refractory platinum.

However, for practical use these grown at low temperature nanowires should be stable at reasonably high T. Our studies of thermal stability of nanowires made of many metals and alloys demonstrated rather unexpected results. In particular, at room temperature nanowires of indium possessing melting point $T_m = 157^0$C exhibit long term stability, while the silver nanowires ($T_m = 960^0$C) fall to "dotted line" of clusters in few hours after their heating up to T = 300K. All results are consistent with the following unusual mechanism of thin metal nanowires decay. In order to destroy the nanowire it is not necessary to bring it to melt. One can achieve that simply moving the atoms along the surface and at a distance slightly greater than interatomic spacing. The motion of atoms on the surface is much less activated than that causing the melting. Therefore, a radical change in the shape of nanowires can occur at temperatures much lower than the melting temperature. However for the destruction of the nanowire by surface mobility a bean-like shape of nanowire should be more energetically favorable than cylindrical one. That is true for metals such as silver, where the surface tension increases rapidly with decreasing radius of the nanowire, and they are destroyed long before their melting. In metals such as indium and platinum, this effect is weak, and they exhibit an enviable thermal stability. The use of alloys can significantly extend the temperature range of metal nanowire stability.

Completely different effect determines the stability of spherical particles, when even melting cannot change their shape. These particles are commonly obtained by cooling the molten metal droplets in a liquid, and a large negative pressure arises inside them during cooling and solidification. Our studies have shown that under weak damage to the integrity of their surface, they break up, ejecting a plurality of nanoparticles.

I - 4

CHARGE STATES AND ENERGY CONVERTION IN ATOMIC AND MOLECULAR CRYOCRYSTALS

V.E. Bondybey[1], I.V. Khyzhniy[2], E.V. Savchenko[2]

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[2] B. Verkin Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., 61103 Kharkov, Ukraine

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In spite of detailed investigation of electronic excitations in atomic and molecular cryocrystals [1,2] the properties and dynamics of charge states, accumulation of uncompensated charge in the samples remained almost unexplored. Our group developed special techniques for investigation of charge states in cryocrystals. It was applied to rare gas solids and solid nitrogen. The correlated in real time measurements of spectrally resolved thermally stimulated luminescence, exoelectron emission, and the desorption yield were performed in combination with cathodoluminescence.

Condensed noble gases as well as solid nitrogen are used as detectors of ionizing radiation and moderators. Interest in research of solid nitrogen is associated with the prospect of its application as a high energy-density material. Investigation of radiation effects in solid nitrogen and rare gas solids is of high interest for astrophysics.

An overview of phenomena affected by charge states in atomic and molecular cryocrystals is presented. We achieved ultrahigh density of charge centers – 10^{15}-10^{16} cm^{-3} in cryocrystals under irradiation with an electron beam. The charge distribution was found to be inhomogeneous. We have shown that excess electrons are localized near the surface of the sample and positively charged centers are on the boundary between the sample and the substrate. The thermally stimulated exoelectron emission from solid nitrogen was detected for the first time [3]. It was found that the main exothermic reactions at low temperatures are electron-ion recombination ones. Energy conversion processes and nature of charge states involved are discussed. A new unusual phenomenon was observed – low temperature “post-desorption” from pre-irradiated solid nitrogen. Its mechanism is suggested. We demonstrated experimentally that localized charge states in cryocrystals are the key species responsible for the effect.

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I - 5

Equilibrium shape of 4He crystal under zero gravity

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We have been promoting the project to seek for the equilibrium shape of 4He crystal under microgravity, which could be available by the parabolic flight of a small jet plane. First of all, we had to overcome the technical issue to develop a refrigerator compatible with a small jet plane. Fortunately enough we successfully constructed a small dilution refrigerator and tested its performance for the parabolic flight. The lowest temperature of 140 mK was not affected by the parabolic flight for 20 seconds. Using this fridge, we were able to observe the 4He crystal under so called zero gravity at 140 mK. After several trials, we obtained beautiful pictures of the crystal with 3 facets, c-, a-, and s-, cut out of the movies. Thanks to getting three facets of the crystal in the probable equilibrium condition, we were able to determine the Wulf's origin with a pretty good accuracy. Using this origin, we estimated the surface energy of each facet. Furthermore, assuming some functional form of the vicinal surface height next to c-facet, we found the size of the c-facet was very small, and then the flat looking plane was the vicinal surface.

I - 6

STUDIES OF OXYGEN AND HYDROGEN AT MULTI-MEGABAR PRESSURES.

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The study of simple archetypal molecular systems having an electronic structure heavily altered by ultra-high compression holds the promise of major breakthroughs in our understanding of matter. Among these systems, oxygen and deuterium are of particular interest due to their abundance in the Universe. We have used optical and synchrotron x-ray diffraction techniques to probe O_2 and H_2 (D_2) to above 300 GPa. Our study on dense oxygen more than doubles the pressure range at which it had been investigated before; the picture we observe is quite different from what was experimentally reported and predicted by theory. Our experiments on dense hydrogen (deuterium) reveal the appearance of a new semiconducting phase at above 220 GPa which persists up to 350 GPa - the highest pressure reached in our studies. This phase is characterized by emergence of intense, well defined low frequency Raman bands, together with the unprecedented softening of the vibron, v_1, and appearance of a secondary vibron, v_2 and slowly closing band-gap. Analysis of the Raman spectra suggests a peculiar graphene-like structure consisting of both atomic and molecular layers.

For both systems we will discuss the differences in results and interpretations which currently present in the literature.

I - 7

UNCONVENTIONAL PHASE TRANSITIONS ON HD AND O2 CRYOCRYSTALS

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Both HD and O2 are molecular solids with an exceedingly well explored phase diagram under pressure. In this talk we focus in two unusual phase transition taking place at high pressures. First we study the unusual reentrant phase transition that the phase diagram of HD exhibits near 50 Gpa where a rotationally ordered ("broken symmetry") crystalline phase surprisingly transforms into a rotationally "disordered" high-symmetry phase upon cooling. While the qualitative reason for reentrance, has been already shown by early mean field studies in this work we aiming at a quantitative understanding of this system using path integral Monte Carlo (MC) constant-pressure calculations. Here we use an efficient sampling method and found the lowest-energy zero-temperature classical state, an structure C2/c similar to that hypothesized by Surh et al. [Phys. Rev. B 55, 11330 (1997)]. Upon turning quantum rotational effects on, we calculate the pressure-temperature phase diagram by monitoring a lattice biased order parameter, and find a reentrant phase boundary in good agreement with experiment. The entropy jump across the transition is found to be comparable with ln 2, the value expected from mean field results. A comparison with earlier studies is also presented, yielding relevant information about the role of factors that quantitatively determine the reentrant part of the phase diagram.

The second part of the talk is devoted to molecular oxygen at high pressures. At low temperatures, the low pressures antiferromagnetic phases below 8 GPa where O2 molecules have spin S=1 are followed by the broad apparently nomagnetic epsilon phase from about 8 to 96 GPa. In this phase which is our focus molecules group structurally together to form quartets while switching, as believed by most, to spin S=0. In this work we present theoretical results strongly connecting with existing vibrational and optical evidence, showing that this is true only above 20 GPa, whereas the S=1 molecular state survives up to at about 20 GPa. The epsilon phase thus breaks up into two: a spinless epsilon_0 (20-96 GPa), and another epsilon_1 (8-20 GPa) where the molecules have S=1 but possess only short range antiferromagnetic correlations. Thus an unconventional and rare local spin liquid-like singlet ground state akin to some earlier proposals and whose optical signature we identify in existing data, is proposed for this phase. Our proposed phase diagram thus has a first order phase transition just above 20 GPa, extending at finite temperature and most likely terminating into a crossover with a critical point near 30 GPa and 200 K.

I - 8

MELTING OF CRYOCRYSTALS AT HIGH PRESSURES. COMPUTER SIMULATION

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Two types of molecular dynamics simulations: single-phase and two-phase carried out and compared to determine the melting temperatures of highly compressed diatomic cryocrystals: nitrogen and hydrogen, as functions of pressure. Solid hydrogen was modeled within non-empirical atom-atom approximation [1], interaction of nitrogen molecules was described by the sum of semi-empirical atom-atom potentials and quadrulole-quadrupole contribution. For both diatomic solids, at different sizes of simulation cells, we observed the same dependence of melting temperature: its raise with increasing density becomes more and more smooth and at megabar pressures goes negative. This effect observed in experiments [2] and known as turnover of the melting line, was reproduced first in recent conventional single-phase molecular dynamics simulation of molecular hydrogen [3]. The same behavior of nitrogen, when polymerization transition ignored, is reported in this work. We discuss possible explanations of this turnover in absence of quantum effects, no changes of interaction and chemical bonding, and analyze its dependence from the rigidity and the length of chemical bonds, structure of the solid phase, and analyze the role of long-range quadrupolar forces.

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I - 9

QUANTUM EFFECTS IN ELASTIC PROPERTIES OF SOLID HYDROGEN UNDER PRESSURE

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We present results of lattice dynamics calculations of the sound velocities and Poisson's ratio in solid hydrogen. Using two complementary approaches - the semi-empirical (SE) many-body calculations and the first-principle density-functional theory calculations we found that the pressure dependencies of Poisson's ratio in solid hydrogen is non-monotonic displaying rather deep minimum.

The entire dependence can be subdivided into three sections obtained with different methods. The small-pressure section was obtained with the SE calculations working well for pressures below approximately 60-70 GPa while DFT works here unsatisfactory; on the contrary, the SE approach does not work at the high-pressure section while the precision of the DFT-GGA approach only increases with pressure. In the intermediate pressure range (100-150 GPa) both approaches fail. In the intermediate pressure range we have a continuous transition from the low-pressure to high-pressure asymptotes.

Normally, Poisson's ratio increases with pressure and tends to 1/2 (the limit of zero compressibility) when pressure goes to infinity. The occurrence of the section with Poisson's ratio decreasing with increasing pressure is a manifestation of a quantum effect. Our explanation of this effect is the following. It is known that the H_2 lattice is swelled due to large zero-point vibrations (ZPV). If ZPV were not present, "classical" solid H_2 would have much smaller zero molar volume V_0 about 7.4 cm^3/mol, i.e. the swelling effect is huge. Until the volume reaches about V_0, the main effect of the external pressure is the suppression of the zero-point vibrations and not the compression of the electron shells.

Thus the pressure dependence of Poisson's ratio establishes a distinct line between pressure ranges with quantum and classical translational motion. In the case of hydrogen this line at zero temperature coincides in fact with the range of existence of phase I.

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I - 10

ENHANCED DESORPTION FROM SOLID DEUTERIUM DRIVEN BY CHARGING WITH keV ELECTRONS

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Films of solid deuterium at a temperature around 3 K have been irradiated by 1.5 or 2 keV electrons. The films were deposited on the silver electrode of a quartz crystal microbalance (QCM) suspended below a pumped liquid helium cryostat [1,2]. The thickness of the films

ranged from 10 nm to up to 5 μm. The initial film thickness and the mass loss as result of desorption were monitored by the QCM. The electron beam current was kept at about or below 100 nA to avoid beam-induced evaporation.

Secondary electron emission was suppressed to a value below 0.01-0.03 electrons/electron by a repeller ring at a bias of – 90 V. However, for films thicker than 3-4 times the range of the bombarding electrons, the electron yield suddenly rose to a value close to 0.40. From this secondary electron yield the voltage potential could be determined unambiguously from secondary electron emission curves obtained by short pulse measurements on fresh films. For the thickest films the charging induced a surface potential of more than 1.0 kV, i.e. one-half of the energy of the bombarding electron. For these thick films the desorption yield increased from the minimum value of 6-10 D_2/electron up to 380 D_2/electron at 1.5 keV and 960 D_2/electron at 2 keV.

The surface potential is induced by electron charge accumulation in the film at large thicknesses from where the electrons no longer are able to migrate to the conductive substrate with a sufficiently high rate.

