ISSN 1563-034X
Индекс 75877; 25877

ӘЛ-ФАРАБИ атындағы ҚАЗАҚ ҰЛТТЫҚ УНИВЕРСИТЕТІ

ҚазҰУ ХАБАРШЫСЫ

Физика сериясы

КАЗАХСКИЙ НАЦИОНАЛЬНЫЙ УНИВЕРСИТЕТ имени АЛЬ-ФАРАБИ

ВЕСТНИК КазНУ

Серия физическая

AL-FARABI KAZAKH NATIONAL UNIVERSITY

KazNU BULLETIN

Physics series

№3(50)

Алматы
«Қазақ университеті»
2014

25.11.1999 ж. Қазақстан Республикасының
Мәдениет, ақпарат және қоғамдық келісім министрлігінде тіркелген

Куәлік №956-Ж.

Жылына 4 рет шығады

Ғылыми басылым

ҚазҰУ ХАБАРШЫСЫ

Физика сериясы

№3 (50)

Шығарушы редакторлары: *Г. Бекбердиева, А. Иманғалиева*
Компьютерде беттеген: *А. Алдашева*

ИБ №7957

Басуға 20.01.2015 жылы қол қойылды.
Пішімі 60х84 $^{1}/_{8}$. Көлемі 8,7 б.т. Офсетті қағаз. Сандық басылыс.
Тапсырыс №35. Таралымы 500 дана. Бағасы келісімді.
Әл-Фараби атындағы Қазақ ұлттық университетінің «Қазақ университеті» баспа үйі.
050040, Алматы қаласы, әл-Фараби даңғылы, 71.
«Қазақ университеті» баспа үйінің баспаханасында басылды.

Арнайы саны

«Cryocrystals and Quantum Crystals» атты
10-шы Халықаралық ғылыми конференцияның тезистері
Алматы, Қазақстан, 31 тамыз – 7 қыркүйек

Специальный выпуск

Тезисы 10-ой Международной научной конференции
«Cryocrystals and Quantum Crystals»
Алматы, Казахстан, 31 августа – 7 сентября

Special Issue

Abstracts of the 10th International
Conference on Cryocrystals and Quantum Crystals
Almaty, Kazakhstan, August 31-September 7

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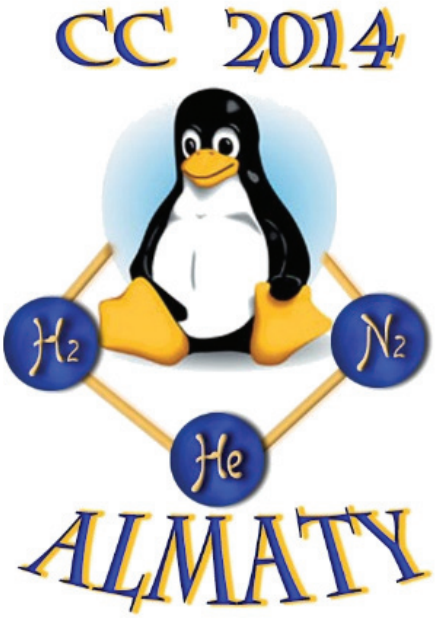

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Almaty 2014

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

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The Republic of Kazakhstan. Almaty, st. Kunaeva 142,

NAS Presidium of the Republic of Kazakhstan.

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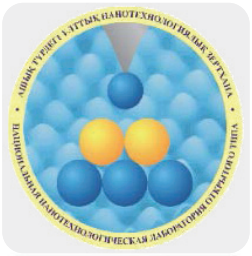

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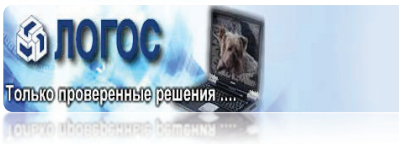

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10th International Conference on Cryocrystals and Quantum Crystals
August 31-September 7, Almaty, Kazakhstan

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 toProf. 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 Polanica Zdrój (September 1997) and in Szklarska Poręba (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-disorder phenomena
– 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-helium condensates
– matrix isolation in cryocrystals
– ultrafast dynamics in crystals
– crystalline and amorphous films, nanoscale systems
– supersolid state
– new emerging materials
– technological applications and instrumentation

CC-2014will 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).

Please check the Almaty-CC2014.kz home page regularly for updates on pertaining information.

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-September 7, Almaty, Kazakhstan

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UDC 533.9.004.14; 621.039.6

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Charge states and energy convertion in atomic and molecular cryocrystals

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.

Key words: charge state, cryogenic, solid nitrogen, radiation exoelectrons.

В.Е. Бондыбей, И.В. Хижный, Е.В. Савченко

Зарядовые состояния и преобразование энергии в атомных и молекулярных криокристаллах

Несмотря на многочисленные исследования, свойства и динамика зарядовых состояний остаются не исследованными. Наша группа разработала специальную методику исследования зарядовых состояний в криокристаллах. Нами была достигнута сверхвысокая плотность зарядовых центров – 1015-1016 $см^{-3}$ в криокристаллах при облучении электронным пучком. Мы показали, что избыточные электроны локализованы вблизи поверхности образца, а положительно заряженные центры - на границе между образцом и подложкой. Термически стимулированное излучение экзоэлектронов твердым азотом было обнаружено впервые. Также нами был обнаружен новый необычный эффект низкотемпературной «пост-десорбции» преварительно облученным твердым азотом. Экспериментально демонстрируется происхождение этого эффекта вследствие влияния локализованных зарядовых состояний в криокристаллах.

Ключевые слова: зарядовое состояние, криокристалл, твердый азот, излучение экзоэлектронов.

В.Е. Бондыбей, И.В. Хижный, Е.В. Савченко

Атомдық және молекулалық криокристалдардағы зарядталған күй және энергияның түрленуі

Көптеген зерттеулерге жүргізілсе де, зарядталған күйлердің қасиеттері және динамикасы әлі де зерттелмеген болып табылады. Біздің тобымыз криокристалдардағы зарядталған күйдің арнайы зерттеу әдістемесін жасап шығарды. Біз электронды шоғырмен сәулелендіре отырып, зарядталған центрдің аса жоғары тығыздығына – 1015-1016 $см^{-3}$ қол жеткіздік. Біз артық электрондар үлгінің бетінің маңайында, ал оң зарядталған центрлер – үлгі мен төсеменің арасындағы шекарада шектетілетінін көрсеттік. Қатты азотпен экзоэлектрондардың термиялық ынталандырылған сәулеленуі алғашқы рет анықталды. Сонымен қатар, біз алдын ала сәулелендірілген қатты азотпен төмен температуралы «постдесорбция» деген жаңа ерекше эффектті анықтадық. Бұл эффектің криокристалдардағы зарядталған күйлердің шектетілген әсердің нәтижесінен болатыны тәжірибе жүзінде көрсетіледі.

Түйін сөздер: зарядталған күй, криокристалл, қатты азот, экзоэлектрондардың сәулеленуі.

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 – 1015-1016 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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UDC 533.9.004.14; 621.039.6

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Claster model of N_2 – Ar, CO – Ar cryoalloys. Comparative analysis

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.

Key words: cluster model, cryogenic, electron diffraction.

Н.С. Мисько, В.В. Данчук, А.А. Солодовник

Кластерная модель N_2 – Ar, CO – Ar криогенных примесей, сравнительный анализ

Растворы криокристаллов, образованные линейными молекулами с атомными компонентами, представляют особый интерес в качестве модельных систем. Для объяснения необычного эффекта зависимости параметра решетки от концентрации в сплавах CO_2 – Ar была использована кластерная модель, учитывающая не только изотропное взаимодействие между частицами, но также и наличие анизотропных сил в молекулярных матрицах. Методами электронной дифракции измерена зависимость параметра решетки от концентрации в системе азот-аргон при 20 К. Изучено влияние парных и тройных кластеров на параметры решетки раствора. Рассмотрены причины искажения, связанные с наличием кластеров в растворах N_2 – Ar, CO – Ar.

Ключевые слова: кластерная модель, криокристалл, электронная дифракция.

Н.С. Мисько, В.В. Данчук, А.А. Солодовник

N_2 – Ar, CO – Ar криогенді қоспалардың кластерлік моделі, салыстырмалы талдау

Атомды құраушылары бар сызықты молекулалардан түзілген криокристалдардың ерітінділері модельдік жүйе ретінде ерекше қызығушылық тудырады. Тор параметрінің CO_2 – Ar құймаларындағы концентрацияға тәуелділігінің ерекше эффектісін түсіндіру үшін бөлшектердің арасындағы изотропты әсерлесуді ғана емес, сонымен қатар молекулалық матрицалардағы анизотропты күштің болуын ескеретін кластерлік модель қолданылды. Электронды дифракция әдісімен 20 К температурада азот-аргон жүйесінде тор параметрінің концентрацияға тәуелділігі өлшенді. Жұптық және үштік кластерлердің ерітіндінің тор параметріне әсері зерттелді. N_2 – Ar, CO – Ar ерітінділерінде кластердің болуына байланысты қателердің себептері қарастырылды.

Түйін сөздер: кластерлік модель, криокристалл, электронды дифракция.

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.

The authors are grateful to M.A.Strzhemechny for discussion of the problem.

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UDC 533.9.004.14; 621.039.6

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Do tunneling states and boson peak persist or disappear in extremely stabilized glasses?

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.

Key words: indomethacin, ultrastable glass, two-level system, the glass transition.

М.А. Рамос, Т. Перес-Кастанеда, Р.Д. Хименез-Риобу,
С. Родригез-Тиноко, Д. Родригез-Виейджо

Сохраняются ли туннельные состояния и бозонные пики в сверхстабилизированных стеклах?

Нами исследовано влияние низких температур на универсальные свойства стекол, а именно, янтарь и сверхстабильные тонкопленочные стекла индометацина.

Мы изучали образцы янтаря, возраст которых 110 миллионов лет, добытые в Эль Соплао (Кантабрия, Испания). Измерения удельной теплоемкости Ср нетронутых, частично или полностью омоложенных образцов проводились в температурном диапазоне 0,07 К<Т<30 К, а также при температуре стеклоперехода Tg 150С. Путем сравнения двух видов высокостабильных стекол мы пришли к выводу, что исчезновение тунелирующих двухуровневых систем в сверхстабильных тонких пленках индометацина может быть вследствие квази-2D и анизотропного поведения этих стекол, что может, в свою очередь, быть подтверждением идеи фононного взаимодействия между двухуровневыми системами, предложенной С.С.Ю и А.Дж. Леджеттом.

Ключевые слова: индометацин, сверхстабильные стекла, двухуровневые системы, стеклопереход.

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Аса тұрақтандырылған шынылардағы туннельдік жағдайлар және бозонды шыңы сақталады ма?

Біз төмен температура кезінде шынылардың температурасының өзгерісінің олардың ерекше қасиеттеріне әсерін зерттедік. Атап айтқанда, екі затты а) кәріптасты және ә) индометациннің аса тұрақты жұқа қабықшалы шыныларын зерттедік.

Біз 110 миллион жыл болған, Эль Соплаода (Кантабрия, Испания) табылған кәріптастың үлгісін зерттедік. Бұрын қолданылмаған, бөлшектей немесе толығымен жасартылған үлгілердің меншікті жылусыйымдылығын Ср өлшеу 0,07 К<Т<30 К температуралық диапазонда, сонымен қатар Tg 150С шыны ауысу температурасында жүргізілді. Жоғары тұрақтандырылған шынының екі үлгісін салыстыру жолымен біз индометациннің аса тұрақтандырылған жұқа қабықшаларында

екі деңгейлі тунельдеуші жүйелердің жоғалуы, өз кезегінде С.С.Ю және А.Дж. Леджет ұсынған екі деңгейлі жүйелердің арасындағы өзара фононды қ әсерлесу идеясын растайтын, осы шынылардың квази-2D және анизотропты тәртібінің әсерінен болуы мүмкін деген қорытындыға келдік.

Түйін сөздер: индометацин, аса тұрақтандырылған шынылар, екі деңгейлі жүйелер, шыныауысу.

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-oldamber samples from El Soplao (Cantabria, Spain). Specific heat C_p measurements of pristine, partially- and fully-rejuvenated samples were conducted in the temperature range $0.07\text{K} < T < 30\text{K}$, 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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UDC 533.9.004.14; 621.039.6

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Dynamic characteristics of the light emission, accompanying the cryocondensation of some gases

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.

Key words: Cryovacuum condensates,cryoemissing, phase transformations, nitrous oxide.

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Динамические характеристики излучения света, сопровождающего процесс криоконденсации некоторых газов

Процессы в тонких пленках криовакуумных конденсатов различных газов и их свойства являются объектом исследования многих ученых более десяти лет. В процессе изучения динамических характеристик фазового превращения газ – твердое вещество было обнаружено, что процессу конденсации закиси азота на металлической подложке сопутствует излучение света в видимом диапазоне.

Ключевые слова: криовакуумные конденсаты, криоизлучение, фазовые превращения, закись азота.

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Кейбір газдардың криоконденсация процесімен қатар жүретін жарықтың сәулеленуінің динамикалық сипаттамалары

Әртүрлі газдардың криовакуумді конденсаттарындағы жұқа қабықшалардағы процестер және олардың қасиеттері ондаған жылдам аса уақыт бойы көптеген ғалымдардың зерттеу нысаны болып келеді. Газ – қатты зат фазалық ауысуының динамикалық сипаттамаларын зерттеу процесінде металл төсемеде азот тотығының конденсация процесіне көрінетін диапазонда жарық сәулеленуі қатар жүретіні анықталды.

Түйін сөздер: криовакуумды конденсаттар, криосәулелену, фазалық ауысулар, азот тотығы.

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 theworking substances, we proceeded from the assumption ofthe possible role ofintrinsic dipolemoment of the moleculesto create the conditionsfor 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 resultsare subject to detailedanalysis and discussion ofthe assumptionsand conclusions.

UDC 533.9.004.14; 621.039.6

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Effect of pseudorotation on isochoric thermal conductivity of hydrocarbons in disordered phases

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.

Key words: isochoric thermal conductivity, hydrocarbon compounds, translation-orientation movement.

В.В. Саган, В.А. Константинов, В.П. Ревякин, А.В. Карачевцева

Влияние псевдовращения на изохорную теплопроводность углеводородов в неупорядоченной фазе

Изохорная теплопроводность твердых пятичленных гетероцикличных соединений была измерена в ориентационно-упорядоченной и ориентационно-разупорядоченной («пластичной») фазах образцов различной плотности в широком интервале температур и давлений. Объектами являлись: фуран – C_4H_4O, циклопентан – C_5H_{10}, тиофен – C_4H_4S. Целью данного исследования было изучение влияния трансляционно-ориентационного движения на поведение изохорной теплопроводности и оценка возможного вклада псевдовращения в общую теплоотдачу.

Ключевые слова: изохорная теплопроводность, углеводородные соединения, трансляционно-ориентационное движение.

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Жалған айналымдардың реттелмеген фазадағы көмірсулардың жылу өткізгіштігіне әсері

Қатты бес мүшелі гетероциклды қосылыстардың изохоралық жылуөткізгіштігі әртүрлі тығыздықты үлгілердің бағдарлы-реттелген және бағдарлы-реттелмеген («пластикалық») фазаларында температураның және қысымның кең аралығында өлшенген. Зерттеу нысаны: фуран – C_4H_4O, циклопентан – C_5H_{10}, тиофен – C_4H_4S болды. Бұл зерттеудің мақсаты трансляциялық-бағдарланған қозғалыстың изохоралық жылуөткізгіштікке әсерін зерттеу және жалған айналымның жалпы жылу беруге үлесін бағалау болды.

Түйін сөздер: изохоралық жылуөткізгіштік, көмірсулы қосылыстар, трансляциялық-бағдарланған қозғалыс.

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

D [1]. A strong translational orientational (TO) coupling contribute significantly to the thermal resistance. This, in turn, leads to large deviations of the isochoric thermal conductivity from the 1/T law owing to its approach to a lower limit min. The concept of the lower limit of the thermal conductivity comes from the idea that 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 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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UDC 533.9.004.14; 621.039.6

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Energy spectrum of the quantum vortices configurations

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

Key words: energy spectrum, the vortex lines, hydrodynamic turbulence, Kolmogorov spectrum.

С.К. Немировский

Энергетический спектр квантовых вихревых конфигураций

В работе предлагается обзор различных моделей, имеющих точное решение по определению энергетического спектра E(k) поля 3D-скорости, вызванного хаотичными вихревыми линиями. Эта проблема тесно связана с сакраментальным вопросом, может ли хаотическое множество вихревых линий имитировать реальную гидродинамическую турбулентность. Мы вводим общий метод расчета энергетического спектра по конфигурациям вихревых линий, рассматриваем несколько простых, но полезных примеров – прямая линия и вихревое кольцо радиуса R.

Ключевые слова: энергетический спектр, вихревые линии, гидродинамическая турбулентность, спектр Колмогорова.

С.К. Немировский

Кванттық құйын тәрізді конфигурациялардың энергетикалық спектрі

Бұл жұмыста құйын тәрізді хаосты сызықтардың әсерінен туындайтын 3D-жылдамдықты өрісінің энергетикалық спектрі E(k)бойынша нақты шешімі бар әртүрлі модельдерді қарастыру ұсынылады. Бұл мәселе көптеген құйын тәрізді хаосты сызықтар шынайы гидродинамикалық турбуленттілікке ұқсайды ма деген киелі сұрақпен байланысты. Біз құйын тәрізді сызықтардың конфигурациясы бойынша энергетикалық спектрінің есептеу әдістемесін енгіземіз, бірнеше қарапайым, бірақ пайдалы мысалдарды – түзу сызық және радиусы R құйын тәрізді шеңберді қарастырамыз.

