B. Verkin Institute for Low Temperature
Physics and Engineering
The National Academy of Sciences of Ukraine

Council of Young Scientists of
B.Verkin Institute for Low Temperature Physics
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# VII International Conference for Young Scientists

# LOW TEMPERATURE PHYSICS

## Conference Program
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## Abstracts book

6-10 June 2016 Kharkiv

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**VII International Conference for Young Scientists**

**"LOW TEMPERATURE PHYSICS - 2016"**

**6 - 10 June 2016**


# Conference Program

# &

# Book of Abstracts

**Kharkiv 2016**

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# CONFERENCE PROGRAM

## MONDAY, 6 JUNE

**8:00-10:00** **Registration**

**10:00-10:15** **OPENING OF THE CONFERENCE**
**Opening remarks from the Administration of the B.Verkin ILTPE NAS of Ukraine**

***CONFERENCE HALL*** **PLENARY LECTURES OF INVITED SPEAKERS**

*Chair* *Mariia Pashchenko*

**10:15-10:55** **MAGNETIC EXITATIONS IN SPIN-1/2 TRIANGULAR-LATTICE ANTIFERROMAGNETS: HIGH-FIELD ESR STUDIES** **42**
S. A. Zvyagin
*Dresden High Magnetic Field Laboratory (HLD) Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany*

**10:55-11:30** ***General Photo and Coffee Break***

***CONFERENCE HALL*** **MAGNETISM AND MAGNETIC MATERIALS**

*Chair* *Tatyana Gaydamak*

**11:30-11:45** **MULTIFERROIC $PrFe_3(BO_3)_4$: STRONG ELECTRON-PHONON COUPLING IN AN EXTERNAL MAGNETIC FIELD PROBED BY TERAHERTZ SPECTROSCOPY** **71**
K. N. Boldyrev[1], M. N. Popova[1], T. N. Stanislavchuk[2], D. Kamenskyi[3], L. N. Bezmaternykh[4]
*[1] Institute of Spectroscopy, Russian Academy of Sciences, Moscow, Russia*
*[2] Department of Physics, New Jersey Institute of Technology, Newark, USA*
*[3] High Field Magnet Laboratory, Radboud University, Nijmegen, The Netherlands*
*[4]Kirensky Institute of Physics, Krasnoyarsk, Russia*

**11:45-12:00** **CLASSIFICATION OF DEGENERATE EQUILIBRIUM STATES OF MAGNETS WITH THE SPIN S=1** **72**
A. V. Glushchenko, M. Yu. Kovalevsky
*Kharkov Institute of Physics and Technology, Kharkiv, Ukraine*

**12:00-12:15** **SPECTRA OF COLLECTIVE EXCITATIONS AND LOW FREQUENCY ASYMPTOTICS OF GREEN'S FUNCTION FOR SPIN S=1 MAGNETICS** **73**
A. V. Glushchenko[1], M. Y. Kovalevsky[1], L. V. Logvinova[2], V. T. Matskevych[1]
*[1]National Science Center "Kharkov Institute for Physics and Technologies", Kharkiv, Ukraine*
*[2]Belgorod State University, Belgorod, Russia*

**12:15-12:30** **MAGNETIC PROPERTIES OF SUPERCONDUCTING NANOSTRUCTURES BASED ON INDIUM IN VARIOUS POROUS DIELECTRICS** **74**

N. Yu. Mikhailin[1,2], V. I. Kozub[1], Yu. A. Kumzerov[1], R. V. Parfeniev[1], A. A. Sysoeva[1], A. V. Fokin[1], D. V. Shamshur[1]
[1]*Ioffe Physical-Technical Institute, Saint-Petersburg, Russia*
[2]*International Laboratory of High Magnetic Fields and Low Temperatures, Wroclaw, Poland*