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I - 11

DO TUNNELING STATES AND BOSON PEAK PERSIST OR DISAPPEAR IN EXTREMELY STABILIZED GLASSES?

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We have investigated how extreme thermal histories in glasses can affect their universal properties at low temperatures. In particular, we have studied two materials which allow us to access highly-stable glassy states, as well as their corresponding conventional glasses, in two different ways: (i) amber [1], the fossilized natural resin, which is a glass which has experienced a hyperaging process for about one hundred million years; and (ii) ultrastable thin-film glasses of indomethacin [2] (an organic molecule commonly used in pharmaceuticals), prepared by physical vapor deposition at temperatures around 85% of its glass-transition temperature.

Specifically, we have studied 110-million-year-old amber samples from El Soplao (Cantabria, Spain). Specific heat C_p measurements of pristine, partially- and fully-rejuvenated samples were conducted in the temperature range $0.07K < T < 30K$, as well as around its glass-transition temperature $T_g \approx 150^oC$. A modest increase of the boson-peak height (in C_p/T^3) with increasing rejuvenation was observed, that can be related to a corresponding increase of the Debye coefficient. The amount of two-level systems, assessed at the lowest temperatures, was however found to be exactly the same for the pristine *hyperaged* amber as for the subsequently *rejuvenated* samples. On the other hand, we have observed an unexpected *suppression* of the two-level systems in the *ultrastable* glass of indomethacin, whereas conventionally prepared thin films of the same material exhibit the usual linear term in the specific heat below 1 K ascribed to these universal two-level systems in glasses.

By comparing both highly-stable kinds of glass, we conclude that the disappearance of the tunneling two-level systems in ultrastable thin films of indomethacin may be due to the quasi-2D and anisotropic behavior of this glass, what could support the idea of a phonon-mediated interaction between two-level systems, as suggested by Yu and Leggett [3].

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I - 12

RELAXATION PROCESSES IN A WEEK SOLUTION OF CRYOCONDENSED WATER, HEAVY WATER AND ETHANOL WITH NITROGEN AND ARGON

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Earlier studies of stability of ethanol molecules in nitrogen cryomatrix showed that the state of immobilized ethanol molecules in the matrix is not stable [1]. A slight increase of temperature of the matrix, long before its evaporation leads to a change in the vibrational spectra in a two-component solid solution of ethanol and nitrogen. This article considers the results of continued research in this direction. Weak solutions of water, heavy water and ethanol in cryomatrix of argon and nitrogen were investigated. The measurements were carried out in the temperature range of 12-40 K and condensation pressures of 10^{-5} Torr. The concentration of the analytes in the matrices was set in the range from 0.5% to 10%. The conclusion about states of molecules was made on the basis of comparison between oscillatory ranges of two-component solid solutions and thin films of pure cryocondensates of the substances. Quantum and chemical calculations were also taken into consideration [2-4].

On the basis of experimental results it is supposed that polyaggregates of different scale are formed in the process of co-condensation of water and ethanol with matrix gases. Thus some molecules, which are forming these units and settling down in a near-surface zone of these clusters, are not connected with the next molecules by intermolecular interaction. As a result they exist in a quasi-free state. Spectral reflection of this fact is an existence of lines of absorption in the oscillatory ranges of the samples which correspond to monomers and linear dimer of water and ethanol. An increasing temperature of the matrix leads to transformations in polyaggregate state that is proved by change of absorption amplitudes at the frequencies of characteristic fluctuations of quasifree molecules of water and ethanol.

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I - 13

MATRIX-ISOLATION STUDIES OF NON-COVALENT INTERACTIONS: MORE SOPHISTICATED APPROACHES

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Matrix isolation is a powerful method to study non-covalent interactions, including hydrogen bonded species. The complexation effect is commonly analyzed by comparing vibrational spectra of the complex and the monomers. Most traditionally, molecular complexes in matrices are prepared by adding two species to the matrix gas and depositing the matrix at somewhat elevated temperatures and/or annealing the matrix after deposition. However, this general strategy is less suitable for the species that are difficult or impossible to prepare in the gas phase, for example, for highly reactive and unstable species. In addition, this method leads to relatively small amounts of the 1:1 complexes with an interference of monomers and larger clusters.

We describe sophisticated approaches allowing studies of complexes that are problematic for the traditional method. For example, photolysis of a suitable precursor can lead to a large concentration of 1:1 complexes, which are otherwise very difficult to prepare (e.g., $H_2O\cdots O$) [1].

Photolysis of two species combined with annealing can produce complexes of radicals via reactions of primary complexes with mobile atoms (e.g., $H_2O\cdots HCO$) [2]. Interaction of noble-gas hydrides HNgY with other species can be studied in solid matrices (e.g., $N_2\cdots HArF$), and the blue shift of the H–Ng stretching mode is a normal effect in this case [3]. Many complexes and dimers have been prepared for the higher-energy conformer of formic acid *cis*-FA [4], even the *cis*-FA solid [5], by using selective vibrational excitation of the lower-energy (trans) form. The higher-energy conformer can be efficiently stabilized in complexes with strong hydrogen bonding. We also discuss specific cases when spectral shifts are very small (e.g., phenol···Xe) [6], and the direct spectroscopic evidence of the complex formation is not available.

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I - 14

EXCITON TRANSPORT AND ORIENTATIONAL GLASSIFICATION POINT IN DOPED C_{60}

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Below 95 K, pristine fullerite C_{60} is in the state of orientational glass with all molecules performing rotational oscillatory motion. However not all the mutual orientations of pairs of molecules are energetically favorable. Saturation of fullerite with gases changes the situation. There were controversies [1,2] concerning what happens with the orientational glass state when C_{60} is stuffed with, for instance, with CO or NO. We used XRD and luminescence techniques to study the process of intercalation of C_{60} with hydrogen [3], nitrogen, and carbon monoxide as well as the consequences brought about by the intercalation, which was affected at elevated temperatures up to 350°C (varying with the species being stuffed to avoid chemisorption) and at a pressure of 30 atm.

Our results [3] showed that the saturation mechanism for H_2 differ essentially from those for N_2 and CO. Equally, the consequences differ as much. Saturation with hydrogen proceeds in two stages, on the earlier of which octahedral voids are filled (at 250°C it takes approximately 50 hours). After that double filling of octahedral voids begins, which has been clearly documented by the lattice parameter vs, time measurements. At that time point the integrated luminescence spectra as a function of temperature begin to change significantly. Unlike in pure C60, in which at the glassification point of Tg = 95 K the spectra start to decay with increasing T, the intensity stays virtually constant to a higher temperature the longer is the saturation time. we came to the following conclusions. First, the mechanism of luminescence suppression above Tg consists in the breaking of exchange paths of mobile excitons that produce the respective luminescence components, thereby stopping them and letting to get de-excited without emission. Second, Tg inevitably goes up until higher temperatures become capable of initiating molecular rotations.

In the case of N_2 or CO, the molecules are too big to occupy a single octahedral cavity with two intercalant particles. They can only expand slightly the cage thereby facilitating molecular rotations. Therefore, as show our luminescence experiments with these two intercalants the point Tg shifts to lower temperatures, more pronouncedly in the case of carbon monoxide.

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I - 15

NANOCLUSTER IMPURITY GELS IN SUPERFLUID HEII

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Nanocluster impurity helium condensates in superfluid He-II (impurity gels) which are created in the process of condensation of the gas mixture "He-4 + vapors of the impurity under investigation" on the surface and in the bulk of superfluid helium cooled below 1.8 K are a new form of a soft matter. In our report we plan to present and discuss the recent results of investigations of the structure and properties of the gels as well as any perspectives of the future studies.

I - 16

MULTIPLY CHARGED CLUSTERS IN CONDENSED MATTER

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Discussed are the details of the structure (both similarities and differences) of various multiply charged complexes in condensed matter: multielectron bubbles and dimples in liquid helium, spherical and cylinder-shaped charged clusters (colloids and DNA molecules) in electrolytes.

I - 17

TURBULENCE ON THE SURFACE OF CRYOGENIC LIQUIDS IN RESTRICTED GEOMETRY OF EXPERIMENTAL CELL

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We report on results of experimental investigations of nonlinear phenomena on the surface of liquid hydrogen and helium. The first result is experimental observation of two bottleneck effects near the high frequency boundary of the inertial range on the spectrum of the turbulence in the system of capillary waves on the surface of liquid hydrogen and superfluid helium driven by a harmonic force. Both effects are manifested as a local maximum on the spectrum of pair correlation function of the surface elevation. On the surface of liquid hydrogen the local maxima can be seen only during reconfiguration of the turbulent cascade caused by a generation of waves below the driving frequency. The other one observed in the steady state spectra of capillary turbulence on the surface of superfluid helium is explained by detuning between harmonics in turbulent cascade and resonant modes of the experimental basin.

The second result is experimental registration of low-frequency harmonics on the surface of liquid hydrogen in a square cell and on the surface of superfluid helium in a cylindrical cell excited by monochromatic force. It was shown that conditions for generation of waves in the low-frequency range can be found experimentally by variation of the frequency of driving force and a discreteness of the spectrum of surface waves changing the boundaries of experimental cells. As on the surface of superfluid helium, and on the surface of liquid hydrogen low-frequency harmonics are generated mainly due to three-wave interactions. Energy from range of excitation is transferred simultaneously towards high frequencies in direct cascade and towards low frequency harmonics.

I - 18

ELEMENTS AT HIGH PRESSURE REVISITED

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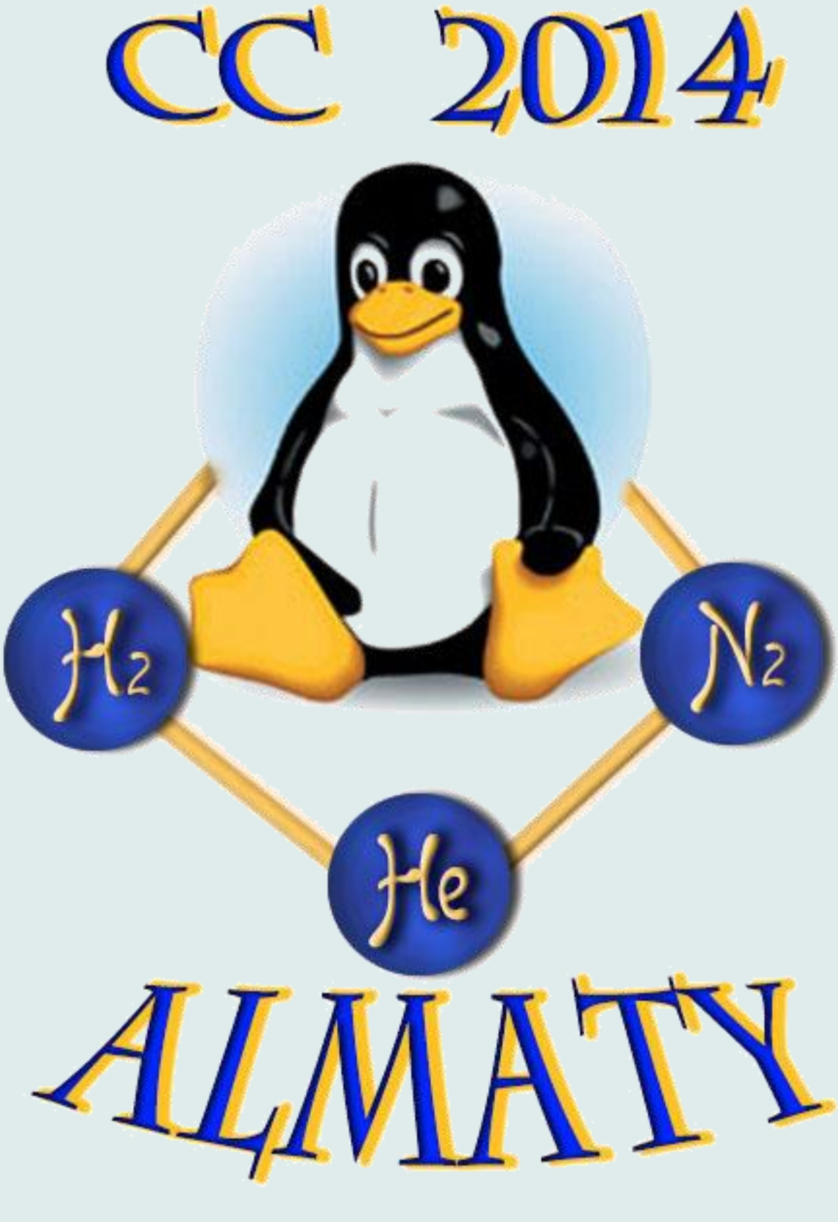
Theoretical studies of low-Z materials will be presented, for which the interplay among anharmonic effects, quantum ion dynamics, and not-trivial exchange interactions are projected to play significant role in the ensuring high-pressure properties. The phase diagram of oxygen has been reexamined, resulting in a consistent picture between theory and experiment up to 100 GPa, and new candidate structures for oxygen are proposed above 100 GPa. For lithium, we elucidate the role of quantum ion dynamics for its low temperature melting behavior at high pressure. Hydrogen iodide is determined to metallize between 20 and 25 GPa at zero temperature, which differs significantly from existing experimental data.