Түйін сөздер: энергетикалық спектр, құйын тәрізді сызықтар, гидродинамикалық турбуленттілік, Колмогоров спектрі.

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 $E(k) = k^{-5/3}$. These are works, based on both the vortex filament method and the Gross-Pitaevskii equation. 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 [3,4]. 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 work we introduce the general method for calculation of the energy spectrum via the vortex line configuration, then we consider the couple of simple but useful examples -the straight line and vortex ring of radius R. Then we study uniform and nonuniform vortex arrays, the straight line with excited Kelvin wave on it and then we study the case of the reconnecting vortex filaments. We demonstrate that the spectra E(k), generated by the these configurations, is very close to the Kolmogorov dependence varproptok$^{-5/3}$, and discuss the reason for this as well as the reason for deviation.

The study was performed by grant from the Russian Science Foundation (project N 14-29-00093).

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UDC 533.9.004.14; 621.039.6

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Enhanced desorption from solid deuterium driven by charging with keVelectrons

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 m. 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.

Key words: desorption of solid deuterium, the surface potential of the film cryocrystals.

Йоргенсен Скоу, Бирджит Зестрап

Улучшенная десорбция твердого дейтерия, обусловленная зарядкой электронами

Пленки твердого дейтерия при температуре около 3 К облучались электронами 1,5 или 2 кэВ. Пленки осаждались на серебряный электрод микровесов с кристаллом кварца (МКК), свободно подвешенный ниже откачиваемого гелиевого криостата. Толщина пленок варьировалась в пределах от 10 нм до 5 мкм. Поверхностный потенциал вызван накоплением электронного заряда в пленках большой толщины, откуда электроны более не способны мигрировать к проводящей подложке с достаточно высокой скоростью. Линейное увеличение поверхностного потенциала может быть объяснено только поведением конденсатора.

Ключевые слова: десорбция, твердый дейтерий, поверхностный потенциал, пленки криокристаллов.

Йоргенсен Скоу, Бирджит Зестрап

кэВ-электрондармен зарядталуға негізделген қатты дейтерийдің жақсартылған десорбциясы

3К температурада қатты дейтерийдің қабықшасы 1,5 немесе 2 кэВ электрондармен сәулеленген. Қабықшалар кварц кристалды микросалмақты күміс (КМК) жинақталатын гелий криостаттан төмен ілінген электродқа отырғызылған. Қабықшаның қалыңдығы 10 нм-ден 5 мкм-ге дейін түрлендірілген. Беттік потенциал қабықшадан электрондар өткізгіш төсемеге жеткілікті жоғары жылдамдықпен өте алмайтын қалың қабықшаға электр зарядының жинақталуынан туындаған. Беттік потенциалдың сызықтық артуы тек конденсатордың әрекетімен түсіндірілуі мүмкін.

Түйін сөздер: десорбция, қатты дейтерий, беттік потенциал, криокристалдардың қабықшалары.

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 D2/electron up to 380 D2/electron at 1.5 keV and 960 D2/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. The interesting point is that the surface potential increases linearly with film thickness and that the increase corresponds to 600 MV/m for both bombardment by 1. 5 keV electrons and 2 keV electrons. This internal field is very high, even though one has to consider that solid deuterium is an extremely bad conductor. The electron-induced field starts at a thickness of 1.9 μm, which should be compared with an average penetration depth for 1.5 keV electrons of 350 nm. For 2 keV electrons the field (as well as the charging) starts at 2.3 μm, which reflects the larger penetration depth of a 2 keV electron. The linear increase of the surface potential can only be explained by a capacitor behavior: the accumulated electrons are located close to the surface within a limited thickness while the space between the charges close to the surface and the metal substrate (the electrode of the QCM) is essentially free of any charge.

It is not clear how the electrons are trapped. As discussed by R. L. Brooks and coauthors [3] the electrons can be trapped in existing vacancies as «bubbles» or by polarons, which are somewhat more mobile. The density of these more and less immobile electrons is 1017 electrons/cm3. This density could actually provide an intrinsic field of the magnitude that has been measured experimentally, provided that the accumulated electrons are located within 0.5 μm from the surface.

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UDC 533.9.004.14; 621.039.6

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Equilibrium crystal shape of 4He under microgravity

The growth coefficient of 4He crystal which is grown from the superfluid becomes divergently large towards T=0, and the crystal relaxes to the equilibrium state in a very short period. We have succeeded in cooling 4He crystal down to 150 mK by the specially designed dilution refrigerator under microgravity of parabolic flight for 20 seconds. Using this fridge, we were able to obtain beautiful pictures of the crystal with 3 facets, c-, a-, and s-, under the equilibrium condition at 150 mK for the first time.

Key words: 4He crystal, microgravity, superfluidity, vicinal surface.

Юши Окуда

Равновесная кристаллическая форма 4He в условиях микрогравитации

Коэффициент роста 4He кристалла, выращенного из сверхтекучей жидкости, становится дивергентно большим вблизи T=0 К, и кристалл переходит в равновесное состояние за очень короткое время. Мы успешно охладили 4He кристалл до 150 мК специально разработанным рефрижератором растворения в условиях микрогравитации в процессе полета по параболе за 20 сек. Используя эту охлаждающую систему, мы впервые смогли получить прекрасные изображения кристалла гелия с 3-мя гранями, c-, a- и s-, в условиях равновесия при 150 мК. Полученные изображения показали, что 4He кристалл на Земле сильно деформируется гравитацией.

Ключевые слова: 4He кристалл, микрогравитация, сверхтекучесть, вицинальная поверхность.

Юши Окуда

Микрогравитация шарттарында 4He бірқалыпты кристалдық формасы

Аса аққыш сұйықтықтан алынатын 4He кристалының арту коэффициенті T=0 К маңайында дивергентті үлкен мәнге ие болады және кристалл өте аз уақытта бірқалыпты жағдайға өтеді. Біз 4He кристалын 150 мК дейін арнайы жасалған еріту рефрижераторында 20 сек ішінде микрогравитация жағдайында парабола бойынша ұшу процесінде сәтті суыттық. Осы суытқыш жүйені пайдалана отырып біз ең бірінші рет150 мК кезінде тепе-теңдік жағдайында c-, a- және s-, 3-қырлы гелий кристалының айқын бейнесін алдық. Алынған суреттер 4He кристалы Жерде гравитациямен өте күшті өзгеретінін көрсетті.

Түйін сөздер: 4He кристалл, микрогравитация, асқын аққыштық, вицинал бет.

The growth coefficient of 4He crystal which is grown from the superfluid becomes divergently large towards T=0, and the crystal relaxes to the equilibrium state in a very short period. We have succeeded in cooling 4He crystal down to 150 mK by the specially designed dilution refrigerator under microgravity of parabolic flight for 20 seconds. Using this fridge, we were able to obtain beautiful pictures of the crystal with 3 facets, c-, a-, and s-, under the equilibrium condition at 150 mK for the first time. The movies revealed that the 4He crystal on the ground is largely deformed by the gravity. Thanks to obtaining crystal with three facets in the probable equilibrium condition, we were able to determine the Wulff's origin with a pretty good accuracy. Once the origin is determined, the surface energy of each facet is derived, using the known c-facet surface energy as a reference. At the same

time, the facet size (c-facet) and the functional form of the vicinal surface next to c-facet were determined. Surprisingly, the size of c-facet of the crystal was very small, and then the flat looking plane was found to be the vicinal surface, not the facet.

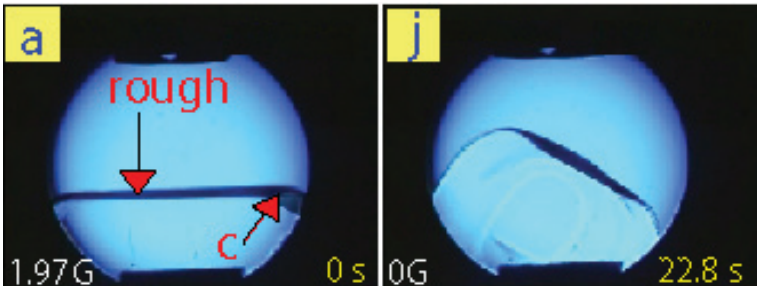

Figure 1 – Left: 4He crystal under 1G. The horizontal flat surface is the rough surface. T=150 mK. Right: The same crystal under microgravity. There are three facets appearing

This work is done in cooperation with Takuya Takahashi and Ryuji Nomura. We would like to thank JAXA for the support as «Ground-based Research Announcement».

UDC 533.9.004.14; 621.039.6

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Exciton transport and orientationalglassification point in doped C60

Below 95 K, pristine fullerite C60 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 C60 is stuffed with, for instance, with CO or NO.

Key words: glass transition point, excitons, X-ray analysis, luminescence.

М.А. Стржемечный, П.В. Зиновьев, В.Н. Зорянский

Перенос экситонов и приблизительная точка стеклования электронов в легированном C60

В настоящей работе мы использовали методы рентгеноструктурного анализа и люминесценции для изучения процесса интеркалирования C60 и водорода, азота, CO, а также последствий, вызванных интеркаляцией, воздействующей при высоких температурах до 350C и давлении 30 атм. Наши результаты показали, что механизм насыщения для H_2 значительно отличается от такового для N_2 и CO. Также наши эксперименты с люминесценцией с N_2 и CO в роли интеркалирующей добавки показали, что точка стеклования Tg смещается в область более низких температур, причем более явно в случае оксида углерода.

Ключевые слова: точка стеклования, экситоны, рентгеноструктурный анализ, люминесценция.

М.А. Стржемечный, П.В. Зиновьев, В.Н. Зорянский

Легирленген C60 электрондарының шынылаудың жуық нүктесі және экситондарды тасымалдау

Бұл жұмыста біз C60 және сутегінің, азоттың, CO интеркалировкалау процесін, сонымен қатар жоғары температурада 350C және қысымда 30 атм әсер ететін интеркаляцияның нәтижесін зерттеу үшін рентген құрылымдық талдау және люминисценция әдістерін пайдаландық. Біздің нәтижелеріміз H_2 үшін қанығу механизмі N_2 және CO қарағанда айтарлықтай ерекшеленетінін көрсетті. Сонымен қатар біздің интеркалировкалау қоспасы ретінде N_2 және CO қолданылған люминисценциямен тәжірибелеріміз Tg шынылау нүктесі көміртек оксиді қолданған жағдайға қарағанда айтарлықтай төмен температура аумағына ауысатынын көрсетті.

Түйін сөздер: шынылау нүктесі, экситондар, рентген құрылымды талдау, люминесценция.

Below 95 K, pristine fullerite C60 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 C60 is stuffed with, for instance, with CO or NO. We used XRD and luminescence techniques to study the process of intercalation of C60 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 350^0C (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 H2 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 250^0C 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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UDC 533.9.004.14; 621.039.6

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Field-emission source of chages based on nanotubes for low temperature experiments

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.

Key words: avtoemission charges, nanotubes, cryocrystals.

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Источник автоэмиссионных зарядов на основе нанотрубок для низкотемпературных экспериментов

В настоящем докладе мы представляем два способа производства автоэмиссионных источников заряда на основе углеродных нанотрубок, которые могут быть использованы в низкотемпературных исследованиях свойств инжектированных зарядов в криогенных жидкостях и кристаллах. Измерения I-V (ток-напряжение) зависимости источников первой серии показали, что в сверхтекучем гелии He-II ток отрицательных зарядов на уровне 10-12 А появляется при напряжении на источнике U = -120 В, и увеличивается до 10-9 А с увеличением U до -170 В. Таким образом, наблюдаемая зависимость существенно сильнее, чем квадратичная зависимость I(U), что может быть объяснено наличием в объеме образца большого количества дефектов, которые могут улавливать инжектируемые заряды.

Ключевые слова: автоэмисионные заряды, нанотрубки, криокристисталлы.

Д.Н. Борисенко, П.М. Уолмслей, А.И. Голов, Н.Н. Колесников, Ю.В. Котов,
А.А. Левченко, М.Д. Феер

Төмен температуралы тәжірибелер үшін нанотүтікшелер негізінде автоэмиссиялы зарядтардың көзі

Бұл баяндамада біз криогенді сұйықтарда және кристалдардағы инжектрлік зарядтардың қасиетін төмен температуралы зерттеулерде қолданылуы мүмкін көміртек негізіндегі нанотүтікшелердің автоэмиссиялық көзін алудың екі жолы туралы айтамыз. I-V бірінші серия көздерінің тәуелділіктерін өлшеулер (ток-кернеу) асқын аққыш гелийде He-II10-12 А деңгейіндегі теріс зарядтардың тогы көзде U = -120 В кернеу болған кезде көрінетіні және U -170 В дейін артқанда 10-9 А дейін артатынын көрсетті. Осылайша, бақыланып отырған тәуелділік квадраттық тәуелділікке қарағанда айтарлықтай күшті болады. Бұл үлгінің көлемінде инжектрленген зарядтарды ұстайтын ақаудың көп болуымен түсіндіріледі.

Түйін сөздер: автоэмиссионды зарядтар, нанотүтікшелер, криокристалдар.

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.

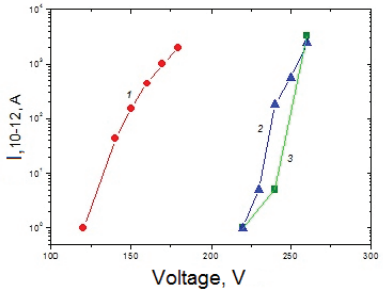

Figure 1 – The dependence of current through the diode in superfluid helium He-II on voltage applied to the source at T=1.3K. Curve 1 – negative charges, curve 2 – positive charges. Curve 3 – current of negative charges in three weeks after first test.

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 = -120 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>220 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. Voltage dependence of negative charges current at voltages above 250V can be described by a power-law function, $I \sim U^{\eta}$, where ηis closed to 7.5. The observed significantly stronger than quadratic dependence of I(U) can be associated with the presence in the volume of the sample of a large number of defects that can trap injected charges [1].

Authors are grateful to A.V. Lokhov for help in preparing experimental setup and L.P. Mezhov-Deglin for useful discussions. The work is partially supported by RFBR #12-02-00581.

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UDC 533.9.004.14; 621.039.6

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Glassy crystals of adamantane derivatives induced by thermal treatment

Observing a first-order transition between the supercooled liquid state and a new amorphous phase, the "glacial state" has been one of the most interesting focus during the last decades. At present the glacial state is seen as an interrupted crystallization due to the low crystal growth rate from the glass state. In this work, we will describe the first glacial state obtained from a plastic crystal for two materials - adamantane derivatives.

Key words: glassy state, adamantane, first order phase transition, plastic crystal.

Д. Шевчук, А. Ежовски

Стекловидные свойства кристаллов производных адамантана, вызванные тепловой обработкой

Наблюдаемое в процессе фазового перехода первого рода между сверхпереохлажденной жидкостью и новой аморфной фазой «стекловидное состояние» является одним из наиболее интересных явлений последние десятилетия. В настоящей работе описывается первое стекловидное состояние, полученное из пластичного кристалла для двух материалов – производных адамантана. Результаты измерений теплопроводности веществ показали, что данный метод чувствителен к типу разупорядоченности, присутствующей в исследуемых молекулярных системах. Попеременное охлаждение и нагревание образца в несколько раз улучшает степень кристаллизации ранее быстро охлажденного пластического кристалла.

Ключевые слова: стекловидное состояние, адамантан, фазовый переход первого рода, пластический кристалл.

Д. Шевчук, А. Ежовски

Өндірістік адамантанның жылулық өңдеуден пайда болған шыны тектес қасиеттері

Аса суытылған сұйық және жаңа аморфты фазаның арасындағы фазалық ауысу процесі кезінде бақыланатын «шыны тектес жағдай» соңғы онжылдықта ең қызықты құбылыстардың бірі болып табылады. Бұл жұмыста екі материал үшін пластикалық кристалдан алынған өндірістік адмантанның бірінші шыны тектес жағдайы сипатталады. Заттардың жылу өткізгіштіктерін өлшеу нәтижелері бұл әдіс зерттелініп отырған молекулалық жүйелерде бар реттелмегендік типіне сезімтал болатындығын көрсетті. Ауыспалы кезектесіп жүргізілетін үлгіні суыту және қыздыру бұрында суытылған пластикалық кристалдың кристалдану дәрежесін бірнеше есе жақсартады.

Түйін сөздер: шыны тектес жағдай, адамантан, бірінші текті фазалық ауысу, пластикалық кристалл.

Observing a first-order transition between the supercooled liquid state and a new amorphous phase, the «glacial state» has been one of the most interesting focus during the last decades. At present the glacial state is seen as an interrupted crystallization due to the low crystal growth rate from the glass state. In this work, we will describe the first glacial state obtained from a plastic crystal for two materials – adamantane derivatives.

The thermal conductivity of 2-adamantanone ($C_{10}H_{14}O$) and 1-cyanoadamantane ($C_{10}H_{15}CN$) disordered crystals has been measured for temperatures between 4.2 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 $C_{10}H_{15}CN$ 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.

The results of thermal conductivity measurements showed that the technique is very sensitive to type of disorder that appears in investigated molecular systems. Furthermore thermal treatment given to the sample resulted in emergence of two completely different states: one – crystalline, the other one – amorphous. Additionally alternately cooling and heating the sample several times improves the crystallinity of the previously quenched plastic crystal. The so far obtained results seems to be a very good beginning for further analyze of glass transition phenomenon in investigated plastic molecular crystals.