**12:30-12:45** **DOMAIN WALL MOTION IN MAGNETIC HELICES UNDER ACTION OF RASBHA TORQUE** **75**

O. V. Pylypovskyi[1], D. D. Sheka[1], V. P. Kravchuk[2], K. V. Yershov[2,3], D. Makarov[4], Y. Gaididei[2]
[1]*Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
[2]*Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, Kyiv, Ukraine*
[3]*National University of "Kyiv-Mohyla Academy", Kyiv, Ukraine*
[4]*Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Dresden, Germany*

**12:45-13:00** **REORIENTATION PHASE TRANSITION IN PERMALOY SPHERICAL SHELL** **76**

M. I. Sloika[1], D. D. Sheka[1], V. P. Kravchuk[2], Y. B. Gaididei[2]
[1]*Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
[2]*Bogolyubov Institute for Theoretical Physics, Kyiv, Ukraine*

**13:00-13:15** **CURRENT DRIVEN DOMAIN WALL MOTION IN MAGNETIC HELIX** **77**

K. V. Yershov[1,2], V. P. Kravchuk[1], D. D. Sheka[3], Y. Gaididei[1]
[1]*Bogolyubov Institute for Theoretical Physics of NAS of Ukraine, Kyiv, Ukraine*
[2]*National University of «Kyiv-Mohyla Academy», Kyiv, Ukraine*
[3]*Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*

**13:15-14:00**  ***Time for Lunch***

## *CONFERENCE HALL* PLENARY LECTURES OF INVITED SPEAKERS

*Chair* *Denis Laptev*

**14:00-14:40** **EXOTIC MAGNETIC PHASES IN FRUSTRATED $J_1$-$J_2$ CHAIN MAGNET $LiCuVO_4$** **40**

L. E. Svistov
*P.L. Kapitza Institute for Physical Problems RAS, Moscow, Russia*

**14:40-15:20** **FERROMAGNETIC RESONANCE: APPLICATION FOR STUDY OF MAGNETIC SHAPE MEMORY ALLOYS** **32**

V. O. Golub
*Institute of Magnetism NAS of Ukraine and MES of Ukraine, Kiev, Ukraine*

## *CONFERENCE HALL* THEORY OF CONDENSED MATTER PHYSICS

*Chair* *Denis Laptev*

**15:20-15:35** **ELECTROMAGNETIC WAVE ABSORBTION AND SURFACE PLASMON PROPAGATION IN A DOUBLE LAYER GRAPHENE SYSTEM WITH ELECTRON-HOLE PAIRING** **181**
K. V. Germash, D. V. Fil
*Institute for Single Crystals of NAS of Ukraine, Kharkiv, Ukraine*

**15:35-15:50** **SHUTTLE INSTABILITY INDUCED BY TEMPERATURE GRADIENT** **182**
O. A. Ilinskaya
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**15:50-16:05** **OPTIMAL EFFICIENCY OF THERMOELECTRICS BASED ON THERMOMAGNETIC EFFECT IN TUNNELING OF SPIN-POLARIZED ELECTRONS THROUGH A QUANTUM DOT IN EXTERNAL MAGNETIC FIELD** **183**
Yu. D. Zubov[1], O. A. Ilinskaya[2]
*[1] V.N. Karazin Kharkiv National University, Kharkiv, Ukraine*
*[2]B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**16:05-16:20** **INVESTIGATION OF STRUCTURAL AND ELECTRONIC PROPERTIES OF BN COMPOUND UNDER HIGH PRESSURE: AN AB-INITIO MOLECULAR DYNAMICS STUDY** **184**
C. Kurkcu, H. Ozturk
*Ahi Evran University, Faculty of Arts and Sciences, Department of Physics, Kirsehir, Turkey*

**16:20-16:35** **JOSEPHSON EFFECTS IN ATOMTRONIC CIRCUITS** **185**
O. Y. Matsyshyn[1], Y. M. Bidasyuk[2], M. Weyrauch[2], A. I. Yakimenko[1]
*[1]Department of Physics, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
*[2]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany*

**16:35-16:50** **REALIZATION OF COMPOSITE FERMION TYPE (QUASI) PARTICLES BY DEFORMED FERMIONS. ENTANGLEMENT MEASURES** **186**
Yu. A. Mishchenko, A. M. Gavrilik
*Bogolyubov Institute for Theoretical Physics of NAS of Ukraine, Kyiv, Ukraine*