Work supported by LLNL, NSERC and ACEnet. Work at LLNL performed under the auspices of the US DOE under contract No. DE-AC52-07NA27344.



Selected lectures

S - 1

PHOTOELECTRIC EMISSION FROM GAS SOLIDS

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Electron photoemission from rare gas solids (RGS) is obtained using VUV open discharge sources. Temperature dependencies of the photoyield are measured by recording the ECR absorption of free electrons emitted from the RGS surfaces.

Study of the electron emission property of solid Ne finds that the photoemission from pure Ne is governed by the surface processes. The effect is due to the exceptionally large path lengths of free excitons and CB electrons in the bulk. Comparative study of the temperature dependencies of the photoelectron yield in the "solid Ne – Ne discharge" and "solid Ne – He discharge" experiments revealed two different mechanisms, intrinsic and extrinsic, responsible for the electron emission in these experiments: escape of the electrons photoexcited into the conduction band, in the former one, and exciton assisted emission, in the latter one. The intrinsic emission from solid Ne shows no temperature dependence in the range 2 – 4.2 K, while the extrinsic one is temperature dependent: the photoyield is found to decrease with decreasing sample temperature.

Our studies show an effect which sample temperature has on the photoelectron yield in "solid Ar – He discharge" and "solid Kr – He discharge" experiments. The threshold energies for photoelectron emission, 13.9 eV and 11.9 eV, in pure Ar and Kr, respectively, are far below the photon energies of the most intense He_I VUV lines at 58.43 and 53.70 nm. Hence, intrinsic photoelectron emission takes place in these systems. The photoemission was found to be temperature dependent and sensitive to the trapping of CB-electrons in the bulk.

The present experiment with CO doping corroborates our previous finding that impurities with negative electron affinity, $E_a(CO)$ = -1.8 eV, hamper the electron emission. An effect of a dopant having large positive affinity on the yield is also studied using molecular oxygen. Summarizing results of the present and previous studies, we conclude that impurities with either negative or positive electron affinities suppress the electron emission from the solid Ne excited over the band gap. In case of the dopant molecules and atoms which have negative or small positive affinities, an effect of the "deterioration" of the surface sites responsible for the electron emission prevails over the bulk effects these impurities have, while the impurities with large positive affinities quench the photoemission by scavenging CB electrons in the bulk.

S - 2

STUDIES OF H_2, HD AND D_2 AT MULTI-MEGABAR PRESSURES

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The recent discovery of the mixed atomic and molecular phase IV of hydrogen (deuterium) is exemplary of how the studies of hydrogen at multi-megabar pressures is constitutive to the understanding of simple systems at extreme compressions[1]. Through a series of high pressure Raman spectroscopic experiments we have conducted isotopic comparisons between

hydrogen, hydrogen deuteride and deuterium in phase IV. Isotopic studies not only reveal differences in phase stability, imposing constraints on the P-T phase diagram, but also provide strong evidence for structural phenomena[2,3].

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S - 3

PHASE DIAGRAM OF POLYMERIZING NITROGEN - A THEORETICAL PREDICTION

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Polymerization of nitrogen molecules in both solid and liquid phases, which was discovered in dynamic and static experiments, and predicted in ab initio simulations, stimulated discussion on a new configuration of phase diagram of nitrogen at high pressures. We consider the high-pressure phase diagram of solid nitrogen, which has long been discussed in theoretical studies, and only in the last decade began to investigate experimentally. The aim of this paper is to demonstrate the possibility of predicting the phase diagram of polymeric nitrogen based on a combination of computer Monte Carlo simulations and theoretical equations of state describing thermodynamic properties of the polymer and molecular nitrogen at high pressures and temperatures.

Location of the molecular crystal - polymeric crystal transition line, for polymer having cubic gauche (CG) structure, on the phase diagram of nitrogen is predicted. Parameters of the phase transition line were determined by the conventional double-tangent procedure. Canonical equations of state of the molecular high-pressure nitrogen phase and polymer CG-crystalline phase (modified Mie-Grueneisen equation [1]), were calibrated on available ab initio data.

The role of structure in the location and slope of the molecular-to-polymeric solid phase transition line on the nitrogen phase diagram was investigated.

The generality of idea, which explains the phenomenon of polymerization in liquid and solid phases and use of canonical equations of state for both phases, allows also predicting the melting line of polymeric nitrogen [2]. In this work we applied the new equation of state of high-pressure polymeric liquid, also calibrated on ab initio simulations [3]. We analyzed the predicted P-T-relation, calculated volumes of the coexisting phases and the entropy jump on the melting line of polymeric nitrogen. The predicted P-T dependencies of two phase transition lines: 1) molecular solid into the hypothetical A7-polymeric structure, having positive slope, and 2) the same transition into CG-polymeric solid, demonstrating the negative slope, were compared. It was found that this qualitative difference is due to negative thermal expansion of CG-polymeric solid. The predicted volume jump on the transition from the molecular to the polymeric phase is in good agreement with experimental data.

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S - 4

PHONON SPECTRUM AND VIBRATIONAL CHARACTERISTICS OF LINEAR NANOSTRUCTURES IN SOLID MATRICES

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Nowadays, the structures with one-dimensional or quasi-one-dimensional nanoinclusions in various crystalline or amorphous matrices attract attention of researchers. Under real relations between the interactions of the atoms of embedded quasi-periodic systems with each other and with the atoms of the matrix, the features, inherent to one-dimensional systems, can appear in the quasi-particle spectra of these structures. The one-dimensional chains are known to be unstable (e.g. [1]) and such a behavior of the phonon spectrum can significantly reduce the dynamic stability of the system, namely, enlarge the root-mean-square (rms) amplitudes of atomic displacements. Therefore, the existing of quasi-one-dimensional features in the systems with high stability seems to be important and interesting problem.

In the present paper, the atomic dynamics of linear chains embedded in a crystalline matrix or adsorbed on its surface is studied. A linear chain formed by substitutional impurities in a surface layer and at the same time offsetting from this layer was analyzed particularly. This system models the actively studied experimentally structures in which gas molecules (monatomic or diatomic) are adsorbed on the walls of the bundles of carbon nanotubes located in certain medium [2].

It is shown that the quasi-1D features are typical for the chains in which the interatomic interaction is 2÷3 times higher than the interaction between the atoms of the chain and the atoms of the crystal matrix. On the local phonon density of atoms of the chain, the transition to quasi-one-dimensional behavior has the form of the kink. In other words, it is the first (lowest-frequency) van Hove singularity, which in 3D structures (the system under consideration is generally three-dimensional) corresponds to the transition from closed to open constant-frequency (quasi-plane) surfaces. The local phonon densities of atoms in the chain have one-dimensional character at frequencies higher than the frequency of the van Hove singularity.

The rms-amplitude of embedded chains atoms vibrations is calculated and the behavior of the atomic vibrations contribution in the low-temperature heat capacity of the system is analyzed. The influence of substitutional impurities in quasi-one-dimensional nano-inclusions on their phonon spectra was studied, in particular, the conditions of forming and the characteristics of the localized states in both the high-frequency and low-frequency regions of the phonon spectrum of the system.

Analytical expressions for the phonon spectral densities of the atoms of linear chains with defects in periodic external field are obtained.

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S - 5

HIGH PRESSURE STABILITY OF OXYGEN CLATHRATE

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Gas clathrates are a family of compounds in which small molecules are held within a cage framework of water molecules and have major implications to planetary science, in particular the study of icy moons [1]. In oxygen clathrate the voids in the cage are occupied by diatomic oxygen molecules; it was first observed in 1960 at low pressures and temperatures below ambient [2]. We have investigated the oxygen water system at, and above, room temperature in a diamond anvil cell up to a pressure of 8 GPa. We observe a new oxygen clathrate structure followed possibly by a transition to a filled ice structure. We have measured the thermal decomposition curve at high pressure over both clathrate phases. This study opens the possibility that the interiors of icy moons may have a considerably higher oxygen content than previously thought.

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NMR RESEARCH OF CONFINED DIFFUSION IN LIQUID INCLUSIONS IN hcp ^{3}He-^{4}He MATRIX

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Previously, it has been shown the inclusions of non-equilibrium liquid phase are contained in the fast quenched helium hcp crystals[1]. Objects mentioned can play an important role in the newly discovered phenomenon, defined as a possible "supersolidity" effect in solid helium. The study of nuclear magnetic relaxation and diffusion processes in such two-phase sample of quenched solid 1 % of ^{3}He-^{4}He mixture by a pulse NMR method [2-4] confirmed the liquid nature of mentioned inclusions.

The aim of this work is the estimation of the size and configuration of the liquid inclusions mentioned as well as the analysis of the dynamics of their changes before the liquid inclusions have transformed into a disordered solid phase [2]. The spin-echo decay measurement over time t allows to calculate the ^{3}He true self-diffusion coefficient D if the liquid sample size $a >> (2Dt)^{1/2}$. Otherwise, the measurements pass to the mode with “restricted” diffusion coefficient measured $D' \sim 1/t^2$. The transition to the second mode depends on both the size and shape of inclusions. In the work it’s shown that in a few hours the average size of liquid inclusions is reduced from 70 mkm to 20 mkm, while the total amount of liquid is reduced by 10 %. In liquid inclusions the true value self-diffusion soefficient is $D = 1 \cdot 10^{-4}$ cm^2/s at 1.3 K. The evaluation of experimental dependence $D(t)$ indicates that the shape of the inclusions is closest to the cylindrical one.

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S - 7

Phononic band gap structures based on compacted nanoceramics

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Nowadays considerable attention is paid to the creation of a new class of nanostructured materials in which one can control the heat flow. Since it is believed that the basic element of such thermocrystals [1] should be phononic lattices with a wide forbidden gap, it is an urgent task to find new methods for their synthesis that strikes a balance between the thermocrystal efficiency and ease of fabrication. One of the methods for obtaining phononic band gap structures is the compaction of ceramics from nanopowders. For the first time, the possibility of existence of a forbidden gap in the phonon spectrum of compacted oxide nanoceramics was suggested in [2]. This idea was then experimentally confirmed in a study of the transport properties of weakly nonequilibrium phonons at helium temperatures by the phonon spectroscopy method [3].

In this work it is shown both theoretically and experimentally that the compacted ceramics can exhibit the properties of a phononic lattice, i.e., a forbidden gap may arise in the phonon spectrum. The position and width of the gap in such systems are determined by the average grain size of ceramics, as well as by the thickness and elastic properties of the grain boundaries.

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S - 8

LOW-TEMPERATURE THERMODYNAMICS OF XENON DOPED FULLERITE C_{60}

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Using a model of the fullerene C_{60} molecule with carbon atoms uniformly and spherically distributed over its surface, the potentional energy of atoms of the noble gases in an octahedral void (O-void) is calculated. At the first stage of our calculations we neglect the wave function anisotropy. Within the framework of three-dimensional harmonic oscillator, the lowest energy levels are estimated and the contribution of xenon impurity atoms to the heat capacity temperature dymamics of Xe-C_{60} system is determined.