UDC 533.9.004.14; 621.039.6

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Heat capacity of fullerite C60

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.

Key words: fullerenes, the specific heat, the crystal lattice, libration.

М.И. Багатский, М.С. Барабашко, В.В. Сумароков

Теплоемкость фуллерита С60

Теплоемкость фуллерита С60 исследована в температурном интервале 1–120 К с использованием адиабатного калориметра. Проведен анализ полученных данных и литературных источников, предполагая, что поступательные, вращательные и внутримолекулярные степени свободы вносят дополнительный вклад в теплоемкость фуллерита. Обнаружено, что температурная зависимость теплоемкости может быть выражена как сумма линейных и кубических термов при температуре ниже 3 К. Вклад внутримолекулярных колебаний становится существенным при температуре выше 50 К.

Ключевые слова: фуллерит, теплоемкость, кристаллическая решетка, либрации.

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С60 фуллериттің жылусыйымдылығы

С60 фуллериттің жылусыйымдылығы 1-120К интервалында адиобатты калориметрді пайдалана отырып зерттелінді. Үдемелі, айнымалы және молекула ішіндегі еркіндік дәрежелері фуллериттің жылусыйымдылығына қосымша үлес қосады деп болжам жасай отырып, алынған мәліметтердің және әдебиет көздерінің талдауы жүргізілді. Жылусыйымдылықтың температуралық тәуелділігі 3К төмен температура кезінде сызықтық және кубтық термдердің қосындысы ретінде көрсетілуі мүмкін екені анықталды. Молекула ішіндегі тербелістердің үлесі 50К жоғары температурада біліне бастайды.

Түйін сөздер: фуллерит, жылусыйымдылық, кристалдық тор, либрациялар.

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 fulleriteorientational 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 . 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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UDC 533.9.004.14; 621.039.6

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Heat transfer in Ar and N_2 doped solid CO

Investigations of thermal conductivity of dielectric crystals play a special role in solid state physics. The obtained information can be interesting both for theory and experiment. Introducing an impurity in the crystal enables to study influence of the thermal excitations modified by the impurity on the thermal conductivity or scattering of the heat carrier by the impurities.

In CO-Ar solution the isotopic effect occurs, i.e. effect caused by the difference of the masses of the impurities and the host atoms. This leads to additional mechanism of phonon scattering.

Key words: thermal conductivity, defects, phonon scattering, impurity.

Т. Романова, П. Стаховяк, А. Ежовски, В. Цебятовски

Теплообмен в твердом CO, легированном Ar и N_2

Исследования теплопроводности диэлектрических кристаллов играют особую роль в физике твердого тела. В растворе CO-Ar существуют изотопические эффекты, вызванные разницей масс примесей и атомов матрицы. Это приводит к дополнительному механизму рассеяния фононов. Раствор CO-N_2 позволяет напрямую исследовать взаимодействие фононов с примесями без изотопических эффектов из-за одинаковых масс веществ. Полученные зависимости теплопроводности от температуры типичны для диэлектрических кристаллов. Обнаружено, что фононное рассеяние точечными дефектами увеличивается с ростом концентрации примеси для обоих твердых растворов.

Ключевые слова: теплопроводность, дефекты, фононное рассеяние, примеси.

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Қатты CO, легирленген Ar және N_2 жылуалмасу

Диэлектрлік кристалдардың жылуөткізгіштігін зерттеу қатты дене физикасында өте маңызды орын алады. CO-Ar ерітіндісінде қоспалардың массасының және матрица атомдарының айырмашылығынан туындайтын изотоптық эффектілер бар. Бұл фонондардың қосымша шашырау механизміне алып келеді. CO-N_2 ерітіндісі заттардың массасының бірдей болуының есебінен фонондардың қоспаларымен тікелей әсерлесуін зерттеуге мүмкіндік береді. Қол жеткізілген жылусыйымдылықтың температураға тәуелділіктері диэлектрлік кристалдарға тән болып табылады. Нүктелік ақаулармен фонондық шашырау қатты ерітінді қоспаларының екеуі үшін де концентрацияның артуымен жоғарылайды.

Түйін сөздер: жылуөткізгіштік, ақаулар, фонондық шашырау, қоспалар.

Investigations of thermal conductivity of dielectric crystals play a special role in solid state physics. The obtained information can be interesting both for theory and experiment. Introducing an impurity in the crystal enables to study influence of the thermal excitations modified by the impurity on the thermal conductivity or scattering of the heat carrier by the impurities.

In CO-Ar solution the isotopic effect occurs, i.e. effect caused by the difference of the masses of the impurities and the host atoms. This leads to additional mechanism of phonon scattering.

CO-N_2 solid solution allows to investigate the interaction of phonons with impurities directly, without isotopic effect, because carbon monoxide and nitrogen have the same masses (28 a.u.).

Measurements of the 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 by steady-state heat flow method. The samples were grown and measured in a thin-wall stainless ampoule placed in a LHe cryostat. In the experiment the crystals were grown from the gaseous phase at the rate of approximately 1mm/h. After growth the samples were cooled down to the region of the measurements temperature at a rate of 0,2 K/h.

The results of the measurements of the thermal conductivity coefficient on temperature of pure carbon monoxide and carbon monoxide doped by nitrogen and argon at different concentration are presented.

The obtained dependences of the thermal conductivity on temperature show a typical behavior for a dielectric crystal. Characteristic maximum is observed. The magnitude of its 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-N_2 and CO-Ar solid solutions at different concentrations was estimated using Callaway's equation in the framework of the Debye model. It was found that the scattering of phonons by point defects increases with increasing concentration of the admixture for both solid solutions. The scattering by the disordered molecules for crystals doped by nitrogen, first increases with increase of the admixture concentration, then decreases. For crystals doped by nitrogen, this scattering decreases with increasing of the admixture concentration.

UDC 533.9.004.14; 621.039.6

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Investigation of Al_2O_3 nanoparticle influence on caloric properties of isopropanol

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.

Key words: nanoparticles, isopropanol, specific heat, melting temperature.

Н.А. Шимчук, В.П. Железный

Исследование влияния наночастиц Al_2O_3 на калорические свойства изопропанола

Целью настоящей работы является экспериментальное изучение калорических свойств модели наносистемы – изопропиловый спирт с наночастицами оксида алюминия с различными концентрациями наночастиц. Полученные экспериментальные данные показывают, что примеси наночастиц влияют на параметры фазового перехода твердое тело – жидкость, а также на теплоемкость изопропилового спирта. Наибольшее влияние наночастиц на параметры перехода наблюдается при низких концентрациях оксида алюминия. Авторами предложена новая методология определения температуры плавления, основанная на нахождении минимума производной функции, описывающей полученную термограмму.

Ключевые слова: наночастицы, изопропанол, теплоемкость, температура плавления.

Н.А. Шимчук, В.П. Железный

Al_2O_3 нанобөлшектерінің изопропанолдың калорикалық қасиеттеріне әсерін зерттеу

Бұл жұмыстың мақсаты концентрациясы әртүрлі нанобөлшектермен алюминий оксидінің нанобөлшектерімен изопропил спирті – наножүйесінің моделінің калорикалық қасиеттерін тәжірибе жүзінде анықтау болып табылады. Алынған тәжірибелік мәліметтер нанобөлшектердің қоспалары қатты дене – сұйықтық фазалық ауысуының параметріне, сонымен қатар изопропил спиртінің жылусыйымдылығына әсер ететінін көрсетеді. Нанобөлшектердің ауысу параметріне айтарлықтай көп әсері алюминий оксидінің төмен концентрациясында байқалады. Авторлар алынған термограмманы сипаттайтын функцияның туындысының минимумын анықтауға негізделген балқу температурасын анықтаудың жаңа әдістемесін ұсынған.

Түйін сөздер: нанобөлшектер, изопропанол, жылусыйымдылық, балқу температурасы.

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.

UDC 533.9.004.14; 621.039.6

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Investigations of thermal properties of simple van der waals crystal based nanocomposites

Physical properties of the objects featuring nanometric linear dimensions have been being intense investigated for over ten years. The reason for the scientific interest is twofold:

• basic science – the objects of dimensions of tens of nanometers display new physical properties, usually very much different than their macroscopic counterparts

• possible applications – the new properties of such the objects make it possible to design new devices. The nanostructured materials along with their new properties utilized as a base for new technologies have recently caused an unprecedented acceleration in some of their fields.

Key words: thermal conductivity, nanopowders, cryocrystals crystal lattice.

П. Стаховяк, А. Ежовски, Р. Никонков, Т. Романова

Исследование термических свойств нанокомпозитов на основе простых кристаллов Ван-дер-Ваальса

Относительная простота кристаллографической структуры матрицы и взаимодействия между составляющими делает криокристаллы с внедренными нанопорошками идеальными объектами фундаментальных физических исследований. В настоящей работе представлен экспериментальный метод исследования теплопроводности нанопорошков диэлектриков и металлов со средним диаметров в пределах от 10 до 50 нм, внедренных в кристаллическую решетку неона, аргона, азота и метана. Измерения проводились в температурном диапазоне 1-40 К стационарным методом.

Ключевые слова: теплопроводность, нанопорошки, криокристаллы, кристаллическая решетка.

П. Стаховяк, А. Ежовски, Р. Никонков, Т. Романова

Ван-дер-Ваальстің қарпайым кристалдарының негізіндегі нанокомпозиттердің термиялық қасиеттерін зерттеу

Матрицаның крситаллографикалық салыстырмалы түрде қарапайымдылығы және құраушыларының арасындағы өзара байланысы енгізілген криокристалды ноноұнтақтары бар криокристалдарды негізгі физикалық зерттеулердің идеал зерттеу нысаны болуына себеп болады. Бұл жұмыста диэлектриктердің және металдардың орташа диаметрі 10-нан 50нм-ге дейін неонның, аргонның, азоттың және метанның кристал торына енгізілген наноұнтақтарының жылуөткізгіштіктерін зерттеудің тәжірибелік әдісі көрсетілген. Өлшеулер 1-40К температуралық интервалда тұрақты әдіспен жүргізілді.

Түйін сөздер: жылуөткізгіштік, нанұнтақтар, криокристал, кристалдық тор.

Physical properties of the objects featuring nanometric linear dimensions have been being intense investigated for over ten years. The reason for the scientific interest is two fold:

• basic science – the objects of dimensions of tens of nanometers display new physical properties, usually very much different than their macroscopic counterparts

• possible applications – the new properties of such the objects make it possible to design new devices. The nanostructured materials along with their new properties utilized as a base for new

technologies have recently caused an unprecedented acceleration in some of their fields.

For the similar reason more complex nanostructured materials are also of great interest and therefore are subject to intense investigations.

A particular example of nanostructured material arecryocrystals with nanopowders immersed in their volume. A relative simplicity of crystallographic structure of the matrix and interactions between the constituents make them ideal objects for basic physics investigations. 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 determine, in particular, the influence of the size of nanoparticles and their intrinsic transport properties on the resultant thermal conductivity of the nanostructured material. The role of the parameters of the crystalline matrix, such as the interaction strength between its atoms (molecules), 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. Here we present experimental technique which will be used to investigate thermal conductivity of nanopowders of dielectrics and metals of average diameter ranging from 10 to 50nm, embedded in crystalline matrixes of neon, argon, nitrogen and methane. The measurements will be carried out in the temperature range ~1 to 40K with steady-state method.

The preliminary results of the measurements carried out on sample of methane with 30nm nanoparticles of hydroxyapatite embedded in the crystal volume showed a low value of the coefficient at temperatures below 10K, lower than that of amorphous solids. Also some kinks of the dependence of the thermal conductivity coefficient on temperature of unknown origin were noticed.

UDC 533.9.004.14; 621.039.6

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

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.

Key words: low-frequency internal friction HTSC ceramics, cryocrystals superconducting transition, phase transformations.

А.В. Леонтьева, А.И. Эренбург, А.Ю. Прохоров

Низкочастотное внутреннее трение (НЧВТ) как экспресс-метод идентификации криокристаллов в порах твердых тел

Криокристаллы (затвердевшие газы) образуют относительно небольшую группу материалов находящихся в газообразном состоянии при комнатной температуре и в твердом состоянии при криогенных температурах. Эта группа веществ включает атомные криокристаллы (He, Ne, Ar, Kr, Xe), простейшие молекулярные криокристаллы (водород, азот, CO, кислород), а также некоторые кристаллы больших молекул (CO_2, N_2O, CH_4, NH_3).

В результате НЧВТ исследования (при f=10-20 Гц) ОМИБ ВТСП керамики обнаружено, что кроме пика при T= 90-95К, относящегося к сверхпроводящему NS-переходу, наблюдаются также несколько повторяющихся пиков вблизи температур 24, 44 и 54 К, соответствующих температурам фазовых превращений и тройной точки твердого кислорода. Данный факт позволяет идентифицировать наличие кислорода в порах оксида Y-Ba-Cu-O.

Ключевые слова: низкочастотное внутреннее трение, ВТСП керамика, криокристаллы, сверхпроводящий переход, фазовые превращения.

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Төмен жиілікті ішкі үйкелістер (ТЖІҮ) қатты денелердің қуыстарындағы крисокристалдарын жылдам сәйкестендіру әдісі ретінде

Криокристалдар (қатып қалған газдар) бөлме температурасында газ тектес күйде, криогенді температураларда қатты күйде болатын материалдардың салыстырмалы түрде кішкентай тобын құрайды. Заттардың бұл тобына атомдық криокристалдар (He, Ne, Ar, Kr, Xe), қарапайым молекулалық криокристалдар (сутегі, азот, CO, оттегі), сонымен қатар үлкен молекулалардың кейбір кристалдары (CO_2, N_2O, CH_4, NH_3) жатады.

ТЖІҮ зерттеу (f=10-20 Гц кезінде) ОМИБ ЖТАӨ керамиканың T= 90-95К кезіндегі асқын өткізгіш NS ауысуға сәйкес келетін шыңы, сонымен қатар фазалық ауысулардың және қатты оттегінің үштік нүктесіне сәйкес келетін 24, 44 және 54 К температураның маңайында бірнеше қайталанатын шыңдарда да байқалады. Бұл факт оттегінің қуыстарында Y-Ba-Cu-O бар екенін сәйкестендіруге мүмкіндік береді.

Түйін сөздер: төмен жиілікті ішкі үйкеліс, ЖТАӨ керамика, криокристалдар, асқын өткізгіш ауысу, фазалық ауысулар.

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 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 ~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 ~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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UDC 533.9.004.14; 621.039.6

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Magnetic resonance study of atomic hydrogen stabilized at high densities in solid H_2 and D_2 matrices

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 supersolidbehaviour. This may happen at high enough densities of atomic hydrogen.

Key words: atomic hydrogen, quantum crystals, quantum tunneling, magnetic resonance.

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Магнитно-резонансное исследование атомарного водорода, стабилизированного при высоких плотностях в твердых матрицах H_2 и D_2

Водород и дейтерий в твердом состоянии при низких температурах представляют особый класс квантовых кристаллов, в которых, благодаря большим нулевым колебаниям и малой массе, эффект квантового туннелирования играет важную роль. Мы обнаружили, что квантовые изотопические реакции обмена $D+H_2=H+HD$ и $D+HD=H+D_2$ проходят с достаточно высокими скоростями при температурах ниже 1 К и значительно увеличивают концентрацию атомарного водорода в пленках смеси H;D; H_2;D_2. Мы полагаем, что взаимодействие электронов атома водорода с магнитными моментами орто-дейтериевых молекул существенно улучшает возможности существования запрещенных состояний.

Ключевые слова: атомарный водород, квантовые кристаллы, квантовое туннелирование, магнитный резонанс.

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Тұрақтандырылған H_2 және D_2 қатты матрицаларында жоғары тығыздық кезінде атомдық сутегіні магниттік-резонансты зерттеу

Қатты күйдегі сутегі мен дейтерий төмен температура кезінде нөлдік тербелістің және кіші массасының арқасында кванттық тунельдік эффект маңызды болып табылатын кванттық кристалдар класы болып табылады. Біз $D+H_2=H+HD$ және $D+HD=H+D_2$ кванттық изотоптық алмасу реакциялары 1 К төмен температурада айтарлықтай жоғары жылдамдықпен өтетінін және H;D; H_2;D_2 қоспасының қабықшасында атомдық сутегінің концентрациясының артатынын анықтадық. Біз сутегі атомының электрондарының орто-дейтерийдің магниттік моментімен өзара әрекеттесуі тыйым салынған жағдайлардың болу мүмкіндігін айтарлықтай жақсартады деп болжаймыз.

Түйін сөздер: атомдық сутегі, кванттық кристалдар, кванттық туннельдеу, магниттік резонанс.

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 supersolidbehaviour. This may happen at high enough densities of atomic hydrogen. In our previous work we succeeded in reaching record high densities of atoms 4•1019 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 (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, 2) we deposited a thin film of solid molecular (ortho-D_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 D2 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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UDC 533.9.004.14; 621.039.6

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Matrix-isolation studies of non-covalent interactions: more sophisticated approaches

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.

Key words: matrix isolation, hydrogen bond, Cryocrystals hydrates.

Л. Хриачтчев

Исследование нековалентных взаимодействий методом матричной изоляции: более сложные подходы

Матричная изоляция является мощным методом изучения нековалентных взаимодействий, включая виды водородных связей. В настоящей работе мы описываем сложные подходы, позволяющие изучать комплексы, являющиеся проблематичными для исследования традиционными методами. Взаимодействие гидратов инертных газов с другими веществами может быть изучено в твердой матрице. Конформеры с более высокой энергией могут быть стабилизированы в комплексах с сильной водородной связью. Мы также обсуждаем особые случаи, при которых спектральные сдвиги небольшие, и прямое спектроскопическое доказательство образования комплексов не доступно.