**16:50-17:05** **MODELING OF KINETICS OF THE MATERIALS FRAGMENTATION MODES AT SEVERE PLASTIC DEFORMATION** **187**
A. V. Khomenko, D. S. Troshchenko, I. O. Solonar
*Sumy State University, Sumy, Ukraine*

**17:05-18:00** **POSTER SESSION I**

# TUESDAY, 7 JUNE

## *CONFERENCE HALL* — PLENARY LECTURES OF INVITED SPEAKERS

*Chair* *Mariia Pashchenko*

**10:00-10:40** **TRANSPORT PROPERTIES IN SUPERCONDUCTING HYBRID NANOSYSTEMS** **29**

A. Braggio[1,2]
[1]*CNR-SPIN Dipartimento di Fisica, Genova (Italy)*
[2]*INFN, Sezione di Genova, Dipartimento di Fisica, Genova (Italy)*

**10:40-11:20** **ABRIKOSOV FLUXONICS IN WASHBOARD NANOLANDSCAPES** **30**

O. V. Dobrovolskiy[1,2], M. Huth[1], V. A. Shklovskij [2]
[1] *Physikalisches Institut, Goethe University, Frankfurt/M, Germany*
[2] *Physics Department, V. N. Karazin National University, Kharkiv, Ukraine*

**11:20-11:40** *Coffee Break*

## *CONFERENCE HALL* — ELECTRONIC PROPERTIES OF CONDUCTING AND SUPERCONDUCTING SYSTEMS

*Chair* *Valentin Koverya*

**11:40-11:55** **PSEUDOGAP AND FLUCTUATION CONDUCTIVITY IN $Y_{1-X}Pr_XBa_2Cu_3O_{7-\delta}$ SINGLE CRYSTALS WITH DIFFERENT PRASEODYMIUM (Pr) CONTENT** **45**

L. V. Omelchenko[1], A. V. Solovjov[1], R. V. Vovk[2]
[1]*B. Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*
[2]*Physics Department, V.N. Karazin Kharkiv National University, Kharkiv, Ukraine*

**11:55-12:10** **SPECIFIC FEATURES OF THE EXCESS CONDUCTIVITY AND PSEUDOGAP BEHAVIOR IN $FeSe_{0.94}$ IRON-BASED SUPERCONDUCTORS** **46**

E. V. Petrenko[1], V. B. Stepanov[1], A. L. Solovjov[1], K. Buchkov[2], E. Nazarova[2]
[1]*B. Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*
[2]*Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria*

**12:10-12:25** **INFLUENCE OF ALTERNATING MAGNETIC FIELD ON PHYSICAL AND MECHANICAL PROPERTIES OF CRYSTALS** **47**

V. I. Karas[1,2], E. V. Karasyova[1], A. V. Mats[1], V. I. Sokolenko[1], A. M. Vlasenko[1], V. E. Zakharov[3,4]
[1]*National Science Center «Kharkov Institute of Physics and Technology», Kharkiv, Ukraine*
[2]*V.N. Karazin Kharkiv National University, Kharkiv, Ukraine*
[3]*P.N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia*
[4]*L.D.Landau Institute for Theoretical Physics of the Russian Academy of Sciences, Chernogolovka, Russia*

**12:25-12:40** **PECULIARITIES OF AVALANCHES DYNAMICS OF MAGNETIC FLUX IN HARD SUPERCONDUCTORS** **48**
E. I. Kuchuk
*O.O. Galkin Donetsk Institute for Physics and Engineering of NAS of Ukraine, Kyiv, Ukraine*

**12:40-12:55** **SPIN-CURRENT INDUCED SWITCHING BETWEEN STATES OF THE NONCOLLINEAR ANTIFERROMAGNET IrMn** **49**
V. Kuchkin[1], O. Gomonay[1,2]
[1]*National Technical University of Ukraine "KPI", Kyiv, Ukraine*
[2]*Institut fur Physik, Johannes Gutenberg Universitat at Mainz, Mainz, Germany*