We have shown that the contribution of the Xe dopants to the temperature dependence of the total heat capacity is essential compared to that of pure fullerite [1] and, as a result, the heat capacity of the doped sample has a substantially different shape.

Using data on the energy spectrum of a Xe atom in an O-void with account of the anisotropy of the interaction [2] between the impurity and octahedral surrounding, we have estimated and taken into account the Gruneisen parameters Γ for all the energy levels, the lowermost triplet being characterized by negative Γ. We compare these results of our calculations with the available low-temperature expansivities [3] measured on a C_{60} sample doped with 38% of Xe.

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S - 9

DYNAMIC OF ETHANOL PHASE TRANSITION IN SOLID STATE.

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We have studied the phase transition ethanol samples from amorphous to monoclinic phase. The ethanol very simple transmits into unstable amorphous state at quick cooling liquid. In our experiments we investigated by X-ray diffraction the temperature dependence of rate of the amorphous -->crystal transition for pure ethanol samples prepared by different methods. In the first set of experiments we prepared samples by quick cooling bulk liquid from room temperature to the T of liquid nitrogen. Another samples were prepared by quick freezing of mixture of small amount of ethanol vapor in a big volume of helium gas down to helium temperatures. This procedure formats nanoparticles of amorphous ethanol with size of the order of 10-30 nm.

We found that the velocity of the phase transition R strong depends from the temperature and may be described as $R=dc_{cr}/dt\sim exp(-\Delta/T)$, where $c_{cr} = V_{cr}/(V_{cr}+V_{am})$ – concentration of crystalline phase, and the energy Δ - depends from size of the amorphous particles.

In the report the possible mechanisms of phase transitions and nature of the size dependence of the Δ will be discussed.

S - 10

APPLICATION OF IMPEDANCE SPECTROSCOPY FOR STUDYING OF CHARGED NANOCLUSTERS IN IMPURITY-HELIUM CONDENSATES

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The new experimental technique for the impedance measurements of impurity-helium condensates is presented. It allows to measure the electrical properties of the condensates in superfluid and gaseous helium. The first experimental results will be presented.

S - 11

MELTING OF HYDROGEN AT MULTI-MBAR PRESSURES

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It was theorized, that at high compressions, the increased zero-point oscillations in hydrogen would destabilize the solid lattice and form a ground fluid state at 0 K[1]. Theory also predicts this fluid would have very unusual properties governed by quantum effects[2,3]. By combining Raman spectroscopy and *in-situ* high temperature techniques at high pressures, we have investigated the behavior of dense hydrogen above 200 GPa and above 300K, *P*-*T* conditions previously inaccessible in experiments. The novel data lead to a significant revision of the phase diagram of hydrogen above 200 GPa and suggest unusual physics in the molecular liquid and solid phases.

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S - 12

ENERGY SPECTRUM OF THE QUANTUM VORTICES CONFIGURATIONS

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A review of various exactly solvable models on the determination of the energy spectra *E (k)* of 3D-velocity field, induced by chaotic vortex lines is proposed. This problem is closely related to the sacramental question whether a chaotic set of vortex filaments can mimic the real hydrodynamic turbulence [1]. The quantity **v(k)v(-k)** can be exactly calculated, provided that we know the probability distribution functional ***P***({**s**(\xi ,t)}) of vortex loops configurations [2,3]. The knowledge of ***P***({**s**(\xi ,t)}) is identical to the full solution of the problem of quantum turbulence and, in general, P({s(\xi ,t)}) unknown. In the paper we discuss several models allowing to evaluate spectra in the explicit form. These cases include the standard vortex configurations such as a straight line, vortex array and ring. Independent chaotic loops of various fractal dimension as well as interacting loops in the thermodynamic equilibrium also permit an analytical solution. We also describe the method of an obtaining the 3D velocity spectrum induced by the straight line perturbed with chaotic Kelvin waves on it. Especial attention will be paid to the spectrum produced by the collapsing and reconnected lines. It is shown that reconnecting lines generate spectrum *E (k)* close to the famous Kolmogorov spectrum *E (k)* = *k*^(-5/3).

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S - 13

GLASSY CRYSTALS OF ADAMANTANE DERIVATIVES INDUCED BY THERMAL TREATMENT

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The thermal conductivity of 2-adamantanone ($C_{10}H_{14}O$) and CN-adamantane ($C_9H_{15}CN$) disordered crystals has been measured for temperatures between 4 K and 275 K. Such a range comprises the signature of a dynamical change involving the statistical intrinsic disorder concerning the site occupancy of the oxygen and nitride atom for $C_{10}H_{14}O$ and $C_9H_{15}CN$ respectively. The reported results encompass measurements performed within monoclinic crystal phases attained by crossing such transition from above, as well as within the ergodic phases of the materials, where large-angle molecular reorientations have been evidenced.
The long-range ordered lattices exhibited by these materials below the transition temperatures show a significant amount frozen disorder as far as the molecular orientations are concerned, which is shown to account for the features observed in the dynamic and thermodynamic properties of translationally ordered and orientationally disordered crystals. The data analysis is carried out in terms of several phonon scattering channels contributing to a resistive relaxation rate, which can be represented by two contributions, one due to propagating phonons whose mean-free path exceeds half the phonon wavelength, the additional one attributed to additional modes as localized short wavelength or diffusive vibrational modes.

S - 14

PHYSICAL MODELING OF THE FORMATION OF THE CLATHRATE HYDRATES OF METHANE

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Nowadays natural gas hydrates attract special attention as a possible source of fossil fuel. According to various estimates, the reserves of hydrocarbons in hydrates exceed considerably explored reserves of natural gas. Due to the clathrate structure the unit volume of the gas hydrate can contain up to 160-180 volumes of pure gas. In recent years interest to a problem of gas hydrates has considerably increased. Such changes are connected with the progress of searches of alternative sources of hydrocarbonic raw materials in countries that do not possess the resources of energy carriers. Thus gas hydrates are nonconventional sources of the hydrocarbonic raw materials which can be developed in the near future.

At the same time, mechanisms of methane clathrate hydrates formations have not reached an advanced level, their thermophysical and mechanical properties have not been investigated profoundly [1]. Regarding this experimental modeling of the processes of formational clathrate hydrates of methane in water cryomatrix in the process of co-condensation from gas phase on cooled substrate was carried in the range of condensation temperatures T=(12-60) K and pressures $P=(10^{-4}-10^{-6})$ Torr. In this experiment concentration of methane in water varies in the range of 1-10%. The thickness of a film was 30-60 mcm. The vibrational spectra of two-component thin films of cryovacuum condensates of CH_4+H_2O were measured and analyzed.

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S - 15

THERMALLY STIMULATED TRANSFORMATIONS IN THIN FILMS OF CRYOVACUUM CONDENSATES OF METHANE

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Solid methane belongs to a group of crystals which contains molecules of hydrogen, whose macroscopic properties (thermal expansion, etc.) are greatly caused by spin interaction of nucleus of hydrogen. In particular, the methane molecule, which has four protons with spin I = 1/2, has three total spin modifications: para-, ortho- and meta- states with three values of the total spin moments of 0, 1 and 2, accordingly. As a result of conversion between these states, an equilibrium concentration ratios set corresponding to the temperature of the system. Identification of connection between the speed of conversion and conditions of formation and

In this report the results of optical researches of thin films of methane cryovacuum condensates, which were formed at a temperature of a substrate of T=16 K and subjected further to thermostimulated influences, are offered to discussion. The obtained features allow to make the assumption that during temperature increase the sample undergoes the transformations caused by spin conversion.

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S - 16

THERMAL CONDUCTIVITY OF MOLECULAR SOLIDS: REGULARITIES AND SINGULARITIES

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The review is devoted to experimental studies of thermal conductivity of molecular solids at low temperatures: structural and orientational glasses, glass – like crystals and crystals with different degrees of orientational disorder.

The new effects (isomeric, mass and isotopic) have been detected and studied in the thermal conductivity of glassy alcohols. 1) The low temperature thermal conductivity of structural glass in the temperature region where the heat transferred by phonons is very sensitive to the mass of the alcohol molecule. [1] 2) A change in the structure of the molecular carbon skeleton and the position of the hydroxyl group –OH on the skeleton of the alcohol molecule affects significantly the value of the thermal conductivity of molecular glass in the temperature region where the heat is transferred by phonons, but it does not influence the thermal conductivity in the temperature region of hopping and diffusive heat transfer. [2] 3) Substitution of deuterium atoms by hydrogen atoms in the ethanol molecule results in a significant increase in the thermal conductivity in the temperature interval of hopping and diffusive heat transfer. [3]

New universal temperature dependences of the thermal conductivity of molecular glasses have been revealed: a universal behavior in terms of the soft potential model.

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S - 17

EFFECT OF PSEUDOROTATION ON ISOCHORIC THERMAL CONDUCTIVITY OF HYDROCARBONS IN DISORDERED PHASES

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The isochoric thermal conductivity of solid five-membered heterocyclic compounds has been measured in orientationally ordered and orientationally disordered («plastic») phases on samples of different density in a wide interval of temperatures and pressures. The objects were: furan - C_4H_4O, cyclopentane - C_5H_{10}, thiophene - C_4H_4S. The aim of this research was to study the influence of the translation-orientational motion on the behavior of the isochoric thermal conductivity and to estimate the possible contribution of pseudorotation to the total heat transfer. Pseudorotation as a large amplitude motion may significantly affect the translation-orientation (TO) coupling in molecular crystals, and therefore on the thermal conductivity, as much as it is determined by the nature as translational and orientational motion of molecules).

Long-term studies of the isochoric thermal conductivity established the basic regularities in the heat transfer of simple molecular crystals at $T \geq \Theta_D$ [1]. A strong translational orientational (TO) coupling contribute significantly to the thermal resistance $W=1/\kappa$. This, in turn, leads to large deviations of the isochoric thermal conductivity from the $\kappa \propto 1/T$ law owing to its approach to a lower limit κ_{min}. The concept of the lower limit of the thermal conductivity comes from the idea that κ_{min} is reached when the heat transfer occurs as diffusion of thermal energy between neighboring quantum-mechanical oscillators the life time of which is assumed close to one-half the period of the oscillations [2]. In orientationally ordered phases of molecular crystals large part of heat is transferred by «diffuse» modes, and thermal conductivity changes more weakly than the $\kappa \propto 1/T$ dependence. In orientationally disordered («plastic») phases of molecular crystals the «rotational» contribution to the total thermal resistance decreases sharply at gradual transition to weakly hindered rotation (freely rotatable molecules do not scatter phonons), so that the isochoric thermal conductivity increases with increasing temperature [1].

It is shown that the experimental data for all substances can be described in framework of a modified Debye model of thermal conductivity with allowance for heat transfer by both low-frequency phonons and “diffuse” modes. In phase II of cyclopentane the isochoric thermal conductivity is practically temperature – independent, but it increases smoothly with temperature in phase I. We attribute the increase of thermal conductivity to the translation – orientation interaction which becomes weaker as the rotational motion of the molecules enhances and the phonon scattering at the rotational exaltations attenuates. Thus, we can conclude that disinhibition of uniaxial rotation of the molecules in the cyclic hydrocarbons leads to the increase of the thermal conductivity with temperature like “plastic” phases of other molecular crystals.