Ключевые слова: матричная изоляция, водородная связь, криокристаллы, гидраты.

Л. Хриачтчев

Ковалентті емес өзара әрекеттесулерді матрицалық изоляция әдісімен зерттеу: айтарлықтай күрделі тәсілдер

Матрицалық изоляция сутекті байланыстың түрлерін қоса алғанда, ковалентті емес өзара әрекеттесулерді зерттеудің қуатты әдісі болып табылады. Бұл жұмыста біз дәстүрлі әдіспен зерттеуде мәселе тудыратын кешендерді зерттеуге мүмкіндік беретін күрделі тәсілдерді сипаттаймыз. Инертті газдардың гидраттарының басқа заттармен өзара әрекеттесуі қатты матрицада зерттелуі мүмкін. энергиялары жоғарырақ конформерлер күшті сутекті байланысты кешендерде тұрақтандырылуы мүмкін. Сонымен қатар біз спектрлік ауытқулар үлкен емес және кешендердің түзілуінің тікелей спектроскопиялық дәлелденуі қолжетімсіз болатын ерекше жағдайларды талқылаймыз.

Түйін сөздер: матрицалық изоляция, сутекті байланыс, криокристалдар, гидраттар.

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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UDC 533.9.004.14; 621.039.6

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Mechanisms of self-screening in intrinsic semiconductors

Electron-hole pairs (proton-hydroxyl pairs in water) thermally activated in intrinsic semiconductors interact through Coulomb forces which necessarily results in some self-screening that should either be accounted for in a proper way or shown to be negligible. Possible mechanisms of self-screening are considered in this work.

Key words: self-shielding, intrinsic semiconductor, method of Debye-Hyukelya.

И. Чикина, В. Шикин

Механизмы самоэкранирования в собственных полупроводниках

Термически активированные электронно-дырочные пары (протон-гидроксильные пары в воде) в собственных полупроводниках взаимодействуют посредством Кулоновских сил, необходимым следствием этого является некоторое самоэкранирование, которое следует или должным образом учитывать, или считать пренебрежимо малым. Возможные механизмы самоэкранирования рассмотрены в настоящей работе.

Ключевые слова: самоэкранирование, собственный полупроводник, метод Дебая-Хюкеля.

И. Чикина, В. Шикин

Меншік жартылай өткізгіштерде өздігінен экрандалу механизмдері

Меншік жартылай өткізгішті жартылай өткізгіштерде термиялық белсендірілген электронды-кемтікті жұптар (судағы протон-гидроксильді жұптар) Кулон күшінің әсерімен өзара әсерлеседі, бұның қажетті нәтижесі ескерілуге тиісті немесе елемейтіндей аз деп есептейтіндей өздігінен экрандалу болып табылады. Өздігінен экрандалудың бұндай механизмдері осы жұмыста қарастырылған.

Түйін сөздер: өздігінен экрандалу, меншік жартылай өткізгіш, Дебая-Хюкель әдісі.

Electron-hole pairs (proton-hydroxyl pairs in water) thermally activated in intrinsic semiconductors interact through Coulomb forces which necessarily results in some self-screening that should either be accounted for in a proper way or shown to be negligible. Possible mechanisms of self-screening are considered in this work.

1. One of the scenarios for development of self-screening is as follows (the Debye-H¨uckel approach [1]). One of the ions is placed into the origin of the coordinate system, all other ions are allowed to screen it. Then the electric potential $\phi(r)$ satisfies the following equation:

$$\phi(r) = e\exp(-\kappa dr)/r, \qquad (1)$$

where ² is the medium dielectric constant and κ is the donor density.

In the expansion of $\phi(r)$ for small r

$$e\phi\ (r)\ `\ -e^2k + \ldots\ U_{corr} \sim e^2k_{aq} \qquad (2)$$

thefirst term is the self-energy of the central ion, while the second term represents.

[1] the correlation correction U_{corr} we are searching for. Eqs. (1,2) are the starting point for all correlation phenomena in classical systems with Coulomb interaction.

2. An interesting alternative estimate for Ucorr can be taken from the theory of ion lattices [2]. If the charges arising due to dissociation are arranged into a regular lattice suitable for the application of

the Ewald rules, then the correlation energy per pair of ions Ucorr can be written as

$$U_{corr} \sim \gamma e^2 / R_{aq},\ R_{aq} \sim (\alpha_{aq} n_{aq})^{-1} \qquad (3)$$

where γ is a Madelung constant.

The estimates (2) and (3) for the correlation energy U_{corr} have different structures and are substantiated in different ways. Discussed in the present paper are the reasons underlying these differences.

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UDC 533.9.004.14; 621.039.6

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Melting of cryocrystasls at high pressures. Computer simulation

Two types of molecular dynamics simulations: single-phase and two-phase carried out and applied to determine the melting temperatures of highly compressed diatomic cryocrystals: nitrogen and hydrogen, as functions of pressure. Solid hydrogen was modeled by two approximations (1) non-empirical atom-atom potential (AAP) approximation [1], and diatom-diatom (DDP) approximation. Within AAP-model potential energy of hydrogen molecules is represented as a function of interatomic distances between all atoms as a sum of intramolecular (bonding) and intermolecular (non-bonding) parts. Both types of potentials are expressed via known potential energies of two isolated hydrogen atoms in the singlet and triplet states.

Key words: cryogenic, computer simulation, molecular dynamics, the melting point.

Е. Якуб

Плавление криокристаллов при высоких давлениях. Компьютерное моделирование

В данной работе использовались два типа моделирования методом молекулярной динамики: однофазный и двухфазный. Этими методами определялись температуры плавления сильно сжатых диатомных криокристаллов азота и водорода как функций давления. Твердый водород моделировался двумя приближениями – (1) неэмпирическое приближение атом-атомного потенциала (ААП) и (2) диатом-диатомное приближение. Уменьшение температуры плавления при высоком сжатии относится к возросшей роли нецентральных сил и молекулярной жесткости.

Ключевые слова: криокристалл, компьютерное моделирование, молекулярная динамика, температура плавления.

Е. Якуб

Жоғары қысымда криокристалдардың балқуы. Компьютерлік модельдеу

Бұл жұмыста молекулалық динамиканың модельдеуінің екі түрі қолданылды: бірфазалы және екіфазалы. Бұл әдістермен қатты қысылған қысым функциясы ретіндегі сутегінің және азоттың диатомды криокристалдарының балқу температурасы анықталды. Қатты сутегі екі жақындастырылумен (1) эмпирикалық емес атом-атомды потенциалдың (ААП) және (2) диатом-диатомды жақындастырылумен модельдендірілген. Жоғарғы қысыммен қысқанда балқу температурасының кішіреюі центрлік емес күштердің және молекулалық қаттылықтың рөлінің артуына жатады.

Түйін сөздер: криокристалл, компьютерлік модельдеу, молекулалық динамика, балқу температурасы.

Two types of molecular dynamics simulations: single-phase and two-phase carried out and applied to determine the melting temperatures of highly compressed diatomic cryocrystals: nitrogen and hydrogen, as functions of pressure. Solid hydrogen was modeled by two approximations (1) non-empirical atom-atom potential (AAP) approximation [1], and diatom-diatom (DDP) approximation. Within AAP-model potential energy of hydrogen molecules is represented as a function of interatomic distances between all atoms as a sum of intramolecular (bonding) and intermolecular

(non-bonding) parts. Both types of potentials are expressed via known potential energies of two isolated hydrogen atoms in the singlet and triplet states. In turn, singlet and triplet potential curves are well known from classical *ab initio*variational calculations.

DDP approximation is actually a more general version of AAP-model [2] which takes into account the overlap of electronic shells of two atoms forming a diatomic molecule. Within this approximation non-bonding short-range intermolecular interaction depends on instant distances between bonded atoms. Both AAP- and DDP-models were extended by inclusion of long-ranged quadrupole-quadrupole interaction. Interaction of nitrogen molecules was also described within AAP-model by the sum of semi-empirical atom-atom potentials and quadrupole-quadrupole contribution.

For both diatomic solids, at different sizes of simulation cells, we observed the same non-monotonous 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 [3] and known as turnover of the melting line, was reproduced first in our recent conventional single-phase molecular dynamics simulation of molecular hydrogen [4].

The same behavior of nitrogen, when polymerization transition ignored, is reported in this work. We discuss possible explanations of this turnover in absence of changes of interaction and chemical bonding, and analyze its dependence on the rigidity and the length of chemical bonds, structure of the solid phase, and analyze the role of long-range quadrupolar forces.

We conclude that turnover in the melting line observed in diatomic solids has a general reason. It can be explained on the basis of simple molecular models. The decrease of the melting temperature at high compressions is related to the increasing role of non-central forces and molecular rigidity. Energy stored in frustrated chemical bonds is released during melting and this effect becomes more pronounced at higher densities leading to the progressive decrease of the relative crystalline lattice stability, melting temperature and vibronic frequency. Inclusion of quadrupole-quadrupole interactions rises the melting temperature and affects both the nature of the molecular rotation in the solid phase and the type of the most stable crystalline structure.

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UDC 533.9.004.14; 621.039.6

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Molecular dynamics simulation of thermodynamic and transport properties of H-bonded low-temperature substances

The results of modeling of water clusters in nitrogen cryomatrix are presented. Earlier, our experimental studies of water in cryomatrix [1] have shown that changes in the concentration of an analyte in matrix leads to a splitting of the absorption bands characteristic frequencies of the molecules in the IR spectrum. Moreover the multiplicity of characteristic absorption bands in the IR spectrum remained unchanged during heating of the samples from the condensation temperature to the sublimation temperature of the matrix element.

Key words: molecular dynamics, hydrogen bond, cluster, matrix isolation.

А.Ж. Тыченгулова, А.У. Алдияров, А.С. Дробышев

Моделирование термодинамических и транспортных свойств водородосвязанных низкотемпературных веществ методом молекулярной динамики

В работе представлены результаты моделирования кластеров воды в криоматрице азота. В проведенных нами ранее экспериментах по изучению состояния воды в криоматрице было обнаружено влияние концентрации воды в матрице, приводящее к расщеплению полос поглощения характеристических частот молекул в ИК-спектре. Также в работе объясняется обнаруженная экспериментально стабильность образованных кластеров воды в матрице в процессе нагревания пленок вплоть до температуры испарения молекул матрицы. Обнаружено, что наиболее стабильным кластером молекул воды, образованным водородной связью, является пентамер.

Ключевые слова: молекулярная динамика, водородная связь, кластер, матричная изоляция.

А.Ж. Тыченгулова, А.У. Алдияров, А.С. Дробышев

Төмен температуралы сутекті байланысқан заттардың термодинамикалық және транспорттық қасиеттерін молекулалық динамика әдісі бойынша модельдеу

Жұмыста азот криоматрицасындағы судың кластерлерін модельдеу нәтижелері келтірілген. Біз бұрын жүргізген криоматрицадағы судың күйін зерттеу тәжірибелерінде ИҚ-спектрде молекулалардың сипаттамалық жиіліктерін жұтылу жолақтарының ыдырауына алып келетін матрицадағы судың концентрациясының әсері анықталды. Сонымен қатар, жұмыста матрицадағы судың қабықшаларды тіпті матрицаның булану температурасына дейін қыздыру кезінде түзілген тәжірибе жүзінде анықталған кластерлерінің тұрақтылығы түсіндіріледі. Сутекті байланыспен түзілген су молекуласының ең тұрақты кластері пентамер екені анықталды.

Түйін сөздер: молекулалық динамика, сутекті байланыс, кластер, матрицалық изоляция.

The results of modeling of water clusters in nitrogen cryomatrix are presented. Earlier, our experimental studies of water in cryomatrix [1] have shown that changes in the concentration of an analyte in matrix leads to a splitting of the absorption bands characteristic frequencies of the molecules in the IR spectrum. Moreover the multiplicity of characteristic absorption bands in the IR spectrum remained unchanged during heating of the samples from the condensation temperature to the sublimation temperature of the matrix element. In order to find out what the structure of clusters is

responsible for the immutability of the absorption bands in the vibrational spectrum during thermal cycling of the samples computer research of water molecules enclosed in nitrogen cryomatrix by the molecular dynamics simulation was conducted.

For this purpose, theoretical studies were carried out using computer software packages of HyperChem 8.1, that implement used by us semi empirical and ab initio molecular dynamics methods [2]. As a result of the research, the data must be obtained are of theoretical interest for summarizing the physico-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 [3].

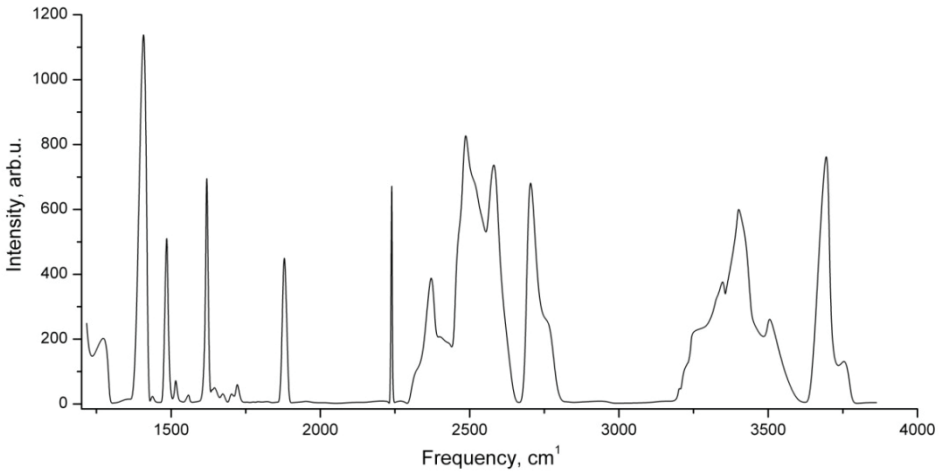

Figure 1 – Linear vibrational absorption spectrum of ice formed by 20 molecules at 16 K calculated in HyperChem using the PM3 method. Three intramolecular modes are preserved in ice, the bending vibration and the overlapped symmetric and asymmetric stretching vibrations and one intermolecular mode (librations).

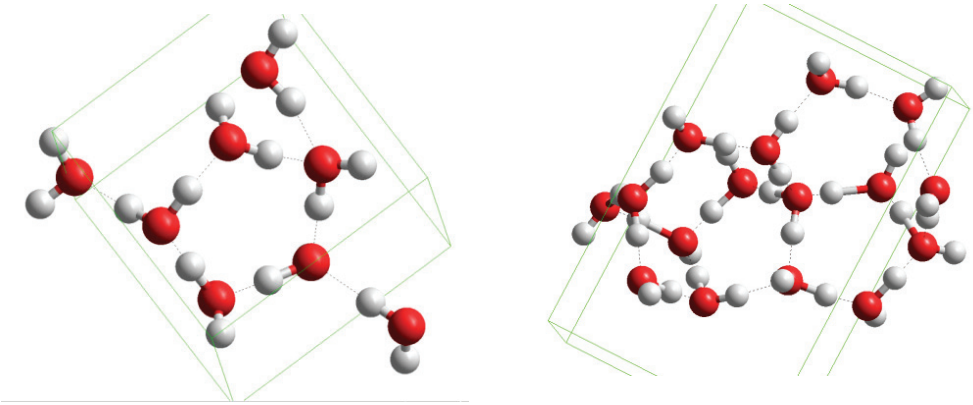

Figure 2 – Water pentamers

Calculations also showed that due to the ability of water molecules to form hydrogen bonds this system has a great variety of structures with substantially different binding energy and heat capacity. Most stable ring structures among them is pentamer ring structure shown in Figure 2, which has only one proton molecules involved in the formation of hydrogen bonds.

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UDC 533.9.004.14; 621.039.6

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Nanocluster impurity gels in superfluid He-II

We discuss here some results of our SANS studies of structure of the impurity-helium condensates, gel samples, prepared by condensation of the gas mixture 4He + 2% of the impurity (D_2, O_2, vapors of D_2O or C_2D_5OD) on the surface of superfluid He-II cooled below 1.8 K. The impurity nanoclusters covered by a layer of solidified He form the backbone (a dispersive system) of the gel, and liquid helium in the nanopores between the cluster aggregates serves as a dispersion medium.

Key words: superfluid helium, neutron scattering, nanocluster, cryocondensates.

Л.П. Межов-Деглин, В.Ф. Ефимов, А.В. Лохов, В.В. Несвихевский,
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Нанокластеры примесных гелей в сверхтекучем He-II

В данной работе обсуждены результаты наших исследований методом МНР (малоуглового нейтронного рассеяния) примесь-гелиевых конденсатов, образцов геля, приготовленных конденсацией газовой смеси 4He + 2% примеси (D_2, O_2, пары D_2O или C_2D_5OD) на поверхности сверхтекучего He-II, охлажденного до температуры ниже 1,8 К. Нанокластеры примеси, покрытые слоем твердого He, образуют основу (дисперсную систему) геля, а жидкий гелий в нанопорах между кластерными агрегатами служит дисперсной средой. Численная оценка характеристических размеров D_2O или C_2D_5OD кластеров в образце геля дает результат в диапазоне 10-15 нм.

Ключевые слова: сверхтекучий гелий, нейтронное рассеяние, нанокластер, криоконденсат.