## *SMALL CONFERENCE HALL* BIOPHYSICS AND PHYSICS OF MACROMOLECULES

*Chair* *Valentyna Zobnina*

**11:40-11:55** **EFFECT OF DIVALENT CATIONS ON THE PROTON TRANSPORT IN ISOLATED ERYTHROCYTE** **149**
D. F. Astapovich, V. P. Berest
*V. N.Karazin Kharkiv National University, Kharkiv, Ukraine*

**11:55-12:10** **PHARMACEUTICAL INTERACTIONS IN MODEL LIPID BILAYERS BY MEANS OF DIFFERENTIAL SCANNING CALORIMETRY** **150**
L. V. Budianskaia, O. V. Vashchenko
*Institute for Scintillation Materials of NAS of Ukraine, Kharkiv, Ukraine*

**12:10-12:25** **LUMINESCENCE ENHANCEMENT FROM CARBON NANOTUBES INDUCED BY THIOL COMPOUNDS** **151**
N. V. Kurnosov, V. S. Leontiev, V. A. Karachevtsev
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**12:25-12:40** **CORRELATION OF SOME MOLECULAR PARAMETERS OF BIOLOGICALLY RELEVANT SUBSTANCES AND THEIR EFFECT ON MODEL LIPID MEMBRANES** **152**
A. O. Sadchenko, O. V. Vashchenko, N. A. Kasian
*Institute for Scintillation Materials of NAS of Ukraine, Kharkiv, Ukraine*

**12:40-12:55** **COMPARISON OF NONCOVALENT INTERACTIONS OF LINEAR HETEROCYCLIC ORGANIC MOLECULES WITH CARBON NANOTUBES OR WITH GRAPHENE** **153**
E. S. Zarudnev, S. G. Stepanian, V. A. Karachevtsev
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**13:00-14:00**  ***Time for Lunch***

**14:00-15:00**  ***LAB TOUR***

## *CONFERENCE HALL* PLENARY LECTURES OF INVITED SPEAKERS

*Chair* *Valentyna Zobnina*

**15:00-15:40** **ONE-MOLECULE SHOW: NOVEL APPLICATIONS OF METHYLENE BLUE DYE IN PHARMACOLOGY AND NANOBIOPHYSICS** **34**
M. V. Kosevich
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

## *CONFERENCE HALL* ELECTRONIC PROPERTIES OF CONDUCTING AND SUPERCONDUCTING SYSTEMS

*Chair* *Valentin Koverya*

**15:40-15:55** **SOLITON DYNAMICS IN AN ASYMMETRIC ARRAY OF JOSEPHSON JUNCTIONS** **50**
I. O. Starodub, Ya. O. Zolotaryuk
*Bogolyubov Institute for Theoretical Physics of NAS of Ukraine, Kiev, Ukraine*

**15:55-16:10** **SUPERCONDUCTING VORTEX ORBITS VISUALIZED BY SCANNING TUNNELING MICROSCOPY** **51**
T. Samuely[1], M. Timmermans[2], D. Lotnyk[1], B. Raes[2], J. Van de Vondel[2], V.V. Moshchalkov[2]
[1]*Centre of Low Temperature Physics, Faculty of Science, P.J. Šafárik University in Košice, Slovakia*
[2]*Institute for Nanoscale Physics and Chemistry (INPAC), KU Leuven, Belgium*

**16:10-16:25** **THE EFFECT OF SINTERING IN DIFFERENT ATMOSPHERE ON SUPERCONDUCTIVITY PARAMETERS OF YBCO** **52**
M. Başoğlu[1], İ. Düzgün[2]
[1]*Gümüşhane University, Department of Energy Systems Engineering, Gümüşhane, Turkey*
[2]*Gümüşhane University, Department of Physics Engineering, Gümüşhane, Turkey*