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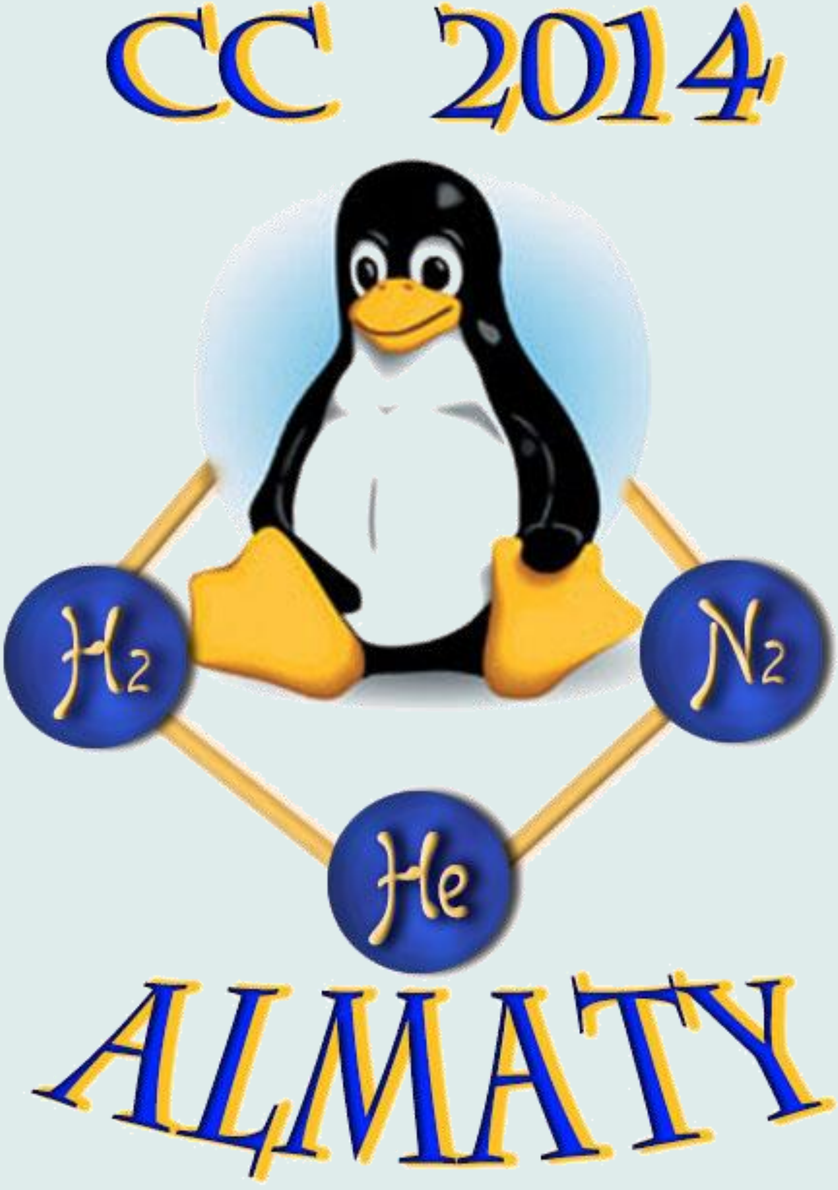

Poster presentation

P - 1

QUANTUM ROTOR IN SOLID GASES: MATRIX EFFECTS ON EPR

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Our study(a) deals with the methyl radical – the simplest organic radical, which is often observed as a transient intermediate species in chemical reactions. Consequently, it has been widely studied both theoretically and experimentally through decades. Theoretical studies of the spin density distribution showed that the radical possesses large anisotropy of the proton hyperfine coupling with three different principal values of the *hf* coupling tensor. However, in case of the free rotation, the components average out leaving an isotropic EPR spectrum. The trapped radical is another story: the methyl radical EPR spectrum lineshape depends on the radical surroundings which impose restriction on CH_3 rotation and contribute to the shifts of the EPR parameters. The residual anisotropy is a fingerprint of the interaction between the trapped radical the matrix surrounding which hinders the radical rotation. In the present report, we go through matrices of inert gases, solid para-H_2 and matrices of linear molecules to show how complex the rotation of the radical is, and how it is governed by matrix properties. The study relies on high-resolution EPR spectra of trapped CH_3 radicals.

Based on our finding, one may think of a new technique of studying the structural phase transition, orientational order-disorder, in solid gas films at a variety of conditions and on a variety of surfaces using the trapped CH_3 radical as a probe. This technique may provide insight into the structure dynamics at the microscopic level which is poorly understood so far. In order to demonstrate potentials of the idea, we launch an investigation of N_2-Ar solid mixture based on tracking the EPR spectrum shape of the trapped CH_3 radicals. The first results clearly show the order-disorder transition depending on the Ar impurity content and sample temperature. We also suggest new insight into the structure peculiarities of the quench-condensed films of solid Kr which relies on the peculiar EPR shape of isolated CH_3.

(a) The reported study was supported, in part, by the Russian Foundation for Basic Research (RFBR), research project no. 13-02-00373a.

P - 2

Effect of solidified rare gas adsorbed on the surface of a solid on the characteristics of the surface waves

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In the present report we consider effect of a rare gas adsorbed on the surface of a crystal on the dispersion relations and surface waves propagation velocity. Such researches are of great interest in nanotribological studies, i.e. atomic-scale friction caused by the solidified rare gases (including He) [1,2]; precise gravimetrical measurements of a negligible mass amount in chemical sensors and biosensors application [3,4], etc.

Face-centered cubic crystal with central interaction between the nearest neighbors with an impurity monolayer adsorbed on its surface is considered as a model. Influence of the surface monolayer (cryocrystals, in particular) on propagation velocity of surface waves of SH polarization is studied. The particular calculations are made for Ne-Ag system ($m_0/m = 1/5$ where m_0 is the impurity mass and m is the host one). We have analyzed the cases of deeply penetrating surface waves (long wavelength limit) and strongly localized ones (short wavelength limit). Similar researches may be carried out for different rare gases by varying m_0/m parameter.

The value $m_0{}^*$ of the adsorbed surface monolayer is obtained beginning from which $m_0 < m_0{}^*$ the surface wave splits off the upper edge of volume spectrum and attenuates non-monotonicly (with oscillation) when penetrating into the crystal.

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P - 3

CLASTER MODEL OF N_2 – Ar, CO – Ar CRYOALLOYS. COMPARATIVE ANALYSIS.

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Cryocrystall solutions formed of linear molecules with atomic components are of considerable interest as convenient model systems. It is known that in some cases Vegard's rule and Prigogine theory are insufficient and in this connection novel approaches are needed. One of the deviations from an ideal solution manifests itself through the anomalous behavior of the lattice parameter as a function of the composition. For explanation of the unusual concentration dependence of the lattice parameter in CO_2 – Ar alloys the cluster model was used. This semiquantitative theory takes into account not only isotropic interaction between particles, but also the presence of anisotropic forces in the molecular matrices [1]. In recent study on the CO_2 – Kr solutions the theoretical analysis [2, 3] considering three mechanisms of interaction of Kr cluster with crystalline environment of CO_2 matrix was in a good agreement with the experiment. The possibility to study not only molecular matrix but and atomic may be realized in an investigation of nitrogen – rare gas alloys. According preliminary results [4] the theory describes well the behavior concentration dependence of the lattice parameter only for Kr in α – N_2. Additional experimental data are needed for N_2-Ar system. The comparison with CO-Ar alloy is interesting because this system is nearest analog. N_2 and CO have identical crystal structures, however the barriers which hinder the rotation of the molecules in an α – N_2 lattice are almost twice as small as in α – CO [5]

Observations were carried out in a standard electron diffractograph equipped with a helium cryostat. The deposition regime was chosen in order to obtain random distributions of impurity. The samples were grown *in situ* by depositing gaseous mixtures on Al substrate at T=20 K. The error in the lattice parameter measurements was usually 0.1%.

Detailed electron diffraction studies have been carried out for the nitrogen-argon system. The concentration dependence of the lattice parameter are measured at T=20 K for low concentrations. Using this data and obtained earlier [6] the relative lattice parameter change per unit impurity fraction is determined for investigated systems. The influence of pair and triple clusters on the lattice parameter of solutions has been studied. The distortion mechanisms related with the presence of clusters in the N_2-Ar, CO-Ar solutions are examined.

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P - 4

HEAT TRANSFER IN AR AND N_2 DOPED SOLID CO

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Investigation of influence of impurities on thermal conductivity of simple molecular crystals is of great importance as a potential source of information about lattice dynamics. Measurements of thermal conductivity coefficient in solid carbon monoxide with argon and nitrogen impurities were carried out in the temperature range from 1.5 to 40 K. The dependences of thermal conductivity as a temperature function for these solutions are presented. The results are typical for dielectric crystals. Each curve has a characteristic maximum. The magnitude of this maximum decreases along with increasing concentration of the admixture and shifts towards higher temperatures. The contribution of various mechanisms of phonon scattering to the thermal conductivity of CO - Ar and CO-N_2 solid solutions at different concentrations was calculated using Callaway method. A discussion of the results is given.

P - 5

DYNAMIC CHARACTERISTICS OF THE LIGHT EMISSION, ACCOMPANYING THE CRYOCONDENSATION OF SOME GASES

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Processes of thin films cryovacuum condensates of different gases, as well as their properties are the object of attention of researchers for more than a decade.

Previously, we conducted studies in which it was found interesting behavior of nitrous oxide in the process of condensation and thermal cycling of the condensed sample. In the course of studying the dynamic characteristics of the phase transformations gas-solid, it was found that the condensation of nitrous oxide into the metal substrate is accompanied by the emission of light in the visible spectrum.

In these studies, we report our new results in the study cryoradiation accompanying the condensation of some gas. The main objectives of this research is: (a) - check a broader range of substances for their ability to cryoradiation; (b) - the study of the nature of radiation and its relaxation characteristics; (c) - the study of thermally stimulated processes in condensed samples. Studies have been carried on the installation and according to the procedure previously described by us in detail. The main unit of the installation is a cylindrical vacuum chamber with diameter and height of 450 mm. The ultimate vacuum in the chamber is reached a value better than $P = 10^{-8}$ Tor. The condensation pressure is adjusted to $P = (10^{-4} - 10^{-2})$ Tor. In the center of the chamber, a cryogenic system of Gifford-Mc Mahon is mounted, on the top flange of which a metal substrate, which serves as the condensation surface, is mounted. Diameter of the substrate d=60 mm. The condensing temperature T = 16 K. The temperature measurement was carried out with silicon sensor DT 670-1.4 using a temperature controller M335/20s. Intensity of radiation was measured by photomultiplier tubes P25a-SS-0-100 with a frequency 10^5 times per second.

When selecting the working substances, we proceeded from the assumption of the possible role of intrinsic dipole moment of the molecules to create the conditions for emergence of cryoradiation. Therefore we investigated dipole molecules (nitrous oxide, water, ethanol), and molecules with zero intrinsic dipole moment (nitrogen, carbon dioxide, argon). The experimental results are subject to detailed analysis and discussion of the assumptions and conclusions.

P - 6

MAGNETIC RESONANCE STUDY OF ATOMIC HYDROGEN STABILIZED AT HIGH DENSITIES IN SOLID H2 AND D2 MATRICES.

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Hydrogen and deuterium solids at low temperatures represent a special class of quantum crystals, where due to the large zero point oscillations and light mass, the effects of quantum tunnelling play important role. Behaviour of atomic impurities in these crystals attracts special attention due to possibility of reaching collective quantum phenomena related with Bose-Einstein Condensation (BEC) or so-called supersolid behaviour. This may happen at high enough densities of atomic hydrogen. In our previous work we succeeded in reaching record high densities of atoms $4 \cdot 10^{19}$ cm^{-3}[1]. This was done by implementing a novel method of in-*situ* dissociation of H_2 or D_2 molecules by low temperature (<1 K) RF discharge. H and D are the simplest atomic systems where magnetic resonance methods may be utilized for the characterization of the sample properties. In this work we present the first ESR study of H/D-impurities stabilized in solid H_2 and D_2 matrices below 1K

Samples of H and/or D in solid H_2/D_2 crystals were created in two stages: 1) we deposited a thin film of solid molecular para-H_2 (ortho-D_2) onto a cold (<1 K) surface of a quartz microbalance crystal, which served also as a mirror of 128 GHz Fabry-Perot resonator; 2) we dissociate part of the molecules in the film by running an RF discharge in the miniature helical resonator located nearby [2].