Л.П. Межов-Деглин, В.Ф. Ефимов, А.В. Лохов, В.В. Несвихевский,
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Асқын аққыш He-II қоспалы гельдердің нанокластерлері

Бұл жұмыста АНШ (аз бұрышты нейтронды шашырау) әдісімен жасалған гелийлі конденсаттардың, 4He + 2% газ қоспасының конденсациясының 1,8 К төмен температураға дейін суытылған асқын аққыш He-II бетіне араластырылуымен (D_2, O_2, D_2O немесе C_2D_5OD булары) жасалған гель үлгілерін зерттеулеріміздің нәтижелері талқыланған. Қатты Не қабатымен жабылған нанокластерлер қоспалары гельдің негізін (дисперсті жүйені) құрайды, ал кластерлік агрегаттардың арасындағы наноқуыстардағы сұйық гелий дисперсті орта болып табылады. Гель үлгісінде D_2O немесе C2D5OD сипаттамалық өлшемдерін сандық бағалау 10-15 нм аралықта нәтиже береді.

Түйін сөздер: асқын аққыш гелий, нейтронды шашырау, нанокластер, криоконденсат.

We discuss here some results of our SANS studies of structure of the impurity-helium condensates, gel samples, prepared by condensation of the gas mixture ^{4}He + 2% of the impurity (D_2, O_2, vapors of D_2O or C_2D_5OD) on the surface of superfluid He-II cooled below 1.8 K. The impurity nanoclusters covered by a layer of solidified He form the backbone (a dispersive system) of the gel, and liquid helium in the nanopores between the cluster aggregates serves as a dispersion medium. From the results of the SANS measurements we found that the characteristic sizes of the D_2 or O_2clusters are distributed in a wide range from 100 to 1 nm. The numerical estimations for the characteristic sizes of

D_2O or C_2D_5OD clusters in the gel sample give the range of 10 – 15 nm.

The weakly connected impurity nanoclusters in bulk of the sample in He-II cooled below a few mK might be used for cooling of cold neutrons below the ultra-cold temperature level. The reasons for significant interplay between nanocluster condensate with slow neutrons are, on one hand, in an approximate equality of wavelength of the last and characteristic size of inhomogeneities in gels and, on another hand, relatively high cross-section of neutrons scattering on a backbone of the condensate. For example, we've observed strong changes in angular distribution of neutrons scattered on D2O sample of size 2.8 cm with variation in the neutron energy: At low energies $E < 0.5$ K neutrons show isotropic s-scattering, whereas the increase of neutron energy up to 5 K results in strongly anisotropic scattering where ~ 90% of neutron beam is scattered into the small angle of a few degrees.

A thick layer of a fine-grained ice powder, which is formed during the gel disintegration, could also be used as coverage of the inner walls of cold neutron guides to decrease the neutron losses.

From the numerical estimations it follows that the magnetic susceptibility of 100 nm-size oxygen clusters at temperatures below 2 K is enough high. In effect, and oxygen gel samples in He-II could form a magnetic structure in an external magnetic field $H > 200$ G, and this structure might be close to a ferromagnetic structure. This opens new opportunities for further studying of the impurity gel samples with the use of spin polarized neutrons.

UDC 533.9.004.14; 621.039.6

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On the equilibrium density of ions in raining clouds

On e of the debatable issues in meteorology is the source of enhanced ion density in storm clouds. This source is obviously related in some way to the density of rain drops in the storm cloud. It is also clear that all charging phenomena should involve free protons which are the highest mobility ions in the problem. Discussed in the present paper is the approach providing a nite ion density in the system of rain drops. The corresponding model for the storm cloud can be referenced as a "proton semiconductor" by analogy with electronic crystal semiconductors where charge is carried by light particles, i.e. electrons and holes.

Key words: ion density, charge phenomena semiconductor.

И. Чикина, В. Шикин

О равновесной плотности ионов в дождевых облаках

Одним из обсуждаемых вопросов метеорологии является источник повышенной плотности ионов в грозовом облаке. Данный источник, очевидно, относится в некоторой степени к плотности дождевых капель грозового облака. Также ясно, что во все зарядовые явления вовлекаются свободные протоны, которые являются наиболее подвижными ионами в задаче. Обсуждаемый в настоящей работе подход позволяет определить конечную плотность ионов в системе дождевых капель. Соответствующая модель грозового облака может рассматриваться как «протонный полупроводник» по аналогии с электронными кристаллическими полупроводниками, в которых заряд переносится легкими частицами, т.е. электронами и дырками.

Ключевые слова: плотность ионов, зарядовые явления, полупроводник.

И. Чикина, В. Шикин

Жаңбыр бұлттарындағы иондардың бірқалыпты тығыздықтары туралы

Метеорологияның көп талқыланатын сұрақтарының бірі найзағайлы бұлттың ионының тығыздығының жоғарылауының көзі болып табылады. Бұл көз, белгілі бір дәрежеде найзағайлы бұлттың жаңбыр тамшыларының тығыздығына да қатысты болып табылады. Барлық зарядталған құбылыстарға тапсырмадағы ең жылжымалы иондар болып табылатын еркін протондар еліктірілетіні де белгілі. Осы жұмыста талқыланатын тәсіл жаңбыр тамшыларының жүйесіндегі иондардың соңғы тығыздығын анықтауға мүмкіндік береді. Найзағайдың бұлтының сәйкес моделі заряд жеңіл бөлшектермен, яғни электрондармен және кемтіктермен тасымалданатын электронды кристалдық жартылай өткізгіштерге ұқсас «протонды жартылай өткізгіш» ретінде қарастырылуы мүмкін.

Түйін сөздер: иондардың тығыздығы, зарядтық құбылыстар, жартылай өткізгіш.

On e of the debatable issues in meteorology is the source of enhanced ion density in storm clouds. This source is obviously related in some way to the density of rain drops in the storm cloud. It is also clear that all charging phenomena should involve free protons which are the highest mobility ions in the problem. Discussed in the present paper is the approach providing a finite ion density in the system of rain drops. The corresponding model for the storm cloud can be referenced as a «proton

semiconductor» by analogy with electronic crystal semiconductors where charge is carried by light particles, i.e. electrons and holes [1].

1. The basic quantity involved in finding properties of the «proton semiconductor» is the water molecule ionization energy in the gas phase Evac. According to available literature [2], this energy is about

The thermal ionization probability for a molecule possessing this binding energy is practically zero, so that water vapor in a clean atmosphere could not be a source of any noticeable number of protons. However, the energy (1) proves to be quite suitable for use as the energy gap of an intrinsic proton semiconductor.

In the proton semiconductor model, water drops play the role of shallow donors capable of releasing free protons into the conduction band of doped semiconductor. A quantitative estimate is as follows. Just as in a gaseous media, the water molecule ionization reaction is exothermic requiring absorption of the energy from the heat bath. By simultaneously considering the free proton level positions on the same energy scale for both gaseous and liquid phases, one can easily discern all the basic semiconductor principles. This «proton semiconductor» is characterized by the intrinsic gap (1) donor energy level (2) within the forbidden band, bulk donor density nd equal to the rain drops density in the cloud, and the effective proton mass to be used in the semiconductor statistics [1] which has the scale of the free proton mass in vacuum. The donor ionization degree is calculated within the standard statistical methods [1].

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UDC 533.9.004.14; 621.039.6

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Application of impedance spectroscopy for studying of charged nanoclusters in impurity-helium condensates

A gas jet consisting of a mixture of helium and impurity (~ 1% of H_2, N_2, Ne, Kr, Xe, etc.) gases was directed onto the surface of superfluid helium (HeII) contained in the glass beaker. During condensation of the impurity particles in the bulk superfluid helium the so–called impurity–helium condensate is formed [1].

Recently in 2013, charges were detected for the first time during destruction of the nitrogen-helium samples [2]. For further investigations it was proposed to use methods of the impedance spectroscopy. We used a sensor of planar geometry with two conductive meanders (the sensor capacity was of 7.9 pF).

Key words: impedance spectroscopy, superfluid helium impurity-helium condensates.

А.А. Пельменев, Р.Е. Болтнев, И.В. Быхало, И.Н. Крушинская

Применение импедансной спектроскопии для изучения заряженных нанокластеров примесь-гелиевых конденсатов

Газовая струя, состоящая из смеси гелия и примеси (~ 1% of H_2, N_2, Ne, Kr, Xe, и т.д.), направляется на поверхность сверхтекучего гелия (He-II), находящегося в стеклянной мензурке. В процессе конденсации частиц примеси в объеме сверхтекучего гелия формируется так называемый примесь-гелиевый конденсат. Результаты работы подтверждают гипотезу о существовании заряда на стадии разрушения примесь-гелиевых образцов. Природа зарядов и механизмы их появления все еще остаются открытыми и требуют дальнейшего изучения.

Ключевые слова: импедансная спектроскопия, сверхтекучий гелий, примесь-гелиевый конденсат.

А.А. Пельменев, Р.Е. Болтнев, И.В. Быхало, И.Н. Крушинская

Импедансты спектроскопияны гелий-қоспалы конденсаттардың зарядталған нанокластерлерін зерттеу үшін қолдану

Гелийден және қоспалардан (~ 1% of H_2, N_2, Ne, Kr, Xe, және т.б.) тұратын газдық ағыс шыны мензуркада орналасқан асқын аққыш гелийдің (He-II) бетіне бағытталады. Қоспаның бөлшектерінің конденсация процесінде асқын аққыш гелийдің көлемінде гелий-қоспалы конденсат түзіледі. Жұмыстың нәтижелері гелий-қоспалы үлгілердің бұзылу сатысында зарядтың болуы туралы болжамды растайды. Зарядтардың табиғаты және олардың пайда болу механизмдері әлі де толық ашылмаған болып табылады және әрі қарай зерттеуді қажет етеді.

Түйін сөздер: импедансты спектроскопия, асқын аққыш гелий, қоспа-гелийлі конденсат.

A gas jet consisting of a mixture of helium and impurity (~ 1% of H_2, N_2, Ne, Kr, Xe, etc.) gases was directed onto the surface of superfluid helium (HeII) contained in the glass beaker. During condensation of the impurity particles in the bulk superfluid helium the so–called impurity–helium condensate is formed [1].

Recently in 2013, charges were detected for the first time during destruction of the nitrogen-helium samples [2]. For further investigations it

was proposed to use methods of the impedance spectroscopy. We used a sensor of planar geometry with two conductive meanders (the sensor capacity was of 7.9 pF). In the experiments the temporal dependencies of the impedance were carried out at frequencies of 2700 and 3000 Hz. The voltage amplitude was of 5 V.

Synchronously with lowering of helium level in the glass beaker, the sample shrinks and then destroys through explosions accompanied with current pulses and bright flashes. Simultaneously with explosions, temperature and pressure peaks, as well as resistance and capacitance jumps were observed.

These results support the hypothesis of charge existence at the stage the destruction of the impurity–helium samples. The nature of the charges and mechanisms of their appearance are still open questions and demand further study.

The measuring technique with use of the planar sensor has shown good performances and allowed to investigate the behavior of the impurity–helium samples in HeII as well as during their destruction processes.

The described construction of the sensor is very simple, easily reproducible and may be applied in investigations of low-temperature films, coats, and matrices.

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UDC 533.9.004.14; 621.039.6

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Turbulence on the surface of cryogenic liquids in restricted geometry of experimental cell

We report on results of experimental investigations of nonlinear phenomena on the surface of liquid hydrogen and helium. The experiments were carried out at temperature T=1.7 K for superfluid helium and at T=15 K for liquid hydrogen. Helium and hydrogen gases were condensed into the copper cup of inner diameter 30 mm (helium) and 60 mm (hydrogen) and depth 4 mm.

Key words: helium, hydrogen, low temperature kelvin.

Л.В. Абдурахимов, М.Ю. Бражников, Г.В. Колмаков, А.А. Левченко, И.А. Ремизов

Турбулентность на поверхности криогенных жидкостей в ограниченной геометрии экспериментальной ячейки

Мы сообщаем о результатах экспериментальных исследований нелинейных явлений на поверхности жидкого водорода и гелия. Эксперименты проводились при температуре Т=1,7 К при сверхтекучем гелии и при Т=15 К для жидкого водорода. Газы гелия и водорода конденсируются в медную чашку внутренним диаметром 30 мм (гелия) и 60 мм (водорода) и глубиной 4 мм.

Ключевые слова: гелий, водород, низкие температуры, кельвин.

Л.В. Абдурахимов, М.Ю. Бражников, Г.В. Колмаков, А.А. Левченко, И.А. Ремизов

Геометриясы шектелген тәжірибелік ұяшықтағы криогенді сұйықтардың бетіндегі турбуленттілік

Біз сұйық сутегінің және гелийдің бетіндегі бейсызық құбылыстардың тәжірибелік зерттеулерінің нәтижелерін баяндаймыз. Тәжірибелер асқын аққыш гелийде Т=1,7 К температурада және сұйық сутегі үшін Т=15 К температурада жүргізілді. Гелийдің және сутегінің газдары ішкі диаметрі 30 мм (гелийге) және 60 мм (сутегіге) және тереңдігі 4 мм мыс ыдысқа конденсирленеді.

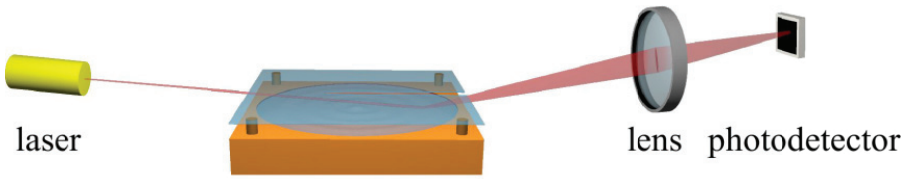
Түйін сөздер: гелий, сутегі, төмен температуралар, кельвин.

We report on results of experimental investigations of nonlinear phenomena on the surface of liquid hydrogen and helium. The experiments were carried out at temperature T=1.7 K for superfluid helium and at T=15 K for liquid hydrogen. Helium and hydrogen gases were condensed into the copper cup of inner diameter 30 mm (helium) and 60 mm (hydrogen) and depth 4 mm. The cup and a copper plate which has been fixed 4 mm above the cup form a flat capacitor. A Source of charges glued to the bottom of the cup ionizes liquid. The surface of liquid is charged with positive ions when DC voltage of about 1 kV is applied between the plates of capacitor. A low-frequency AC voltage applied in addition to the DC voltage excites waves on the charged surface of liquid. Waves are detected by means of a laser beam reflected from the surface of liquid and then focused into a photodetector. Variation of angle between the laser beam and the oscillating surface leads to the modulation of the power of reflected light $P(t)$. As we have shown earlier [1] the power spectrum P^2_ω, obtained by Fast Fourier Transformof the $P(t)$, is proportional to the spectrum of the pair correlation function of the surface elevation.

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 [2] 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 [3] 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.



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UDC 533.9.004.14; 621.039.6

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Unconventional phase transitions on HD and O_2 cryocrystals

Both HD and O_2 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.

Key words: phase diagram, pressure, sample, crystalline phase.

Ю. Креспо, А. Лайо, Г.Е. Санторо, М. Фабрицио, С. Скандоло, Е. Тосатти

Нетрадиционные фазовые переходы в HD и O_2 криокристаллах

Обе молекулы HD и O_2 твердых тел обусловлены хорошо изученной фазовой диаграммой при высоких давлениях. В этом докладе мы фокусируем внимание на двух необычных фазовых переходах, существующих при высоких давлениях. Первоначально мы изучим необычный, возвратный фазовый переход, на фазовой диаграмме HD образцов в окрестности 50 ГПа, где вращение обнаруживает «нарушение симметрии» кристаллической фазы, обусловленное превращением в «неупорядоченной» стадии высокой симметрии при охлаждении.

Ключевые слова: фазовая диаграмма, давление, образцы, кристаллическая фаза.

Ю. Креспо, А. Лайо, Г.Е. Санторо, М. Фабрицио, С. Скандоло, Е. Тосатти

Криокристалдардағы HD және O_2 дәстүрлі емес фазалық ауысулар

HD және O_2 қатты денелердің қос молекулалары жоғары қысымдағы жақсы зерттелген фазалық диаграммаға негізделген. Бұл баяндамада біз жоғары қысымда болатын екі ерекше фазалық ауысуларға назар аударамыз. Алдымен біз, HD үлгінің фазалық диаграммасындағы айналу («симметрияның бұзылуы») ауысуын зерттедік.

Түйін сөздер: фазалық диаграмма, қысым, үлгілер, кристалдық фаза.

Both HD and O_2 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 C_2/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 O_2 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.

UDC 533.9.004.14; 621.039.6

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Vacancy assisted flow of solid helium

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
Key words: helium, solid, temperature, low temperature

Дж. Бенедик, А. Калинин, П. Ниетто, Дж П. Тоенис

Содействие вакансии потоку твердого гелия

Идея, что твердый гелий может стать сверхтвердым веществом, предсказана Андреевым и Лившицем [1]. В 2004 г. Э. Ким, М. Чен начали широкую международную серию соответствующих исследований сверхтвердого вещества по методике экспериментально крутильных осцилляторов [2].
Ключевые слова: гелий, твердое тело, температурный режим, низкие температуры.

Дж. Бенедик, А. Калинин, П. Ниетто, Дж П. Тоенис

Бос орынның қатты гелийдің ағынына көмектесуі

Қатты гелий аса қатты зат болуы мүмкін деген идеяны Андреев және Ливщиц болжап айтқан болатын [1]. 2004 ж. Э. Ким, М. Чен халықаралық осы идеяға сәйкес зерттеулердің топтамасын жүргізген, аса қатты заттың айналатын тәжірибелік осцилляторлардың әдістемесі бойынша зерттеулер жүргізілген [2].
Түйін сөздер: гелий, қатты дене, температуралық режим, төменгі температуралар.