**16:25-16:40** **EFFECT OF Dy SUBSTITUTION AT Ca SITES IN BSCCO CERAMIC SUPERCONDUCTORS** **53**
İ. Düzgün[1], A. Öztürk[2] and S. Çelebi[2]
[1]*Gümüşhane University, Department of Physics Engineering, Gümüşhane, Turkey*
[2]*Karadeniz Technical University, Department of Physics, Trabzon, Turkey*

**16:40-16:55** **JOSEPHSON EFFECT IN GRAPHENE JUNCTIONS** **54**
P. P. Shyhorin, I. P. Dmytruk and Yu. Datsiuk
*Lesya Ukrainka East European National University, Lutsk, Ukraine*

## *SMALL CONFERENCE HALL* BIOPHYSICS AND PHYSICS OF MACROMOLECULES

*Chair* *Valentyna Zobnina*

**15:40-15:55** **INFLUENCE OF FREEZING DOWN TO -196°C ON STRUCTURE AND ANTIOXIDANT POWER OF SEVERAL PROTEINS** **154**
S. V. Narozhnyi, S. L. Rozanova, O. A. Nardid
*Institute for Problems of Cryobiology and Cryomedicine, Kharkiv, Ukraine*

**15:55-16:10** **THE VIBRATIONAL SPECTRA OF 5-FLUOROURACIL MOLECULES ISOLATED IN THE LOW TEMPERATURE Ar MATRICES** **155**

I. I. Shkapo, A. Yu. Ivanov, Yu. V. Rubin, V. A. Karachevtsev
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**16:10-16:25** **MASS SPECTROMETRIC INVESTIGATION OF INTERACTION OF PUTRESCINE WITH OLYGOMERS OF POLYETHYLENE GLYCOL** **156**

V. G. Zobnina[1], O. A. Boryak[1], M. V. Kosevich[1], K. Vekey[2], A. Gomory[2]
[1] *B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*
[2] *Core Technologies Centre of Research Centre for Natural Sciences of the Hungarian Academy of Sciences, Budapest, Hungary*

**16:25-16:40** **THE INFLUENCE OF THE PROTONATION ON THE STABILITY OF THE SPIROPYRAN AND MEROCYANINE MOLECULES** **157**

O. A. Kovalenko[1], Yu. M. Lopatkin[1], P. O. Kondratenko[2]
[1] *Sumy State University, Sumy, Ukraine*
[2] *Aerospace Institute, National Aviation University, Kiev, Ukraine*

## 16:55-18:00 POSTER SESSION II

# WEDNESDAY, 8 JUNE

***CONFERENCE HALL*** **PLENARY LECTURES OF INVITED SPEAKERS**

*Chair* *Mariia Pashchenko*

**10:00-10:40** **OPPORTUNITIES AND TECHNIQUES IN THE NHMFL HIGH B/T FACILITY AT THE UNIVERSITY OF FLORIDA** **35**

J. S. Xia, N. Masuhara, C. Huan, A. Serafin, M. W. Meisel and N. S. Sullivan

*Department of Physics and the National High Magnetic Field, University of Florida, Gainesville, FL, USA*

**10:40-11:20** **TUNEABLE LDHs** **39**

A. N. Salak[1], D. E. L. Vieira[1], A. V. Fedorchenko[2,3], E. L. Fertman[3], A. B. Lopes[1], A. Feher[2], M. G. S. Ferreira[1]

*[1]Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal*

*[2]Institute of Physics, Faculty of Science, P.J. Šafárik University in Košice, Košice, Slovakia*

*[3]B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**11:20-11:40** ***Coffee Break***

***CONFERENCE HALL*** **MATERIALS SCIENCE**

*Chair* *Vusal Geidarov*

**11:40-11:55** **CHANGE OF STRUCTURE OF POLYIMIDE PM-A AFTER EXPOSURE TO LOW TEMPERATURE AND DEFORMATION** **165**

V. G. Geidarov, Y. M. Plotnikova

*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**11:55-12:10** **X-RAY DETERMINATION OF STRUCTURAL PARAMETERS IN CP-TITANIUM UNDER CRYOROLLING** **166**