We found out that quantum isotopic exchange reactions $D+H_2=H+HD$ and $D+HD=H+D_2$ go with high enough rate at temperatures below 1K and effectively increase the concentration of atomic hydrogen in H;D; H_2;D_2 mixture films. Efficient dynamic nuclear polarization (DNP) of H in D_2 matrices was created via both Overhauser and solid effects. We suggest that interaction of electrons of the H atoms with magnetic moments of ortho-D_2 molecules greatly enhances probabilities of forbidden transitions. The presence of D_2 molecules in a close neighbourhood of H and atoms was supported by observation of the holes in both ESR spectra of H and D atoms during pumping the position of the satellite lines which appear due to simultaneous spin flips of the electron of the atom and the deuteron spin on a neighbouring D_2 molecule. In addition, pumping the center of the H spectrum created negative DNP. All attempts to observe DNP via the solid effect and pumping the center of the spectrum in pure H_2 were unsuccessful. We discuss possible explanations of this effect being due to the nuclear polarization transfer between H and D, or strong exchange effects between clusters of H atoms.

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P - 7

HEAT CAPACITY OF FULLERITE C60

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The heat capacity of the fullerite C60 has been investigated in the temperature interval 1 – 120 K using an adiabatic calorimeter. The fullerite is 99.99% pure. The sample mass is equal to about 0.6 g. Analysis of the obtained results and literature data [1-3] in the temperature range 1 – 300 K was carried out assuming that the translational, rotational, and intramolecular degrees of freedom make additive contributions to the heat capacity of fullerite. It was found that the temperature dependence of the heat capacity can be expressed as sum of linear and cubic terms below 3 K. The linear term can be explained by the existence of low energy tunneling levels in the fullerite orientational glass. The calculated Debye temperature is equal to 53 K. The contributions of optical translational and librational vibrations of molecules C60 are noticeable with temperature increasing above 3 K. The contributions of lattice and intramolecular vibrations to the heat capacity of fullerite were determined. The experimental heat capacity, associated to the translational and rotational vibrations, agrees well with the theory of lattice dynamics of the orientational ordered crystal C60 [3] in the temperature range 1 - 25 K. The contribution of the intramolecular vibrations becomes significant above 50 K. Lattice heat capacity is close to the 5R and has weak temperature dependence on the temperature range 50-140 K. This value of heat capacity associated to contribution of translational vibrations and the orientation vibrations of molecular in the plane perpendicular to the direction of type <111>. The contribution of processes of orientational phase disordering to the heat capacity of C60 is increased with temperature increasing above 140 K. The peak observed in the heat capacity near the temperature of 260 K is associated with the orientational phase transition. In the high-temperature orientation-disordered phase of fullerite the heat capacity equaled to near 4.5R, it corresponds to a case in which the rotation of molecules C60 is close to free.

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P - 8

Thermal properties of simple Van der Waals crystal-based nanocomposite materials

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P - 9

INVESTIGATION OF THE SURFACE PROPERTIES OF COMPLEX THERMODYNAMIC SYSTEMS AND CRYOGENIC LIQUIDS

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Results of investigation of surface layer's structure of complex thermodynamic systems with significantly different physic-chemical properties and of cryogenic liquids are presented in the report. Binary solution of dimethyl ether and triethylen glicole (DME/TEG) and the solution of argon and nitrogen (Ar/N_2) have been investigated as the complex thermodynamic system and the cryogenic liquid respectively. For these purposes the gradient theory in a single-fluid approach has been used. Saturated vapor pressure data needed for the gradient theory were calculated using modified Peng-Robinson's cubic equation of state (EOS). The method of calculating EOS parameters is based on the data without involving of critical parameters of substances and solutions. Influence parameters of the inhomogeneous fluid values were calculated with these data. Also local values of the solution density, concentration and partial density of components through the interface thickness z of the solution liquid phase were calculated.

Also authors attempted to develop a theoretically method for determining the effective composition of the solutions' surface layer. The method is based on using of the concept of "standardized" surface segregation. The authors propose to use the coordinates of extrema points of "standardized" surface segregation to determine an equivalent concentration of the solutions' surface layer. Theoretically determined effective composition was compared with data calculated from combining of parachor method with the experimental surface tension of solutions.

P-10

INVESTIGATION OF Al_2O_3 NANOPARTICLE INFLUENCE ON CALORIC PROPERTIES OF ISOPROPANOL

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The aim of this work is the experimental studying the caloric properties of the model nanosystems - isopropyl alcohol with nanoparticles of alumina oxide (Al_2O_3) at different nanoparticle concentrations. Study of thermophysical properties of these model systems is required to assess the of nanoparticle's influence on the phase equilibria parameters and heat caloric properties of working fluids and coolants with nanoparticle additives promising for use in refrigeration systems.

The results obtained for the temperature of phase transition (melting) and heat capacity for the nanofluids are reported in this paper. The components of solution were isopropanol and nanoparticles Al_2O_3. Nanofluid samples have been prepared by dilution of the serially produced nanoalcohol sample (CAS Number 1344-28-1) with the pure isopropanol. The size of nanoparticles in the nanofluid samples did not exceed 50 nanometers. The measurements have been done using experimental calorimetric setup that realizes the direct heating method. Melting temperature definition was performed by the thermogram method. The direct heating method in a calorimeter with a quasi-adiabatic cover was used for determination of the heat capacity of nanofluids.

The obtained experimental data show that nanoparticle admixtures influence on parameters of phase transition solid - liquid and the heat capacity of isopropyl alcohol as well. The results show that the presence of nanoparticles affects the parameters of the solid-liquid phase transition. The greatest effect of nanoparticles on the parameters of the phase transition appears at low concentrations of Al_2O_3. The authors proposed a new methodology to determine the melting temperature. This methodology based on the finding the minimum derivative of the function describing the obtained thermogram.

The analyzes of the obtained results shows that our experimental heat capacity data for the isopropanol are in good agreement with the reference information and other literature data. The additive (0.88 %) of Al_2O_3 nanoparticles to the pure isopropanol leads to changes in absolute value of the heat capacity at constant pressure. The effect was approximately 5% heat capacity decrease in the liquid phase and about 5% increase in the solid phase compared with the heat capacity of pure alcohol. This result should be considered as quite reasonable, because the alcohol molecules are adsorbed on the surface of nanoparticles and form the stable micelles. Thus, the structure of colloidal solution in the liquid phase is more ordered compared with the structure of pure alcohol, which leads to a reduction of heat capacity in the liquid phase. The question of the effect of nanoparticle concentration on isobaric heat capacity of isopropyl alcohol requires additional studies. This research is currently under way in the laboratory of the "Thermophysics and Applied Ecology" Department, Odessa National Academy of Food Technologies.

P-11

Low-frequency internal friction (LFIF) as express method for identification of cryocrystals in pores of the solids

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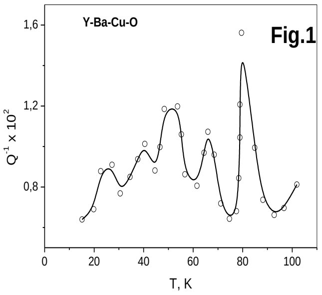
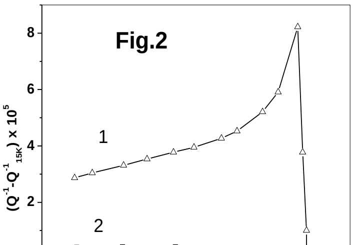
Cryocrystals (solidified gases) form a relatively small group of materials which are gaseous at room temperatures and solids at low ones. They have the triple points at low temperatures because of low weight and small size of their molecules and also weakness of binding forces. This group of solids includes atomic cryocrystals (He, Ne, Ar, Kr, Xe), simplest molecular crystals (hydrogen, nitrogen, CO, oxygen, fluorine), and also few crystals from bigger molecules (CO_2, N_2O, CH_4, NH_3 etc.). Being chemically neutral, the gases fill the pores and becomes cryocrystals under cooling, influencing the properties of the solid matrices. Method of internal friction used in the paper permits to detect a presence of gases in pores of the matrix as the cryocrystals give an additional contribution in the background spectrum of crystal matrix causing an appearance of additional peaks in the spectrum. Temperatures of triple points are the control points for most of the cryocrystals. For molecular cryocrystals, the control points are temperatures of phase transitions as well.



LFIF study (f=10-20 Hz) of YBCO HTSC ceramics [1] reveals (Fig.1), that besides a peak at T= 90-95K, related probably to superconducting NS transition, a few repeating peaks are observed near the temperatures 24, 44 and 54 K corresponding to temperatures of phase transitions and triple point of solid oxygen. This fact allows identifying the presence of O_2 in pores of oxide Y-Ba-Cu-O ceramics. Note that temperatures of these $\mathbf{Q^{-1}}$(T) peaks are independent on frequency and coincides with ones for pure crystalline O_2 [2]. Indeed, according to our study [3], the pores of HTSC ceramic samples are filled with condensed O_2, released by a sample during it's thermal treatment. Porosity of such samples can reach 10% from its volume.



Holter et al. have studied an effect of hydrogen absorption of sample pores on mechanical properties of the steels. LFIF spectra $\mathbf{\Delta Q^{-1}}$(T) of such steel samples obtained at frequencies 100-300 Hz (see Fig.2) show the presence of H_2 in view of a sharp peak near ~14K (curve 1), corresponding to H_2 triple point [4]. In case of an absence of hydrogen in pores of the sample (curve 2) the dependence $\mathbf{\Delta Q^{-1}}$(T) shows a monotonic behavior without any anomalies.

Thus, the LFIF method makes it possible a determination and identification of gases in the studied objects. This method, in particular, is desirable for studying of solids derived from hard-to-reach or remote atmospheres, for instance, samples from ocean bed, mines, or space objects (meteorites).

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P-12

INVESTIGATIONS OF THERMAL PROPERTIES OF SIMPLE VAN DER VAALS CRYSTAL BASED NANOCOMPOSITES

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Investigations of nanocomposites formed of nanoparticles embedded in simple molecular crystals matrixes seem to be very interesting from both basic physics and application point of view. By applying the thermal conductivity experimental technique to investigate such objects one can get an answer to numerous questions regarding the influence of properties and parameters of the components of such nanocomposites on their total thermal conductivity. The results of investigations are going to specify, in particular, the influence of the size of nanoparticles and their intrinsic transport properties on the sum thermal conductivity of the nanostructured material. The role of the parameters of the crystalline matrix, such as the interaction strength between its constituents, the atomic (molecular) mass of the constituents or the type of the excited thermal vibrations of the lattice for the thermal conductivity can be specified.

In the current contribution we present an experimental technique enabling investigations of thermal conductivity of simple molecular crystal based nanocomposites.

P-13

THEED STUDY OF Ar – Kr EQUIMOLAR ALLOY MORPHOLOGY

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Solid Binary mixtures of cryocrystals are of considerable interest for many reasons [1]. One of them is the possibility of the compare the experimental results with theoretical predictions. According theoretical model of rare – gas binary alloys proposed by Prigogine [2] the solutions should separate in the pure components below about 40 K. This critical temperature depends on the concentration and is a maximum for an equimolar solution.

Experimental investigations of binary mixtures of the inert gases are contradictory. In electron diffraction studies [3, 4] a phase separation in the Ar – Kr systems was not observed at T=7 K. However measurements on the diffuse and Bragg scattering of neutrons [5] from Ar – Kr samples indicated the solubility of argon micro clusters in the krypton – rich phase and the solubility of krypton atoms in the argon – rich phase.

THEED (Transmition High Energy Electron Diffraction) investigations were carried out in a standard electronograph EG–100A equipped with a helium cryostat. The deposition regime was chosen in order to obtain random distributions of impurity. The samples were grown *in situ* by depositing gaseous mixtures on Al substrate. The error in the lattice parameter measurements was usually 0.1%. The concentration dependence of the lattice parameter are measured at T=20 K for low concentrations.