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 GalliandReatto 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 4He 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.

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UDC 533.9.004.14; 621.039.6

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Optical spectroscopy and current detection during warm-up and destruction of impurity-helium condensates

It is well known that deposition of rare gases (RG) passed through electrical discharge area onto a cold (~ 4 K) surface, or irradiation of cryofilms by energetic particles (electrons, protons, or photons with energies of 20 eV – 4 MeV) can cause formation and stabilization of neutral radicals and ions. Recent experiments have revealed ion currents accompanied by luminescence during destruction of nitrogen-helium condensates prepared by condensation of nitrogen-helium gas mixtures (after passing through a radio frequency RF discharge zone) into superfluid helium (HeII) bulk [1].

Key words: condensate, spectroscopy, cryocondensates surface.

И.Н. Крушинская, Р.Е. Болтнев, И. Б. Бухало, А.А. Пелменев, Б.Б. Хмеленко, Д.М. Ли

Оптическая спектроскопия и определение тока во время прогрева и разрушения примесь-гелиевых конденсатов

Хорошо известно, что осаждение благородных газов (Rg), прошедших через электрическую разрядную область на холодную (~ 4 К) поверхность, или облучение криопленок энергоемкими частицами (электроны, протоны, или фотонов, с энергией 20 эВ - 4 МэВ), может привести к формированию и стабилизации нейтральных радикалов и ионов. Недавние эксперименты показали, ионные токи, сопровождающиеся люминесценции в процессе распада азотно-гелиевых конденсатов, полученных конденсацией газовых смесей азот-гелий (после прохождения через зону радиочастотного ВЧ разряда) в сверхтекучий гелий (HeII) [1].

Ключевые слова: конденсат, спектроскопия, криоконденсат, поверхность.

И.Н. Крушинская, Р.Е. Болтнев, И. Б. Бухало, А.А. Пелменев, Б.Б. Хмеленко, Д.М. Ли

Оптикалық спектроскопия және қоспа-гелийлі конденсаттардың қыздырылуы және бұзылуы кезіндегі токты анықтау

Электрлік разрядталған аумақтан суық (~ 4 К) бетке өткен асыл газдарды (Rg) тұндыру немесе криоқабықшаларды энергия сыйымдылықты бөлшектермен (электрондар, протондар немесе фотондар, 20 эВ – 4 МэВ энергиямен) сәулелендіру бейтарап радикалдардың және иондардың қалыптасуына және тұрақтандырылуына алып келуі мүмкін екені жақсы белгілі.

Түйін сөздер: конденсат, спектроскопия, криоконденсат, бет.

Introduction

It is well known that deposition of rare gases (RG) passed through electrical discharge area onto a cold (~ 4 K) surface, or irradiation of cryofilms by energetic particles (electrons, protons, or photons with energies of 20 eV – 4 MeV) can cause formation and stabilization of neutral radicals and ions. Recent experiments have revealed ion currents accompanied by luminescence during destruction of nitrogen-helium condensates prepared by condensation of nitrogen-helium gas mixtures (after pass-

ing through a radio frequency RF discharge zone) into superfluid helium (HeII) bulk [1]. We present new experimental results on detection of optical spectra and ion currents during thermostimulated destruction of impurity-helium condensates (IHCs) prepared from nitrogen-argon-helium and nitrogen-xenon-helium gas mixtures.

Experimental Method and Results

The experimental technique of IHC sample preparation was first developed in 1974 [2]. It is based on the injection of a helium gas jet containing impurity particles (Im = N, N_2, H, H_2, Ne, Ar, etc.) into bulk HeII. A gas mixture enters a helium bath region from a quartz capillary cooled with liquid nitrogen inside an atom source. The lower portion of the capillary is surrounded by electrodes to produce an RF discharge (f = 40 MHz, P = 40-90 W). The typical conditions during sample preparation were as follows: the impurity admixture, [Im]/[He] ~ 0.5-1 %, the gas jet flux

(4.5-6)·1019 s-1, the HeII temperature 1.5 K, and the duration of the sample condensation 600-5000 s. The oxygen content in the gas mixtures is mainly a result of contamination of the helium gas. We employ helium gas with an oxygen content of ~ 10 ppm. A gas jet consisting of a mixture of helium and impurity gases was directed onto the surface of HeII contained in a glass beaker placed below the source at a distance of 20-35 mm. Calibrated Lake Shore thermometers were used for the temperature measurements. The sample emission was directly collected by an optical fiber fixed above an IHC sample in the beaker. The spectrometer AvaSpec-ULS2048XL-USB2 allowed us to detect luminescence within the spectral range from 200 to 1100 nm with resolution ~ 2.5 nm.

The spectra observed during destruction of impurity-helium condensates containing stabilized radicals reveal that all of the emitting particles are localized within solid matrices. The spectra of luminescence detected during the destruction of the second sample prepared from a gas mixture [N_2]/[Ar]/[He] = 1/10/1000 were changing on time. The dominance of emission due to species containing oxygen was explained by a multishell structure of impurity clusters: heavier particles (in this case O atoms) are involved in the reactions and the luminescence at the final stage of sample destruction when impurity clusters fuse together.

The luminescence spectra detected during destruction of the sample prepared from a gas mixture [Xe]/[N_2]/[He] = 1/10/2000 has revealed, for the first time, the spectra from molecules XeO*captured in N2 films surrounding the xenon cores of impurity nanoclusters.

The destruction of impurity-helium condensates containing stabilized radicals is accompanied with pressure and luminescence peaks, and current pulses (~ nA).

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UDC 533.9.004.14; 621.039.6

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Penetration of charges through the surface of water

The general goal of this project is experimental investigation of the properties of intrinsic (electric) The general problem of this project is experimental investigation of the properties of intrinsic (electric) carriers in water and development of statistics of liquid electrolytes by analogy with semiconductor statistics. in water and development of statistics of liquid electrolytes by analogy with semiconductor statistics.

Key words: Water surface charge, charge carrier semiconductor.

А.А. Левченко, Д.А. Храмов, В.Б. Шикин, А.М. Лихтер, В.А. Грязнова

Проникновение зарядов через поверхность воды

Общая цель исследований данной работы состоит в экспериментальном обнаружении внутренних электрических свойств, присущих (электрическим) носителям в воде, и изучении развития статистики жидких электролитов по аналогии со статистикой полупроводника.

Ключевые слова: вода, поверхность, заряд, носитель заряда, полупроводник.

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Зарядтардың судың беті арқылы енуі

Бұл зерттеулердің жалпы мақсаты, жалпы мәселесі судағы тән (электрлік) тасымалдаушыларды және сұйық электролиттердің аналогия бойынша жартылай өткізгіштің статистикасымен тәжірибелік анықтау болып табылатын ішкі электрлік қасиеттерді тәжірибе жүзінде анықтау болып табылады.

Түйін сөздер: су, бет, заряд, заряд тасымалдаушы, жартылайөткізгіш.

The general goal of this project is experimental investigation of the properties of intrinsic (electric) The general problem of this project is experimental investigation of the properties of intrinsic (electric) carriers in water and development of statistics of liquid electrolytes by analogy with semiconductor statistics. in water and development of statistics of liquid electrolytes by analogy with semiconductor statistics. The most apparent argument in favor of such development is the absence of the concept of intrinsic electrolyte and, specifically, an agreed definition of «doped electrolyte» properties (by analogy with intrinsic semiconductivity in crystalline media [1]) in modern thermodynamics of electrolyte (see [2,3]) which is important for development of the whole statistics of weakly charged liquid. The proposed set of problems with the general title «Screening properties of pure water» specifies the concept of intrinsic electrolyte by the example of water and provides a practical opportunity to understand its typical features. Such media exhibit a spontaneous probability of nucleation of proton-hydroxyl pairs initiated by the presence of an external field. This property whichis not found in thermodynamics of electrolyte (implying the known Oswald law [2, 3]) is «identity card» of vacuum states: spontaneous nucleation of electron- positron pairs in electromagnetic vacuum [4]; occurrence of «electron-hole» pairs in vacuum of solid [4] or liquid pure solvents; pair excitations in lattice vacuum of ion (molecular) crystals [5]. Some of the observed effects of proton-hydroxyl instability of pure water in external field is discussed and checked both theoretically and experimentally within the framework of the Project.

Experimental studies of penetration of positive charges through a nitrogen-gas/water interface

have been carried out. 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, Fig.1. 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. At voltages above U = 900V surface water discharge is observed: at the instant of breakdown a 10^{-10} coulomb charge Q arrives onto the upper plate, Fig.2. The discharge process reoccurs with a period depending on applied voltage U. The observed periodic surface charge-discharge cycles point to time reproducibility of carriers in the liquid volume.

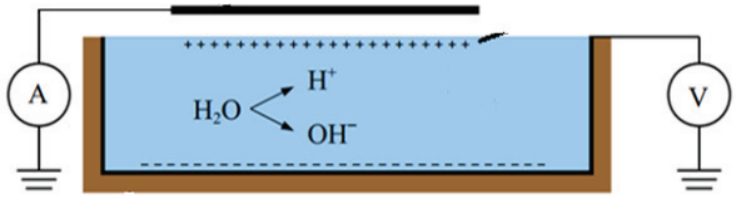

Figure 1 – V– voltage source, A– electrometer

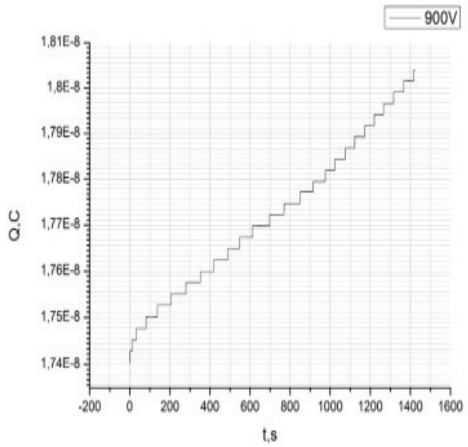

Figure 2

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UDC 533.9.004.14; 621.039.6

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Phase diagram of polymerizing nitrogen – a theoretical prediction

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.

Key words: Nitrogen, the phase diagram, the pressure polymerization.

Л.Н. Якуб

Диаграмма полимеризации азота – теоретическое предсказание

Полимеризация молекул азота как в твердых, так и жидких фазах, которая была обнаружена в динамических и статических экспериментах и предсказана в неэмпирических моделированиях, стимулирована обсуждением новой конфигурации фазовой диаграммы азота при высоких давлениях. Рассмотрим фазовую диаграмму высокого давления твердого азота, который уже давно обсуждается в теоретических исследованиях, и только в последнее десятилетие начали исследовать экспериментально.

Ключевые слова: азот, фазовая диаграмма, давление, полимеризация.

Л.Н. Якуб

Азоттың полимеризациясының диаграммасы – теориялық болжам

Динамикалық және статикалық тәжірибелерде анықталған және эмпирикалық емес модельдеуде болжамдалған азот молекулаларының қатты, сонымен қатар сұйық фазалардағы полимерленуі жоғары қысымдағы азоттың фазалық диаграммасының жаңа конфигурациясының талқылануымен негізделген. Қатты азоттың жоғары қысымдағы бұрыннан теориялық зерттеулерде талқыланған және тек соңғы онжылдықта тәжірибе жүзінде зерттеліп басталған фазалық диаграммасын қарастырайық.

Түйін сөздер: азот, фазалық диаграмма, қысым, полимерлену.

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 work 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 polymeric CG-crystalline phase (modified Mie-Grueneisen equation), were calibrated on available ab initio data. The proposed modification of the Mie-

Grüneisen equation for solid polymeric nitrogen [1] based on the Monte Carlo computer simulation data describes negative thermal expansion and significant deviations of heat capacity from the Dulong-Petit law in CG-phase.

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.

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. It was found that this qualitative difference is closely related to the negative thermal expansion of CG-polymeric solid. Both P-T dependences of transition of molecular solid into polymeric CG-phase and on the melting line of CG-solid have negative slopes due to its negative thermal expansion.

The predicted volume jump on the transition from the molecular to the polymeric phase is in good agreement with experimental data of. The predicted location of the triple point of polymeric nitrogen in the pressure range of 80-100 GPa, is also consistent with available experimental data.

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UDC 533.9.004.14; 621.039.6

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Phonon spectrum and vibrational characteristics of l inear nanostructures in solid m atrices

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.

Key words: Matrix nanostructure crystal structure of amorphous.

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Фононный спектр и колебательные характеристики линейных наноструктур в твердых матрицах

В настоящее время структуры с одномерным или квази-одномерным включением в различных кристаллических или аморфных матрицах привлекают внимание исследователей. В реальных отношениях между взаимодействиями атомов встроенных квазипериодических систем друг с другом и с атомами матрицы особенности, присущие одномерным системам, могу появиться в спектрах квазичастиц этих структур.

Ключевые слова: матрица, наноструктуры, кристалл, аморфная структура.

И.А. Господарев, Е.В. Манжелей, К.А. Минакова, Е.С. Сыркин, С.Б. Феодосьев

Қатты матрицалардағы сызықты наноқұрылымдардың тербеліс сипаттамалары және фононды спектр

Қазіргі уақытта әртүрлі кристалл немесе аморфты матрицаларға бірөлшемді немесе квазибірөлшемді қосылған құрылымдар зерттеушілердің назарын аударып отыр. Кіріктірілген квазипериодты жүйелердің атомдарының бір-бірімен және матрица атомдарымен өзара әрекеттесуінің шынайы қатынастарында бірөлшемді жүйелерге тән ерекшеліктер осы құрылымдардың квазибөлшектерінің спектрлерінде пайда болуы мүмкін.

Түйін сөздер: матрица, наноқұрылымдар, кристалл, аморфты құрылым.

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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UDC 533.9.004.14; 621.039.6

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Photoelectric emission from gas solids

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.

Key words: photoemission, solid gas, free electrons

Ю. А. Дмитриев

Фотоэлектрические выбросы от газовых тел

Фотоэмиссии электронов из редких твердых газов (РГО) получают, используя ВУФ источников открытого разряда. Температурные зависимости от поля измеряются путем записи поглощения ECR свободных электронов, испускаемых с поверхности RGS.

Ключевые слова: фотоэмиссия, твердый газ, свободные электроны

Ю. А. Дмитриев

Газдық денелерден фотоэлектрлік шығарылулар

Сирек қатты газдардан электрондардың фотоэмиссиясын ВУК ашық разрядты көздерін пайдаланып алады. Өрістен температуралық тәуелділіктер RGS бетінен шығарылатын ECR еркін электрондардың жұтылу жазбалары өлшенеді.

Түйін сөздер: фотоэмиссия, қатты газ, еркін электрондар.

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 HeI 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, Ea(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.

UDC 533.9.004.14; 621.039.6

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Physical modeling of the formation of the clathrate hydrates of methane

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.

Key words: hydrate, methane clathrate, energy.

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Физическое моделирование формирования клатратов гидратов метана

В настоящее время природные газовые гидраты привлекают особое внимание как возможный источник ископаемого топлива. По разным оценкам, запасы углеводородов в газовых гидратах значительно превышают разведанные запасы природного газа.

Ключевые слова: гидрат, метан, клатрат, энергетика.

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Метан гидратының клатраттарының қалыптасуын физикалық модельдеу

Қазіргі кезде табиғи газ гидраттар қазбалы отынның мүмкін көзі ретінде ерекше назар аудартып отыр. Әртүрлі бағалаулар бойынша газды гидраттардағы көмірсулардың қорлары барланған табиғи газдың қорынан асып отыр.

Түйін сөздер: гидрат, метан, клатрат, энергетика.

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 temperatures T=(12-60) K and pressures P=(10^{-4}-10^{-6}) Torr. Methane concentration in water varied in the range of 5-90%. 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. According to the comparison of thermal desorption curves and changes in the absorption amplitude of characteristic frequencies of methane vibrations, we made some assumptions relatively the state of methane molecules in the «matrix» of water. We assume, that under these conditions cryoprecipitated methane in solid solution with water can exist in three states. The most significant and interesting temperature ranges are the following:

1. Temperature range from 30 K to 58 K – is the range of solid methane evaporation. This assumption is consistent with the values of methane equilibrium parameters (pressure, temperature) on the phase diagram.

2. Temperature range from 60 K to 130 K – is the range of decrease in the adsorption capacity of amorphous water film at higher temperatures.

3. Temperature range from 130 K to 145 K – is the range of the restructuring of solid phase from water – amorphous state (ASW) through the intermediate state super cold liquid (SCL) to cubic ice [2].

4. In the range from 145 to 160 K the methane concentration in the sample is almost stable. At these high temperatures, methane can exist in the film only in bound state with water, namely in the form of clathrates. Increase of the temperature above 160 K leads to a decrease of methane concentration, which is connected with the transition of cubic ice I_c to regular hexagonal state I_h, which is apparently accompanied by a partial destruction of the clathrates. Narrow temperature range of 172-176 K with constant values of the methane concentration is related with the existence of hexagonal ice containing methane clathrates. Further increase in the temperature leads to evaporation of water film with simultaneous change of methane concentration. The fact that methane evaporates from the sample together with water confirms methane clathrates presence in the samples.

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UDC 533.9.004.14; 621.039.6

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Portable dedvices for cryosurgery and therapy

Cryosurgery is a surgical technique that employs freezing to destroy undesirable tissue. Although the prefix "cryo" (from the Greek word "kruos" for cold) usually refers to temperatures below 120K, cryosurgery deals with temperatures below the freezing temperature of tissue, i.e. about 273K.