Y. M. Plotnikova

*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**12:10-12:25** **INDENTATION SIZE EFFECT IN TITANIUM VT1-0** **167**

A. V. Rusakova

*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**12:25-12:40** **STRAIN HARDENING, STRAIN RATE SENSIITIVITY AND DUCTILITY OF THE NANOCRYSTALLINE TITANIUM** **168**

R. V. Smolianets

*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**12:40-13:30** ***LAB TOUR***

**13:30-14:00** ***Time for Lunch***

## *CONFERENCE HALL* PLENARY LECTURES OF INVITED SPEAKERS

*Chair* *Olena Vatazhuk*

**14:00-14:40** **TERA-MIR RADIATION: MATERIALS, GENERATION, DETECTION AND APPLICATIONS III** **38**
M. F. Pereira
*Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, United Kingdom*

**14:40-15:20** **LOW-TEMPERATURE ACOUSTIC PROPERTIES OF NANOSTUCTURED Cu AND Cu-BASED NANOCOMPOSITES OBTAINED BY DIFFERENT METHODS OF SEVERE PLASTIC DEFORMATION** **37**
P. P. Pal-Val
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

## *CONFERENCE HALL* MATERIALS SCIENCE

*Chair* *Olena Vatazhuk*

**15:20-15:35** **PEIERLS BARRIERS FOR <a>-TYPE SCREW DISLOCATIONS IN MAGNESIUM** **169**
O. M. Vatazhuk[1], A. Ostapovets[2], R. Gröger[2]
[1]*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*
[2]*CEITEC-IPM, Institute of Physics of Materials ASCR, Brno, Czech Republic*

**15:35-15:50** **PECULIARITIES OF PLASTIC DEFORMATION OF UFG AZ31 AT LOW TEMPERATURE** **170**
P. A. Zabrodin
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**15:50-16:05** **EFFECT OF DOPING AMINO ACIDS L-ARGININE ON THE STRENGTH AND NONLINEAR OPTICAL PROPERTIES OF KDP CRYSTALS** **171**
E. I. Kosteniukova, O.N. Bezkrovnaya
*STC ''Institute for Single Crystals'', Kharkiv, Ukraine*

**16:05-16:15** **PLASTIC PROPERTIES OF TUNGSTEN-POTASSIUM IN A WIDE TEMPERATURE RANGE** **172**
S. V. Lebediev[1], T. V. Khvan[1], V. I. Dubinko[2], D. Terentyev[3]
[1]*V. N. Karazin Kharkiv National University, Kharkiv, Ukraine*
[2]*National Scientific Centre Kharkiv Institute of Physics and Technology, Kharkiv, Ukraine*
[3]*Belgian Nuclear Research Centre SCK·CEN*

**17:00-21:00** **WELCOME PARTY**

# THURSDAY, 9 JUNE

***CONFERENCE HALL*** **PLENARY LECTURES OF INVITED SPEAKERS**

*Chair* *Mariia Pashchenko*

**10:00-10:40** **THERMODYNAMIC STUDIES ON THE SUPERCONDUCTIVITY AND THE SPIN LIQUID STATE IN ORGANIC CHARGE TRANSFER COMPOUNDS** **36**
Y. Nakazawa, S. Yamashita, R. Yoshimoto, S. Imajo, H. Akutsu
*Department of Chemistry, Graduate School of Science, Osaka University, Osaka, Japan*

**10:40-11:20** **LOW TEMPERATURE FTIR SPECTROSCOPY IN THE STUDIES OF SURFACE PHENOMENA** **41**
A.A. Tsyganenko
*V.A.Fock Institute of Physics, St.Petersburg State University, St.Petersburg, Russia*