The structure of equimolar solid Ar – Kr equimolar alloys has been investigated at the condensation temperature 5 K and 20 K and in the process of subsequent temperature change right up to sublimation of specimens, which took place at temperature range between T=32 to T=45 K . In the composition range K 40 – 60 mol% Ar, at the condensation temperature T=20 K the face centered cubic phase was observed. In this region the concentration dependence of the lattice parameter was measured. The low temperature equimolar samples were multiphase. Crystallographic structure of observed phase was determined. The obtained results indicate a limiting solubility in Ar – Kr system.

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P-14

MOLECULAR DYNAMICS SIMULATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES OF H-BONDED LOW-TEMPERATURE SUBSTANCES

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Studies of the properties of molecular crystals have a special place in solid state physics. The relative simplicity and understanding of van der Waals forces that bind the molecules in the lattice, caused interest that shows the theory to molecular crystals. Substances selected by us as objects of the study belong to the simplest van der Waals crystals. Due to the nature of their structure cryocrystals are closest to the models, considered by the theory, and are ideal objects for studying the fundamental solid-state physics.

The purpose of this paper is to obtain thermodynamic and structural characteristics of cluster systems formed during the cryocondensation of water vapor and N_2 gases mixture, based on the results of computer simulation. The infrared absorption spectra for these systems will be calculated, as well as the movement of molecules in clusters will be studied.

There are few fundamental problems that will be studied here, such as the processes of water and nitrogen molecules cluster formation in order to identify the basic principles of hydrogen bonded systems interaction at low and ultralow temperatures. For this purpose, theoretical studies were carried out using the computer software packages of Hyper Chem 8.0, that implement used by us semi empirical and molecular dynamics methods.

As a result of the research, the data must be obtained are of theoretical interest for summarizing the physical-chemical properties of systems, consisting of water molecules, and their combination with inert gases, as well as other atoms for studying the properties of molecular crystals composed of small molecules.

P-15

FIELD-EMISSION SOURCE OF CHAGES BASED ON NANOTUBES FOR LOW TEMPERATURE EXPERIMENTS

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In this report we present two methods of production of field-emission charge sources, based on carbon nanotubes, that can be used in low-temperature investigation of properties of injected charges in cryogenic liquids and crystals. The sources were made from metal disks with a diameter of 10 mm and thickness of about 1 mm. The thermal emission on a source does not exceed $E < 10^{-6}$ W. The first series of sources was prepared by the deposition of nanotubes from the arc discharge on a flat copper substrate, and the second series – by a mechanical rubbing of nanotubes in porous metal. In test experiments the sources were placed on inner surface of a plate of the diode with gap 0.5 mm. Measurements of I-V (current-voltage) dependence of sources from first series showed that in the superfluid He-II a current of negative charges at the level of 10^{-12}A occurred when the voltage applied to the source was U = -140 V, and it increased to 10^{-9}A with raising U up to -170 V. When the polarity of voltage was changed the current of positive charges in the diode occurred at the voltage U >240 V. In a source from the second series the current of negative charges at the level of 10^{-12}A in the superfluid He-II was registered at the voltage U= -260 V. We applied the source from the first series to investigate the motion of negative and positive charges in the samples of solid helium at temperatures down to 75 mK. I-V dependences are presented and discussed.

P-16

PENETRATION OF CHARGES THROUGH THE SURFACE OF WATER

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We report the results of experimental studies of penetration of positive charges through a nitrogen-gas/water interface. The measurements were performed on a cylinder capacitor consisting of a 20 mm deep metal cup 50 mm in diameter and an upper metal plate 15 mm in diameter. The water was poured to the rim of the cup. The spacing between the water surface and the upper electrode was 1 mm. The capacitor was placed into a glove box with a nitrogen atmosphere. Positive dc voltage was applied to the metal cup and the incoming charge on the upper electrode was measured by means of an electrometer. Under the action of electric field the positive charges rose to the liquid surface and the negative ones descended into the lower electrode. Charged liquid surface can lose stability at a charge concentration under the surface above a critical value. As electric voltage below U = 900V was applied to the cup, the capacitor was charged by the time law close to the exponential. The characteristic charging time is a function of voltage applied to the cup, amounts to approximately $\tau_{relax} = 10^2$ s and decreases with increasing U. At voltages above U = 900V surface water discharge is observed: at the instant of breakdown a 10^{-10} coulomb charge arrives onto the upper plate. The discharge process reoccurs with a period depending on applied voltage U. The observed periodic surface charge-discharge cycles point to time reproducibility of proton- hydroxyl pairs in the liquid volume.

P-17

THERMAL EFFECTS INDUCED BY DEVELOPMENT OF SCREENING IN ELECTROLYTES

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Appearance of electric field in a cell filled by electrolyte and bounded with blocking electrodes results in the development of screening processes modifying the spatial charge distribution. Total number of arising charges involved in screening grows with time as the stationary screening regime is reached, and goes back to the original number when the external field is turned off. Under these conditions overall cooling of the cell filled with electrolyte becomes inevitable as the stationary screening regime is approached (as well as its heating when the system relaxes to its original state). Discussed in the present paper are details of these thermal effects.

P-18

Numerical Study on the Free Decay of Vortex Tangle at Zero Temperature in Superfluid Helium

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The results of numerical simulation on the free decay of the inhomogeneous vortex tangle when mutual friction is absent are reported. The calculations were performed both with the use of the localized induction approximation (LIA), which neglects the nonlocal effects, and with the use of the full Biot-Savart law. The approximation in the time step was done by the Runge-Kutta method of the fourth order. Different boundary conditions were considered. One of them is an infinite volume, the another one is a cube with smooth walls. It was shown that the number of reconnections result of the breakdown of the loop significantly larger in the case of full Biot-Savart law, than in the LIA approach. We performed the proper monitoring of various mechanisms responsible for attenuation of the vortex line length. They are the changes of length owing to an escape of the small loops from the volume, the reconnection processes, the annihilation of small vortices below the space resolution, the insertion and removing of points. These mechanisms have a numerical nature (e.g. numerical loss of length at reconnection event), but clearly they have also obvious physical meaning. The obtained numerical results demonstrate that the diffusive-like smearing of the vortex tangle into ambient space, initially localized in the small region, is the major mechanism responsible for attenuation of the vortex length. The temporal evolution of vortex line density agrees with the ones, obtained from the solution of diffusion equation.

P-19

THE STANDARDIZATION AND CERTIFICATION PROCEDURES OF CRYOGENIC EQUIPMENTIN IN KAZAKHSTAN

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Creation of the Common Economic Space and functioning within the framework of EurAsEC of industrial enterprises requires forming a common base of normative documents to the Member States. Considering the whole increasing role of the cryogenic technologies in the industrial development of the world's leading powers, it is necessary to carry out the appropriate set of activities of normative ensuring this occupation. Kazakhstan is an active participant in the creating of this normative base, being the members of the Technical Committee TC-114 - Oxygen and cryogenic equipment. In this work is reported the main peculiarities of the implementation tasks assigned by the Technical Committee. Cryogenic equipment is manufactured in the laboratory of cryophysics and cryotechnologies of al-Farabi Kazakh National University subjected to obligatory procedures of standardization and certification.

P-20

OLIGOMERIZATION OF METHYLACRYLATE AND METHYLMETHACRYLATE UNDER THE INFLUENCE OF MOLECULAR CHLORINE AT LOW TEMPERATURE

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Radical polymerization of acetylene (paradietinilbenzene p-DEB, phenylacetylene) and vinyl (acrylamide AA) monomers as it was recently reported takes place at the simple mixing of these monomers with molecular chlorine at low temperatures. Spontaneous formation of radicals occurs apparently due to the chemical bonds breaking in multimolecular intermediate complexes. Present study investigates an ability of radicals formed by mixing of molecular chlorine with methylmethacrylate (MMA) and methylacrylate (MA) at low temperature to initiate the polymerization reaction of these monomers. Exclusional chromatography, elemental analyzes, UV-, VIS- spectroscopy, and calorimetry have been used for this study. The final product obtained after heating of the mixture to 300 K represents a colorless, transparent, viscous mass. The product yield determined by chromatography is ~ 70% in the case of MA and ~ 90% in the case of MMA. Chromatography studies showed that in contrast to the low temperature chlorination of p-DEB and the AA, leading to polymerization, low-temperature chlorination of MA and MMA results only in oligomers having 3-4 monomer units. The reactions of oligomerization and chlorination in MMA + Cl_2 system though begin long below the melting point of chlorine (T_m = 172K) mostly takes place at temperatures 200-240 K (the peak of heat release occurs in the region of MMA melting, T_m = 225K). In the MA + Cl_2 system the reactions start near the chlorine melting point and proceed rapidly in the temperature range 180-190K, near MA melting temperature (T_m) = 198K.

P-21

THERMAL CONDUCTIVITY OF DONOR-DOPED GaN INVESTIGATIONS WITH 3-ω AND STATIONARY METODS

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The thermal conductivity coefficient of three single crystal samples of n-type gallium nitride with electron density 4.0 x10^{16}, 2.6 x10^{18} and 1.1 x10^{20} cm^{-3} has been specified in the temperature range 4-320 K. The measurements were carried out in *ab* plane direction using stationary method. The value of the thermal conductivity coefficient depends strongly on the donor doping concentration. The analysis of phonon-electron scattering was done in the framework of Debye model with the use of Callaway method. Additionally, some results of the measurements in the direction of *c* axes obtained with 3-omega method are presented. The 3-omega method was also utilized for the measurements of thermal conductivity of GaN layers on an Al_2O_3 substrate.

The work was supported by Wroclaw Research Centre EIT+ within the project "The Application of Nanotechnology in Advanced Materials" – NanoMat (POIG.01.01.02-02-002/08) co-financed by the European Regional Development Fund (operational Programme Innovative Economy, 1.1.2)

P-22

DILUTE SOLUTIONS OF WEAK ELECTROLYTES

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Restricted applicability of Ostwald law to the dissociation in dilute aqueous solutions of electrolytes in the limit of vanishing donor (acceptor) concentration (i.e. transition to pure water) is emphasized. Discussed in the paper are available phenomenological approaches to finding the dissociation degree of weak electrolytes beyond the Ostwald approximation where the Ostwald law itself is used to identify the phenomenological constants arising in the theory.

P-23

ENERGY LOSS AND INELASTIC SCATTERING OF PHOTOELECTRONS IN N_2 DOPED SOLID Kr

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The method of matrix isolation of reagents in inert matrix is usually used to study of chemical reaction molecular dynamics along with methods of molecular beams and femtosecond probing spectroscopy [1]. Matrix-assisted energy transfer to matrix-isolated species is one of the most powerful tools for photostimulated chemical reaction control, and rare-gas solids are the most popular media for such investigations [2]. In Rare Gas Solids the energy loss rate of photoelectrons with energies above the band gap energy is mainly determined by electron-electron scattering [3]. The scattering of a hot photoelectron by a valence electron results in the formation of an additional electron-hole pair which can be bound or free. Such processes of multiplication of excitations with well-defined thresholds lead to prominent structures in the photoluminescence excitation spectra [2]. The influence of inelastic electron-electron scattering processes on quantum efficiency of intrinsic photoluminescence have been the subject of continuous interest as a powerful tool to investigate the relaxation mechanisms in Rare Gas Solids [4]. Solid krypton doped with N_2 was extensively used to investigate intra- and intermolecular energy relaxation into the impurity subsystem [5]. Because of the fast electronic relaxation by the intersystem crossing to the lowest excited $A^3\Sigma_u^+$ state and the pronounced Vegard-Kaplan bands emission, N_2 can be used as a sensitive luminescent probe to detect electronic relaxation at an impurity. This paper reports the observation of the influence of inelastic photoelectron scattering on luminescence of N_2 doped solid Kr.