Key words: Cryosurgery, appliance, malignant tissue.

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Портативные приборы для криохирургии и терапии

Криохирургия и принцип хирургической техники направлен на заморозку и уничтожение нежелательных тканей живых организмов. Хотя префикс «крио» (от греческого слова «kruos» для холодной) обычно относится к температуре ниже 120 К, для криохирургии с температурой ниже температуры замерзания ткани, т.е. о 273 К.

Ключевые слова: криохирургия, прибор, злокачественные ткани.

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Криохирургияға және терапияға арналған портативті құралдар

Криохирургия және хирургиялық техниканың принципі тірі организмдердің қалаусыз ұлпаларын жоюға және мұздатуға бағытталған. «Крио» қосымшасы (гректің «kruos» суық үшін сөзінен) әдетте 120К төмен температураға қатысты болады, криохирургия үшін ұлпаның қату температурасынан төмен, яғни 273К жуық болады.

Түйін сөздер: криохирургия, құрал, қатерлі ұлпалар.

Cryosurgery is a surgical technique that employs freezing to destroy undesirable tissue. Although the prefix «cryo» (from the Greek word «kruos» for cold) usually refers to temperatures below 120K, cryosurgery deals with temperatures below the freezing temperature of tissue, i.e. about 273K. The history of cryosurgery is relatively short and is closely intertwined with developments in low temperature physics, engineering and instrumentation that were made during the last century. Thus, cryosurgery appears to advance in jumps triggered by immediately preceding technological advances and now it is a fast growing minimally invasive surgical technique. Low temperature damage in cells can be divided into damage produced by three effects: low temperature; direct effects of freezing; and indirect effects of freezing. The study of life at low temperatures and the study of life at low water contents have some features in common. This is because, in environmental freezing, one of the major causes of damage is freezing induced dehydration.

Introduction of the cryogenic methods of treatment into the practice of municipal outpatient clinics in our countries restrains lack of simple and reliable portable cryoinstruments. In this regard a series of original portable apparatus for different application in cryosurgery and cryotherapy was designed in the ISSP RAS in close cooperation with the surgical clinicians. The series includes contact cryodestructors with the changeable active finger

cooling with liquid nitrogen, which is storing in a special can, simple cryoapplicators with active metal tips cooled preliminary in liquid nitrogen, nitrogen cryosprays. According to the recommendation of the Ministry of Health RF any prototypes of this devices were transferred for approbation to clinics of Moscow and Moscow region. The report includes some results of the test examinations in model surroundings including biological objects as well as of the approbation in real conditions of a few Moscow clinics.

Cryosurgery, sometimes referred to as cryotherapy or cryoablation, is a surgical technique in which freezing is used to destroy undesirable tissues A review of the history of the field will show that.

UDC 533.9.004.14; 621.039.6

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Properties of dilute weak charged solutions

A neutral donor dissociation into charged fragments typical of electrolytes is one of the reversible reactions satisfying the law of mass action (LMA) [1]. Its application to weak electrolytes results into the formula (Ostwald law) for an important characteristic of the electrolyte, its ionization degree [1, 2].

Key words: Electrolyte solution ionization.

В. Шикин

Свойства разбавленных слабо заряженных растворов

Диссоциация нейтральных доноров на заряженные фрагменты типичных электролитов является одной из обратимых реакций, удовлетворяющих закону действия масс (LMA) [1]. Применение слабых электролитов для получения результатов с помощью формулы (закон Оствальда) является важной характеристикой электролита, показывает его степень ионизации [1, 2].

Ключевые слова: электролит, раствор, ионизация.

В. Шикин

Сұйылтылған әлсіз зарядталған ерітінділердің қасиеттері

Диссоциацияның қарапайым электролиттердің зарядталған бөліктеріне бейтарап доноры масса әрекеттерінің заңын қанағаттандыратын қайтымды реакциялардың бірі болып табылады (LMA) [1]. Әлсіз электролиттерде формуладағы (Оствальд заңы) нәтижені алу үшін электролитті қолдануда маңызды сипаттама оның иондалу дәрежесі болып табылады [1, 2].

Түйін сөздер: электролит, ерітінді, иондалу.

A neutral donor dissociation into charged fragments typical of electrolytes is one of the reversible reactions satisfying the law of mass action (LMA) [1]. Its application to weak electrolytes results into the formula (Ostwald law) for an important characteristic of the electrolyte, its ionization degree α [1, 2].

$$K(T) = \alpha^2 C/1 - \alpha. \qquad (1)$$

The ionization degree α is defined as the ratio of the number of ionized donors to the total number of neutral donor molecules, K(T) is the ionization constant which does not depend on C, but strongly depends on temperature T.In the extreme case $C \to 0$ Eq.(1) yields

$$\alpha(C)_{C\to 0} \to 1 \qquad (2)$$

Along with Eqs. (1) and (2) which illustrate the tendency of an individual donor towards complete ionization, there also exist alternative statements. One of them, formulated as the Thomas-Fermi approximation for a single many-electron atom, demonstrates the possibility of the existence of statistically equilibrium confinement of Z electrons by a nucleus containing Z protons [3]. This is also confirmed by the well-known statistically equilibrium Yukawa-type solution to the Poisson equation for a single Coulomb center screened within the electrolyte by counter-ions at the Debye length [1]. Both cases address the properties of a single donor (acceptor) in vacuum or within the intrinsic electrolyte, i.e. exactly the limit (2) with quite the opposite behavior of

$$\alpha(C)_{C\to 0} \to 0. \qquad (3)$$

The present paper provides a detailed discussion of the properties of dilute weak charged solutions in the limit $C \to 0$, settling, among others issues, the indicated alternative between (2) and (3).

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UDC 533.9.004.14; 621.039.6

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Pseudo-rotational motion of cyclic molecules and thermal conductivity of tetrahydrofuran

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), C4H8O, 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

Key words: amplitude, angular forces cyclic molecules.

В.А. Константинов, В.В. Саган, В.П. Ревякин и А.В. Карачевцева

Псевдо-вращательное движение циклических молекул и теплопроводности в тетрагидрофуране

Псевдовращение – движение, которое возникает при постоянном волнообразном движении кольца и стягивает моды в присутствии небольшого барьера на плоскостности молекул. Псевдовращения в тетрагидрофуране (ТГФ), C4H8O, возникают вблизи аннулированных угловых сил деформации вследствие валентных углов в скелете кольца и скручивающих нагрузок из-за отталкивания водород – водорода.

Ключевые слова: амплитуда, угловые силы, циклические молекулы.

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Тетрагидрофурандағы жылуөткізгіштіктің және молекулалардың циклдік жалған-айналатын қозғалысы

Жалған-айналыс, молекула кеңістігінде үлкен емес кедергі жағдайында пайда болатын қайта қалпына келу әсерлесулері болмаса сақина кеңістігінен тыс қозғалыс болып табылады [1]. Тетрагидрофурандағы (ТГФ) жалған айналыс, C4H8O, сақина қаңқасындағы валентті бұрыштардың бұрыштық күштердің салдарынан деформациялануынан немесе сутегі- сутегі [2-3] арасындағы иірілген күштердің арасындағы тебінулер салдарынан пайда болады.

Түйін сөздер: амплитуда, бұрыштық күштер, циклдік молекулалар.

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 C_2/c with 4 molecules in the unit cell) and melts at 164.9 K with a large entropy change on melting $\Delta Sf/R$=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 TD 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 κ_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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UDC 533.9.004.14; 621.039.6

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Quantum effects in the kinetics of ^{3}He, ^{4}He, H_2 and D_2sorption by bundles of single-walled carbon nanotubes

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 kinetics of gas desorption was investigated on a powder of SWNT bundles compacted into plates under P=1.1 GPa.

Key words: nanotubes, carbon, desorption kinetics.

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Квантовые эффекты в кинетике ^{3}He, ^{4}He, H_2 И D_2, захваченных пучками одностенных углеродных нанотрубок

Была исследована низкая температура кинетика сорбции ^{3}He, ^{4}He, H_2 и D_2 газов пучками одностенных углеродных нанотрубок (нанотрубок) и последующей десорбции этих газов из нанотрубок пучков. Кинетику десорбции газа исследовали на порошке нанотрубок пучков, запрессованных в пластины под P = 1,1 ГПа.

Ключевые слова: нанотрубки, углерод, десорбция, кинетика

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Кинетикадағы ^{3}He, ^{4}He, H_2 И D_2 түйінделген бірқабырғалы көміртекті нанотүтікшелердің квантты эффектілері

Төменгі температурадағы ^{3}He, ^{4}He, H_2 И D_2 түйінделген бірқабырғалы көміртекті нанотүтікшелердің десорбция құбылысы қарастырылды. Газ десорбциясының кинетикасын нанотүтікшелердің ұнтағымен зерттелінді, пластина P = 1,1 ГПа қысымымен престелген.

Түйін сөздер: нанотүтікшелер, көміртек, десорбция, кинетика.

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 kinetics of gas desorption was investigated on a powder of SWNT bundles compacted into plates under P=1.1 GPa. The starting powder consisted of closed SWNTs having two basic diameters 1.02-1.06 and 1.69-1.72 nm. The SWNTs in the sample had metallic conductivity. One of the plates of mass 0.07g was heated stepwise to T=500^0 C in dynamic vacuum (~ 10^{-3}Torr) and kept in it for eight hours. This technique allowed us to remove the residual gases from the sample and hence open the ends of the SWNTs. The other plate unaffected by heat pretreatment was irradiated with γ-quanta of ^{60}Co with the dose $1.6\cdot10^7$ rad. The SWNT ends therefore remained closed (c- SWNTs). The irradiation procedure was performed at room temperatures in the H_2 gas medium under the at-

mosphere pressure. This permitted us to increase significantly the rate of radiation defect generation in the SWNTs [1]. The kinetics of gas sorption and desorption was investigated using the technique detailed in [2].

The characteristic times of the sorption-desorption processes coincide within the experimental error. The 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 lowest activation energy was obtained for He isotopes in o- SWNTs (186 K). It was higher (212 and 224 K) for H_2 and D_2 molecules, respectively. The highest value (E_a=336 K) was measured on c-SWNTs irradiated with γ-quanta of ^{60}Co. This high E_a characterizes the H_2 desorption through the barriers at the ends of the interstitial channels of the bundles in which the tube surfaces have radiation-induced defects.

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 have introduced a crossover temperature T_0 below which the quantum correction contributes significantly to the activation energy desorption. The temperature T_0 is a linear function of the inverse mass of the gas molecule, which is consistent with theory [3].

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UDC 533.9.004.14; 621.039.6

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Quantum rotor in solid gases: matrix effects on EPR

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.

Key words: Quantum rotor matrix, radical chemical reaction

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Квантовый ротор в плотных газах: матричные эффекты по ЭПР

Наше исследование имеет дело с метил радикалом – простым органическим радикалом, который часто наблюдается в переходном промежуточном виде в химических реакциях. Следовательно, он был широко изучен как теоретически, так и экспериментально в течение многих десятилетий.

Ключевые слова: квант, ротор, матрица, радикал, химическая реакция.

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Тығыз газдардағы квантты ротор: ЭПР бойынша матрицалық эффектілер

Біздің зерттеуде метил радикалдарымен қарапайым органикалық байланыспен қатысты, ол көп жағдайда химиялық реакциялардың екі өту аралығында байқалады. Демек, көптеген онжылдықтар аралығында ол кеңінен теориялық және эксперименттік тұрғыда зерттелінді.

Түйін сөздер: Квант, ротор, матрица, радикал, химиялық реакция.

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.

Figure 1 evidences how closely the simulation based on the rotation model matches the experimental results. In our simulation, we started from the axially symmetrical *A* and *g*-tensor measured for CH_3 in N_2. Solid Ar and N_2 have near similar physical parameters: lattice structure, lattice constant, polarizability of the matrix particles. This similarity provides nearly equal EPR parameters, *A*- and *g*-tensors, for the trapped rigid CH_3 radical. The main exception between matrices is that the

solid N_2 is a matrix with orientation ordering and, thus, fixes the methyl radical three-fold axis at a certain direction. In that case, the radical is allowed to perform fast rotation about this axes (parallel rotation), while the reorientation about the in-plane axes (perpendicular rotation) is prohibited. As a result, the EPR spectrum takes a characteristic lineshape, Figure 2.

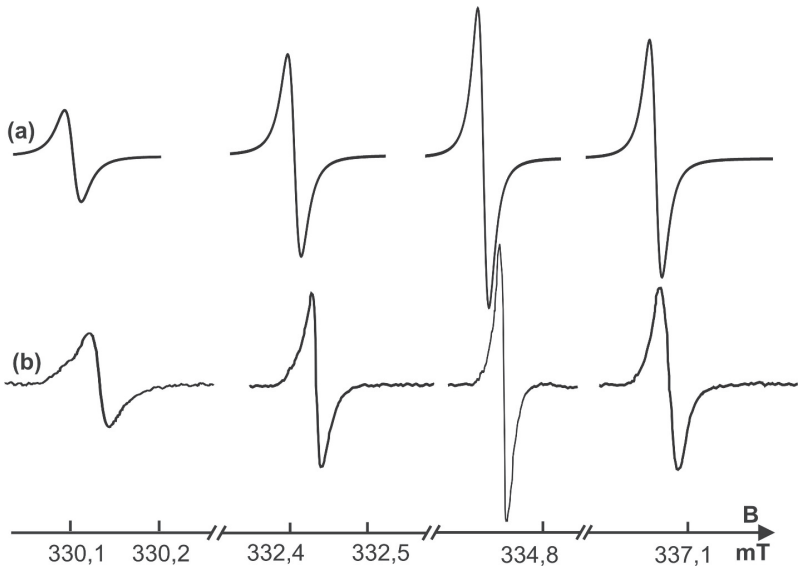

Figure 1. EPR spectrum of CH_3 in solid Ar. (a) an *EasySpin* simulation with parameters as follows: $A_{\perp} = -2.350\,\text{mT}$, $A_{//} = -2.252\,\text{mT}$, $g_{\perp} = 2.00262$, $g_{//} = 2.00225$, $\tau_{\perp} = 14\,\text{ns}$, $\tau_{//} = 1\,\text{ps}$. Here, $\tau_{\perp}$ and $\tau_{//}$ are correlation rimes for the perpendicular and parallel rotations, respectively (see the text for detail). (b) the experimental spectrum for CH_3 in solid Ar at 4.2 K.

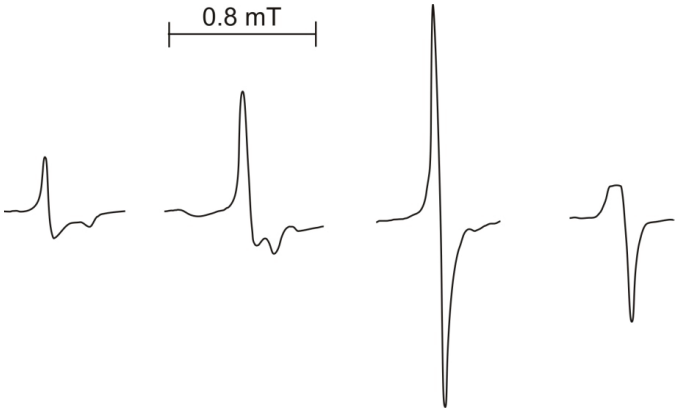

Figure 2 – Axially symmetrical EPR spectrum for CH_3 in solid CO obtained at 4.2 K. This spectrum is characteristic of CH_3 in matrices with orientation ordering, N_2, CO, N_2O, CO_2.

If a slow perpendicular rotation is allowed, the spectrum lineshape transforms into that one depicted in Figure 1.

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.

UDC 533.9.004.14; 621.039.6

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Relaxation processes in a week solution of cryocondensed water, heavy water and ethanol with nitrogen and argon

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-componentsolid solution of ethanol and nitrogen. This article considers the results of continued research in this direction.

Key words: cryomatrix isolation, a weak solution, temperature, evaporation

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Релаксационные процессы в слабых растворах криоконденсатов воды, тяжелой воды и этанола в матрице азота, аргона

Более ранние исследования устойчивости молекул этанола в криоматрице азота показали, что состояние иммобилизованных молекул этанола в матрице не является стабильным [1]. Незначительное повышение температуры матрицы, задолго до ее испарения, приводит к изменению колебательных спектров в двухкомпонентном растворе этанола и азота.

Ключевые слова: Криоматричная изоляция, слабый раствор, температура, испарение.

А. Дробышев, Алдияров, К. Катпаева, Е. Коршиков,
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Су, ауыр су және азот пен аргон матрицаларының криоконденсаторлар әлсіз ерітінділеріндегі релаксациялық үрдістер

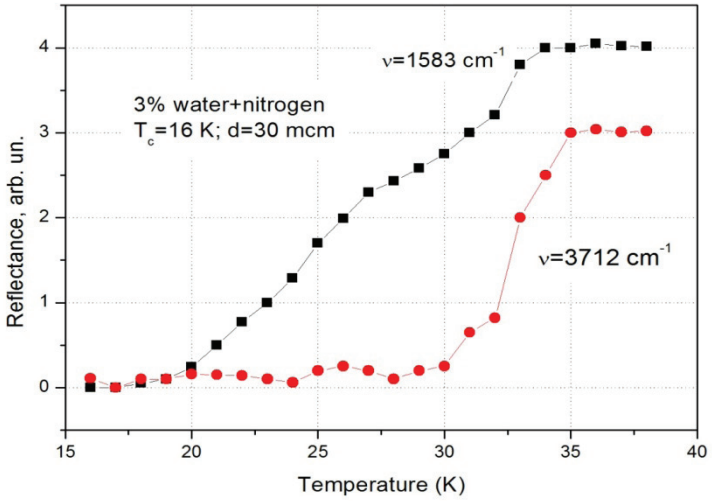
Ертеректе жасалған зерттеулер көрсеткендей, азот криоматрицасындағы этанол молекуласындағы орнықтылығы, иммобилизацияланған этанол молекулаларының азот матрицасында тұрақты емес екендігі көрсетілді [1]. Матрицадағы температураның өзгеруі этанол және азот қоскомпонентті қоспаның тербелмелі спектрлерінің өзгеруіне әкеліп соғады.