**11:20-11:35** ***Coffee Break***

***CONFERENCE HALL*** **QUANTUM LIQUIDS AND QUANTUM CRYSTALS, CRYOCRYSTALS**

*Chair* *Ivan Gritsenko*

**11:35-11:50** **THE THERMAL CONDUCTIVITY OF POLYMORPHS 4-BROMOBENZOPHENONE CRYSTALS** **107**
Yu. V. Horbatenko, O. O. Romantsova, A. I. Krivchikov, O. A. Korolyuk
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**11:50-12:05** **ON THE DIPOLE MOMENT OF QUANTIZED VORTICES IN THE PRESENCE OF FLOWS** **108**
S. I. Shevchenko, A. M. Konstantinov
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**12:05-12:20** **ANALYSIS OF INFLUENCE OF LIQUID DIELECTRIC FILM THICKNESS ON THE CHARACTERISTICS OF THE PHASE TRANSITION TO A SPATIALLY PERIODIC STRUCTURE IN A GAS OF CHARGED PARTICLES ABOVE IT** **109**
D. M. Lytvynenko[1,2]
[1]*Akhiezer Institute for Theoretical Physics NSC KIPT, Kharkiv, Ukraine*
[2]*Kharkiv V.N. Karazin National University, High-Technology Institute, Kharkiv, Ukraine*

**12:20-12:35** **BOSE-EINSTEIN CONDENSATION IN A MIXED FERMION-BOSON SYSTEM OF INTERACTING PARTICLES** **110**
Yu. M. Poluektov, S. N. Shulga
*Akhiezer Institute for Theoretical Physics NSC KIPT, Kharkiv, Ukraine*

**12:35-12:50** **THE ELECTRIC POLARIZATION OF He II WITH MOTION OF SUPERFLUID COMPONENT RELATIVE TO THE VORTICES** **111**
I. N. Adamenko, E. K. Nemchenko
*V. N. Karazin Kharkiv National University, Kharkiv, Ukraine*

**12:50-13:05** **EFFECTS CAUSED BY ORIENTATIONAL DISORDER ON THERMAL CONDUCTIVITY OF MOLECULAR CRYSTALS** **112**
G. A. Vdovychenko, A. I. Krivchikov, O. A. Korolyuk, O. O. Romantsova, Yu. V. Horbatenko
*V. N. Karazin Kharkiv National University, Kharkiv, Ukraine*

**13:05-13:20** **SPONTANEOUS CURRENT OSCILLATIONS IN A PHOTO-EXCITED 2D ELECTRON SYSTEM ON LIQUID HELIUM** **113**
K. Nasyedkin[1], K. Kono[1,2,3]
[1]*RIKEN Center for Emergent Matter Science, Wako, Saitama, Japan*
[2]*Institute of Physics, National Chiao Tung University, Hsinchu, Taiwan*
[3]*Institute of Physics, Kazan Federal University, Kazan, Russia*

## *HALL* — YOUNG SCIENTISTS WORKSHOP

*Chair* *Mariia Pashchenko*

**13:20-14:20** **Workshop devoted to celebration of 100 years anniversary of OSA (Optical Society of America) and Carrier Development opportunities for young scientists and students**

**Mariia Pashchenko**
ILTPE NASU
"Introduction about SPIE and OSA Societies"

**Alexander Semchenkov**
web-manufacture.net
"3D-printer and its potential"

**Prof. Mauro F. Pereira**
Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, United Kingdom
"Special Program for Students"

**14:30-19:00** ***Excursion to ECOPark***

# FRIDAY, 10 JUNE

## *CONFERENCE HALL* PLENARY LECTURES OF INVITED SPEAKERS

*Chair* *Mariia Pashchenko*

**10:00-10:40** **ELECTRON-PHONON COUPLING IN BINARY MOLIBDATES** **33**
D. Kamenskyi[1], A. Pronin[2], K. Kutko[3], S. Poperezhai[3]
[1]*High Field Magnet Laboratory, Radboud University, Nijmegen, The Netherlands*
[2]*Universitat Stuttgart, Stuttgart, Germany*
[3] *B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**10:40-11:20** **CLUSTERING PROCESSES IN HYDROGEN-BONDED LIQUIDS BY MATRIX-ISOLATION FTIR SPECTROSCOPY** **31**
I. Doroshenko[1], V. Pogorelov[1], G. Pitsevich[2], V. Sablinskas[3] and V. Balevicius[3]
[1] *Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
[2] *Belarusian State University, Minsk, Belarus*
[3] *Vilnius University, Vilnius, Lithuania*