The photoluminescence experiments were carried out at the SUPERLUMI experimental station at HASYLAB, DESY, Hamburg [6]. Solid krypton exhibit strong effects of neutral and charged defect formation induced by electronic transitions [2]. Therefore all measurements were carried out after saturation of dose effects at steady concentration of point defects and ionic centers. Under selective excitation by synchrotron radiation the threshold energies for multiplication of electronic excitations were measured. The data obtained suggest that in N_2 doped solid Kr three types of photoelectron scattering exist: (i) long-range photoelectrons are scattered inelastically by the impurity molecules, (ii) short-range photoelectrons with energies about $E_g + E_{exciton}$ form electronic polaron complexes, (iii) photoelectrons with energies above $2E_g$ can create intrinsic ionic centers as a result of formation of secondary electron-hole pairs during scattering. The influence of mean free path of photoelectrons on scattering process is discussed.

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P-24

QUANTUM EFFECTS IN THE KINETICS OF ^{3}He, ^{4}He, H_2 AND D_2 SORPTION BY BUNDLES OF SINGLE-WALLED CARBON NANOTUBES

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The low temperature kinetics of sorption of ^{3}He, ^{4}He, H_2, and D_2 gases by bundles of single-walled carbon nanotubes (SWNT) and the subsequent desorption of these gases from the SWNT bundles has been investigated. The characteristic times of the sorption-desorption processes coincide within the experimental error. The prior annealing of the SWNT samples at T=500 C reduced significantly the characteristic times and changed their temperature dependences. The effect of annealing decreased at the molecular weight of the dissolved gas was increasing. The influence of irradiation of SWNT bundles with γ-quanta upon H_2 sorption is qualitatively similar to annealing effect.

The gases desorption rates obey the Arrhenius law at high temperatures, deviate from it with temperature reduction and become constant at low temperatures. These results indicate the quantum nature of gas outflow from carbon nanotube bundles. We had deduced the crossover temperature below which the quantum corrections to the effective activation energy of desorption become significant. This temperature follows linear dependence against the inverse mass of gas molecule and is consistent with theoretical prediction [1].

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P-25

OPTICAL SPECTROSCOPY AND CURRENT DETECTION DURING WARM-UP AND DESTRUCTION OF IMPURITY-HELIUM CONDENSATES

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New experimental results on synchronous detection of optical spectra and ions during destruction of impurity-helium condensates will be presented. The luminescence flashes observed were accompanied by current pulses of negative and positive amplitudes.

P-26

PORTABLE DEVICES FOR CRYOGENIC SURGERY AND THERAPY

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Methods of local cryoimpact on biological fabrics are widely applied in modern surgery and therapy. Introduction of cryogenic methods of treatment in practice of federal and municipal authorities of Russia restrains lack of simple and reliable domestic cryodevices. In this regard in ISSP Russian Academy of Sciences a series of original portable cryodestructors with cooled liquid nitrogen the hollow active tip, the shipped cryoapplicators, and also the cryosprays of liquid nitrogen intended for fast contactless local freezing of biological fabrics by a stream of cold steam with a temperature of an order a minus 150^0C is developed and patented. These portable devices can find application in practice of usual district clinics of Russia, them it is convenient to use and when developing the combined techniques of treatment, for example, SHF - or laser radiation plus cryoinfluence. According to the recommendation of Ministry of Health of Russia prototypes of these devices were transferred to approbation to clinics of Moscow and the Moscow region. Results of tests of various devices are given in article and is reported about results of their approbation.

P-27

THERMAL CONDUCTIVITY OF CLATHRATE HYDRATES AT LOW TEMPERATURES

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Clathrate hydrates are non-stoichiometric inclusion compounds with the water molecules forming a three-dimension network by hydrogen bounds, where the small guest particles can be encaged in empty voids. The guest particles can be inert gas atoms or small molecules.

Most of the physical properties of clathrate hydrates are similar to those of ice Ih. The exception is the unusually low thermal conductivity whose temperature dependence is unnatural in crystal substances. Gas hydrates can be taken as model systems to investigate and clarify the origin of the glass-like behavior of thermal conductivity in crystal-structure solids.

It has been found that the temperature dependence of thermal conductivity for crystalline hydrates of methane xenon and tetrahydrofuran is typical of amorphous solids. An anomaly in the thermal conductivity behavior of the xenon clathrate hydrate has been observed and explained by the mechanism of resonance scattering of acoustic phonons by local translational vibrations of xenon atoms. It is found for the first time that the mode of cooling the clathrate hydrate of tetrahydrofuran influences the low temperature thermal conductivity of clathrate hydrate. It is probable that this effect is caused by the process of local proton ordering in the clathrate framework. The influence of the potassium hydroxide admixture on the thermal conductivity of tetrahydrofuran clathrate hydrate is investigated. It is established that a negligible quantity of alkali assists to phase transformation in the crystalline lattice of tetrahydrofuran clathrate hydrate. It is shown that temperature dependence of the thermal conductivity of clathrate hydrates at low temperatures shows the behavior predicted by phenomenological soft potential model.

P-28

THE DYNAMIC TRANSITION IN A WIGNER CRYSTAL OVER LIQUID HELIUM

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The surface electrons over liquid helium form a classical two-dimensional Coulomb-interacting system. Such arrangement is of dual interest: on the one hand, it is a good model of a low-dimensional system; on the other hand, it is a suitable object to investigate the surfaces of quantum liquids. The possibility of using the surface electrons for forming cubits in quantum computers has been considered too.

Among its most interesting features, the system can transform under certain conditions into the spatially ordered state of an electron (Wigner) crystal involving a phase order-disorder transition.

The system also exhibits a nonequilibrium phase (dynamic) transition caused by the external electric field below the melting temperature of the crystal. There is no unambiguous interpretation of the nature and the features of the dynamic transitions in a two-dimensional Wigner crystal, which calls for additional experimental investigations.

In this study the dynamic transitions in a two-dimensional Wigner crystal over the liquid helium surface have been investigated under the conditions of incomplete screening of the holding potential. It is found that the critical electric field provoking a transition depends on the surface density of the electron layer and is independent of the holding field. It is assumed that the dynamic transition is primarily connected with the disturbance of the spatial order in the system, which causes delocalization of the electrons and hence affects the features of the electron-ripplon interaction.

P-29

PSEUDO-ROTATIONAL MOTION OF CYCLIC MOLECULES AND THERMAL CONDUCTIVITY OF TETRAHYDROFURAN.

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Pseudo-rotation is a large amplitude motion arising from the interaction of two degenerate, or nearly degenerate out-of-plane ring puckering modes in the presence of a small barrier to planarity of the molecule [1]. Pseudo-rotation in tetrahydrofuran (THF), C_4H_8O, arises from near cancellation of the angular strain forces due to nontetrahedral bond angles in the skeleton ring and torsional forces due to hydrogen-hydrogen repulsion [2-3]. Experimental evidence strongly suggests that in solid THF the pseudo-rotational motion becomes a large-amplitude ring deformation vibration with a fundamental frequency of about 140 cm^{-1}. THF has only one crystallographic modification (monoclinic space group C2/c with 4 molecules in the unit cell) and melts at 164.9 K with a large entropy change on melting $\Delta S_f/R=7.07$ (R is the gas constant) indicating a high degree of order in solid [4-5]. The possible influence of pseudo-rotation on the thermal conductivity was not previously studied.

For correct comparison with theory at $T \geq \Theta_D$ (Θ_D is the Debye temperature) the thermal conductivity must be measured at constant density to exclude the thermal expansion effect. The isochoric thermal conductivity of solid THF was measured on three samples of different densities in the interval from 125 K to the onset of melting. The thermal conductivity was also investigated at saturated vapor pressure on the sample grown under a pressure of several atmospheres. The isochoric thermal conductivity of all three samples decreases with rising temperature by the law much weaker than $\kappa \propto 1/T$, has a bend and then decreases more rapidly. The bend can be associated with the onset of the sample melting. The Bridgman coefficient $g=-(d \ln \kappa / d \ln V)_T$ calculated from our experimental data is 7.7±0.6 at 160 K.

It is shown that the experimental data can be described in framework of a modified Debye model of thermal conductivity with allowance for heat transfer by both low-frequency phonons and "diffuse" modes. The calculated parameters of the model are close to values observed for orientationally ordered phases of other molecular crystals. No significant contribution of pseudo-rotation on the thermal conductivity has been detected.

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August 31	**September 1**	**September 2**	**September 3**	**September 4**	**September 5**	**September 6**	**September 7**
Registration. (6:00 – 22:00)	Breakfast (8:00 – 9:00)	Breakfast. (8:00 - 9:00)	Breakfast. (8:00 - 9:00)	Breakfast. (8:00 - 9:00)	Breakfast. (8:00 - 9:00)	Breakfast. (8:00 - 9:00)	Breakfast. (8:00 - 9:00)
TOGETHER party (18:00 – 22:00)	**OPENING** (9:00 – 10:00)	**Morning Session 3,** **Chair: R. Jochemsen.** (9:00 – 13:00)	9:30 – 17:30 **Excursion to Alatau – Ridge** **Lunch at restaurant "Gate of Needles of Tuyuk-su"**	**Morning Session 4,** **Chair: Y. Okuda.** (9:00 – 13:00)	**Morning Session 6,** **Chair: A.A. Levchenko.** (9:00 – 13:00)	**Morning Session 7,** **Chair: M. Ramos** (9:00 – 13:00)	**Conference Closing** (10:00 – 11:30)
	Morning Session 1 **Chair: M. Strzhemechny** (10:00-13:00)			9:00 **J. Schou** 9:40 **M. Ramos**	9:00 **A. Levchenko** 9:40 **V. Efimov**	9:00 **Szewczyk** 9:40 **Timchenko**	**Barbeque.** (13:00 – 18:00)
	10:00 **P. Toennies** 10:40 **R. Jochemsen**	9:00 **E. Grigoryanz** 9:40 **H. Crespo** 10:20 **E.Yakub**		Coffee break (10:20 – 10:40)	Coffee break (10:20 – 10:40)	Coffee break (10:20 – 10:40)	**Departure of participants.** (18:00)
	Coffee break (11:20 – 11:40)	Coffee break (10:40 – 11:20)		10:40 **S. Bonev** 11:20 **M. Frost** 12:00 **L. Khryashchev** 12:40 **E. Manzhelii**	10:40 **A. Pelmenev** 11:10 **Ph. Dalladay-Simpson** 11:40 **S. Nemirovskii** 12:10 **N.P. Mikhin**	10:40 **Zh.Nurkeyev** 11:10 **Krivchikov** 11:50 **A. Drobyshev**	
	11:40 **E. Gordon** 12:20 **I. Khizhniy**	11:20 **Y. Freiman** 12:00 **R Hovie** 12:30 **L.Yakub**		Lunch (13:00 – 14:00)	Lunch (13:00 – 14:00)	Lunch (13:00 – 14:00)	
	Lunch (13:00 – 14:00)	Lunch (13:00 – 14:00)		**Afternoon Session 5,** **Chair: A. Jeżowski.** (15:40 – 18:00)	**Poster session B,** **Chair: V.B. Shikin.** (16:00 - 18:30)	**Poster session C,** **Chair: A. Aldiyarov.** (16:00 - 18:00)	
	Afternoon Session 2, **Chair: L.P. Mezhov - Deglin.** (15:20 – 16:20)	**Almaty sightseeing** **Visit of Kazakh National University Campus** (14:00 – 17:00)		15:40 **M. Strzhemechny** 16:20 **L. Mezhov-Deglin** 16:40 **V. Shikin** 17:20 **E. Salamatov** 17:40 **M. Klochko**	**Conference Dinner.** (19:00 - 22:00)	Dinner (18:00 – 19:00)	
	15:20 **Y. Okuda** 16:00 **Y. Dmitriev**			Dinner (18:00 – 19:00)		**Concert** (19:00 – 21:00)	
	Poster Session A **Chair: Yu. A. Freiman** (16:20 – 18:00)						
	Dinner (18:00 – 19:00)	Dinner (18:00 – 19:30)					
			Dinner (18:30 – 19:30)				