Түйін сөздер: криоматрицалық оқшаулау, әлсіз ерітінді, температура, булану.

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-componentsolid 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 connectedwith the next molecules by intermolecular interaction. As a result theyexist 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 correspondto monomers and linear dimer of water and ethanol.An increasing temperatureof 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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UDC 533.9.004.14; 621.039.6

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The standardization and certification procedures of cryogenic equipmentin Kazakhstan

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.

Key words: cryogenic equipment, regulations, standards.

А. Шинбаева, А. Дробышев

Процедура стандартизации и сертификации криогенного оборудования в Казахстане

Создание Единого экономического пространства и функционирования в рамках ЕврАзЭС промышленных предприятий требует формирования общей базы нормативных документов в государствах-членах Союза. Учитывая всю возрастающую роль криогенных технологий в промышленном развитии ведущих мировых держав, необходимо провести соответствующий набор мероприятий, нормативно обеспечивающих это занятие.

Ключевые слова: криогенное оборудование, нормативные документы, стандарт.

А. Шинбаева, А. Дробышев

Қазақстандағы криогенді құрылғыларды стандарттау және сертификаттау рәсімдері

Бірыңғай экономикалық кеңістіктің құрылуымен және ЕврАзЭС жиектері бойынша өндірістерде іске асыру үшін ортақ нормативтік құжаттар базасы жасалуы керек. Криогенді технологиялардың өндірісте дамуына сәйкес, қажетті сәйкесінше шаралар ұйымдастырылып, оған қажетті нормативті тәртіптерді орындау қажет.

Түйін сөздер: криогенді құрылғылар, нормативті құжаттар, стандарт.

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.

Procedure of certification represents in written confirmation of compliance of the equipment by authorized body to the requirements established in normative documents (Gosstandart) and consists of the following actions:

1. Application by the applicant in certification authority.

2. Direction to the applicant of the decision on results of consideration of the declaration form. This decision goes to the applicant to 2-week time.

3. Registration of the contract between the applicant and certification authority on work on certification of the equipment. The issued contract goes to the applicant to 2-week time in duplicate.

4. Carrying out selection, identification of samples of the declared equipment and their representation in test laboratory (center). Selection is made by certification authority on a contractual basis. Selection can be made and the applicant by appointment of the competent commission as a part of not less than 3 people from among representatives of the uninterested organizations

5. In necessary cases the body for certification can charge sampling of the accredited test commission.

6. The test laboratory (center) carries out to the terms of test of samples of the declared equipment coordinated with certification authority and sends its results issued in the form of the protocol to body for certification.

7. The analysis of the received results and making decision on possibility of issue of the certificate of conformity.

8. At negative results of test, at least on one of indicators, test for the purpose of certification stop.

Issue of the certificate of conformity and its registration in the State register of GSS of the Republic of Kazakhstan. At positive results of the performed works as the provided scheme of the declared equipment, the certification authority makes out the Certificate of conformity.

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UDC 533.9.004.14; 621.039.6

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Theed study of Ar – Kr equimolar alloy morphology

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.

Key words: Gas mixtures, low temperatures, the binary system.

В.В. Данчук, Н.С. Мисько, А.А. Солодовник, М.А. Стржемечный

Исследование Ar – Kr эквимолярной морфологии сплава

Твердые бинарные смеси криокристаллов представляют значительный интерес по многим причинам [1]. Это возможность сравнить экспериментальные результаты с теоретическими предсказаниями. По теоретической модели газовых бинарных сплавов, предложенных Пригожиным [2], должны выделяться в чистых компонентах ниже температуры 40 К. Эта критическая температура зависит от концентрации и максимума для эквимолярного решения.

Ключевые слова: газовые смеси, низкие температуры, бинарные системы.

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Ar – Kr қоспасының эквимолярлы морфологиясын зерттеу

Криокристалдардың қатты бинарлы қоспалары көптеген себептермен қызығушылық тудырады [1]. Олардың бірі, әрдайым эксперименттен алынған нәтижені теориямен салыстыра алатындығын. Теориялық үлгі бойынша бинарлы қоспалардың, Пригожинның ұсынысымен [2] таза күйінде 40 К төмен температурада ғана бейнеленуі керек. Бұл критикалық нүкте эквимолярлық шешімнің концентрациясымен максимумына тәуелді.

Түйін сөздер: газ қоспалары, төменгі температуралар, бинарлы жүйелер.

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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UDC 533.9.004.14; 621.039.6

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Thermal conductivity of donor-doped GaN – investigations with 3-ωand stationary metods

Gallium nitride due to its unique optical properties and therefore possible applications has been attracting much attention of researchers for over one decade. Thermal conductivity is of interest as a key parameter in the design of high-power devices in which gallium nitride is an important element.

Key words: Thermal conductivity, donor doping.

О. Чурикова, А. Ежовский, П. Стаховиак, Ж. Муча, П. Перлин, Т. Суски, В. Трзибятоски

Теплопроводность доноров легированного GaN - исследования с 3-ω and стационарным методом

Нитрид галлия благодаря своим уникальным оптическим свойствам и, следовательно, возможности применения привлекает большое внимание исследователей более одного десятилетия. Теплопроводность представляет интерес в качестве ключевого параметра в разработке мощных устройств, в которых нитрид галлия важным элементом.

Ключевые слова: теплопроводность, донор, легирование.

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Қосындыланған GaN донорлар жылуөткізгіштігін 3-ω and стационарлық әдіспен зерттеу

Соңғы онжылдықта галлий нитриді өзінің бірегей оптикалық қасиеттерінің арқасында көп қызығушылық тудырды. Галлий нитриді негізгі рөлді атқаратын қуатты құрылғылардың жылуөткізгіштігі бірінші қызығушылық болып табылады.

Түйін сөздер: жылуөткізгіштік, донор, қосындылау.

Gallium nitride due to its unique optical properties and therefore possible applications has been attracting much attention of researchers for over one decade. Thermal conductivity is of interest as a key parameter in the design of high-power devices in which gallium nitride is an important element.

The investigated here samples were prepared byammonothermal method. The thermal conductivity of bulk crystals was measured over the temperature range 4–300K with stationary state heat flow method while the measurements of the thermal conductivity of GaN thin layers was carried out in the temperature range 50 – 320K by 3-omega method. For the later, on the surface of the investigated sample a special electrically conductive pattern featuring a temperature-dependent resistance is prepared. During the measurement the pattern acts both as a heater to create a temperature oscillations and as a sensor to measure the sample's thermal response. An electric current of angular frequency ω flows through the pattern resulting in heating the surface of the sample at frequency 2ω. The appearing signal of frequency of 3ω is measured with a lock-in amplifier. The thermal conductivity of the investigated sample is being obtained from the frequency dependence of the signal.

The value of the thermal conductivity coefficient of three investigated bulk 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} 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. In considering the effect of the oxygen dopant on thermal conductivity of GaN crystal the following three effects were taken into account and discussed:

• additional scattering of phonons by oxygen atoms which replace the original nitrogen atom in gallium nitride structure (Rayleigh scattering of phonons)

• enhancement of the thermal conductivity due to increase of concentration of electrons in the conduction band

• additional scattering of phonons by the extra free electrons. 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)

UDC 533.9.004.14; 621.039.6

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Thermal stability of metallic nanowires and microspheres

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.

Key words: superfluidity, impurity nanotubes

Евгений Б. Гордон

Термическая стабильность металлических нанопроволок и микросфер

Квантованные вихри в сверхтекучем гелии являются идеальным одномерным шаблоном для роста продуктов конденсации каких-либо примесей, взвешенных в HeII только по сердцевине вихря. Тем не менее мы продемонстрировали невозможность в случае с металлом подготовки цепочки отдельных атомов или молекул.

Ключевые слова: сверхтекучесть, примесь, нанопроволка.

Евгений Б. Гордон

Металды наносымдар мен микросфералардың темиялық тұрақтылығы

Асқынаққыш гелийдегі квантты құйындар кез келген қоспаның өсуіне идеалды үлгі болып табылады. Дегенмен, біздің зерттеуіміз бойынша жекелеген атомдар мен молекулаларда бұл тізбектің орындалмай қалуын көрсеттік.

Түйін сөздер: асқынаққыштық, қоспа, наносым.

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 Tm = 1570C exhibit long term stability, while the silver nanowires (Tm = 9600C) 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.

UDC 533.9.004.14; 621.039.6

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Thermally stimulated transformations in thin films of cryovacuum condensates of methane

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.

Key words: Methane, spin, thin film condensation.

А. Дробышев, А. Алдияров, Ж. Нурекеев, А. Тыченгулова

Термостимулированные преобразования в тонких пленках криовакуумных конденсатах метана

Твердый метан принадлежит к группе кристаллов, которые содержат молекулы водорода, чьи макроскопические свойства (тепловое расширение, и т.д.) в значительной степени вызваны спиновым взаимодействием ядер водорода.

Ключевые слова: метан, спин, тонкие пленки, конденсат.

А. Дробышев, А. Алдияров, Ж. Нурекеев, А. Тыченгулова

Криовакуумды метан конденсаттарындағы жұқа үлдірлерде болатын термоынтандырылған түрленулер

Қатты метан құрамында сутегі ядроларының спиндік әсерлесулерінің арқасында (жылулық кеңею және т.б.) қасиеттері өзгерген сутегісі бар кристалдар тобына жатады.

Түйін сөздер: метан, спин, жұқа үлдір, конденсат.

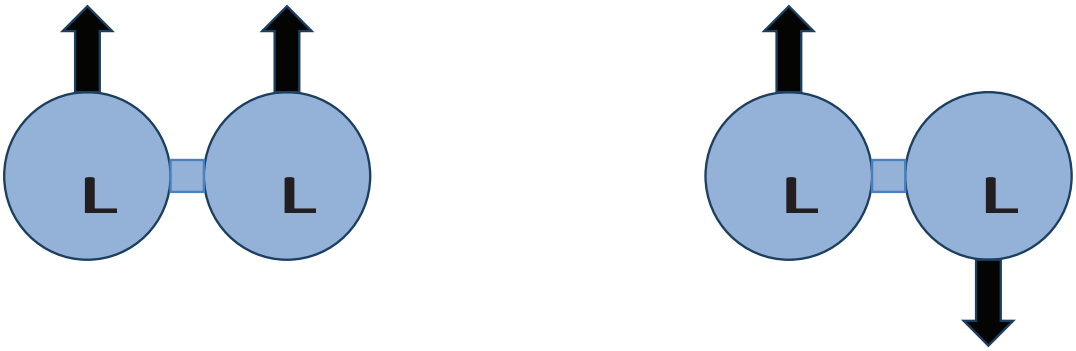
Solid methane belongs to a group of crystals which contains molecules of hydrogen, whose macroscopic properties (thermal expansion, etc.) are greatly caused by spin interaction of nucleus of hydrogen. In particular, the methane molecule, which has four protons with spin I = 1/2, has three total spin 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 existence of solid methane is an object of the research the last 40 years [1, 2].

After this our experimental results will be shown. Despite its simplicity from the point view of organic chemistry, molecule of methane is a quantum object. We have carried out researches of gas hydrates as they are potential energy sources. In the course of research of thin films of methane cryocondensates we have found unusual optical properties in IR-range.

Molecules that possess equivalent nuclei exhibit different nuclear spin states. Well-known case is the nuclear spin isomers of hydrogen molecule. Hydrogen molecule with the nuclear spin number 1 is called orthohydrogen, and those with nuclear spin number 0 is called parahydrogen (Fig.1).

Our object of study is methane molecules. Methane has 4 equivalent nuclei. And spin numbers of isomers are 2, 1 and 0. Last 30-40 years methane has been actively studied. We focus on thin films of

methane at high vacuum. There is an equilibrium of concentrations between nuclear spin states. According to Yuki Miyamoto ratio of concentrations at 4K is 0:1:9. If isomers at equilibrium, and then we change the temperature, isomers will strive to the new equilibrium. This striving process is called nuclear spin conversion. Relaxation time can vary within wide range (Fig.2)..



OrthohydrogenI = 1 ParahydrogenI = 0

Figure 1 – Nuclear spin isomers of H_2

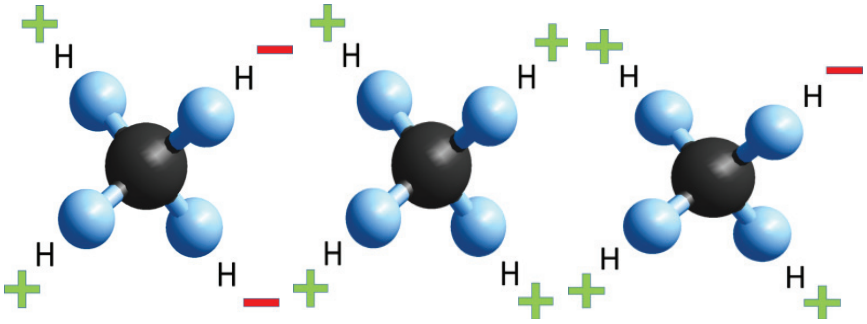


Figure 2

Here you can see some possible transitions between energy levels. It shows us couplings between rotational states and nuclear spin states. Also vibrational states and spin states are coupled according to Mr. Nijman. It is possible due to spin-phonon interaction.

Changing in the position of absorption band of methane cryocondensateslibration varying thickness. Condensation temperature is T = 16 K.

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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UDC 533.9.004.14; 621.039.6

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Unconventional phase transitions on hd and O_2cryocrystals

Both HD and O_2 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 (BSP) surprisingly transforms into a rotationally "disordered" high-symmetry phase upon cooling.

Key words: phase diagram, pressure, sample, crystalline phase.

Ю. Креспо, А. Лайо, Г.Е. Санторо, М. Фабрицио, С. Скандоло, Е. Тосатти

Нетрадиционные фазовые переходы в HD и O_2 криокристаллах

Обе молекулы HD и O_2 твердых тел обусловлены хорошо изученной фазовой диаграммой при высоких давлениях. В этом докладе мы фокусируем внимание на двух необычных фазовых переходах, существующих при высоких давлениях. Первоначально мы изучим необычный, возвратный фазовый переход на фазовой диаграмме HD образцов в окрестности 50 ГПа, где вращение обнаруживает «нарушение симметрии» кристаллической фазы, обусловленное превращением в «неупорядоченной» стадии высокой симметрии при охлаждении.

Ключевые слова: фазовая диаграмма, давление, образцы, кристаллическая фаза.

Ю. Креспо, А. Лайо, Г.Е. Санторо, М. Фабрицио, С. Скандоло, Е. Тосатти

HD және O_2 криокристалдарындағы дәстүрлі емес ауысулар

HD және O_2 молекулалары, қатты денелерде жоғарғы қысымда жақсы зерттелінген. Бұл мақалада жоғарғы қысымда бақыланған, ерекше екі фазалық ауысуға зейін салып отырмыз. Ең алғашқыда қайтымды ерекше HD диаграммасындағы үлгілерді зерттедік.

Түйін сөздер: фазалық диаграмма, қысым, үлгілер, кристалдық фаза.

Both HD and O_2 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 (BSP) 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. Herein we have applied path integral Monte Carlo (PIMC) within both the constant-volume and constant-pressure ensembles to the reentrant phase diagram of the HD solid at high pressures and low temperatures, considering both hcp (realistic) and fcc (fictitious) lattices. We studied the influence of the potential chosen, the translational degrees of freedom, and the choice of the electronic quadrupolequadrupole (EQQ) interaction potential on the BSP transition line. It was found that while the translational degrees of freedom have a small effect on the transition pressure, the choice of lattice and interaction potential strongly affects the transition pressure. Using a metadynamics based MC scheme, we found that a C_2/c ordered structure, containing 16 molecules per cell is, with the best available potentials, energetically preferred for the classical

BSP phase on an hexagonal closed packed (hcp) lattice.

Successive implementation of quantum molecular rotations by PIMC permitted a full calculation of the reentrant BSP-rotationally symmetric phase line. The transition was identified using two order parameters, one dependent on the new structure and the second related to the total quadrupolar moment of the molecule, particularly sensitive to the rotational state of the molecule. The phase line was calculated for both the hcp and the face centered cubic (fcc) lattices, yielding a realistic reentrant behavior in both cases. The best results are obtained with the Burton potential on the hcp lattice, with features of the BSP-symmetric coexistence line in good agreement with experiment.

The orientationally ordered state edge was found at a minimum pressure Pe≈ 56 GPa for the hcp lattice and the Cui-Burton potential, quite close to the experimental value Pe= 53 GPa and in much better agreement than the previous PIMC calculations, which gave Pe= 10 GPa. The edge point temperature Te= 25K is also in good agreement with the experimental one Te= 30 K. Finally, the entropy jump at the phase transition is found to have a maximum value below but not far from ln[2], in agreement with a Pomeranchuk-like, entropy-driven picture of the reentrant transition.

CONTENTS

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