**11:20-11:40** *Coffee Break*

## *CONFERENCE HALL* OPTICS, PHOTONICS AND OPTICAL SPECTROSCOPY

*Chair* *Sergii Poperezhai*

**11:40-11:55** **THz STUDY OF LOW ENERGY EXCITATIONS IN $KEr(MoO_4)_2$** **89**
S. Poperezhai[1], K. Kutko[1], P. Gogoi[2], D. Kamenskyi[2]
[1]*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*
[2]*High Field Magnet Laboratory, Radboud University, Nijmegen, The Netherlands*

**11:55-12:10** **FLUORESCENCE ENHANCEMENT BY J-AGGREGATES** **90**
I. Yu. Ropakova, I. I. Grankina, A. V. Sorokin, Yu. V. Malyukin
*Institute for Scintillation Materials, STC "Institute for Single Crystals", Kharkiv, Ukraine*

**12:10-12:25** **PHOTOLUMINESCENCE PROPERTIES OF THE $Li_2OxGeO_2$ GLASS-CERAMIC DOPED WITH SOME THREE CHARGED IONS** **91**
Ya. Rybak[1], S. Nedilko[1], V. Scherbatskii[1], M. Trubitsyn[2], M. Volnianskii[2]
[1]*Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
[2]*Oles Honchar Dnipropetrovsk National University, Dnipropetrovsk, Ukraine*

**12:25-12:40** **INTEGRATED QUANTUM CORRELATION COUNTER BASED ON MULTI-ELEMENT SUPERCONDUCTING NANOWIRE SINGLE PHOTON DETECTOR** **92**
M. Yu. Mikhailov[1,2], V. Zwiller[1]
[1]*Kavli Institute of Nanoscience Delft, Delft University of Technology, Delft, The Netherlands*
[2]*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**12:40-12:55 INFLUENCE OF ZINC CONCENTRATION ON STRUCTURAL AND OPTICAL PROPERTIES OF POLYCRYSTALLINE CZT THICK FILMS OBTAINED BY THE CLOSE SPACED SUBLIMATION 93**

Y. V. Znamenshchykov, V. V. Kosyak, A. S. Opanasyuk
*Sumy State University, 2, Sumy, Ukraine*

**12:55-13:10 EFFECT OF THE STRUCTURE ON THE CHARACTERISTICS OF THE LANTHANUM-GALLIUM SILICATE GROUP CRYSTALS 94**

O. A. Buzanov[1], A. P. Kozlova[2], N. S. Kozlova[2], E. V. Zabelina[2], N. A. Siminel[2], D. A. Spassky[3]
[1] *Fomos Materials Ltd., Moscow, Russia*
[2]*National University of Science and Technology "MISiS", Moscow, Russia*
[3]*Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow, Russia*

## *SMALL CONFERENCE HALL* NANOPHYSICS AND NANOTECHNOLOGIES

*Chair* *Maxym Barabashko*

**11:40-11:55 LOW TEMPERATURE HEAT CAPACITY OF THE 1D METHANE CHAINS 129**

M. S. Barabashko, M. I. Bagatskii, V. V. Sumarokov
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**11:55-12:10 THE QUANTUM EFFECTS IN HYDROGEN SORPTION BY MESOPOROUS MATERIALS 130**

M. V. Khlistuck, A. V. Dolbin, V. B. Esel'son, V. G. Gavrilko, N. A. Vinnikov, R. M. Basnukaeva
*B.Verkin Institute for Low Temperature Physics and Engineering, Kharkiv, Ukraine*

**12:10-12:25 STRUCTURAL FEATURES OF SURFACE LAYERS THIN FILMS OF YTTRIUM IRON GARNET 131**

O. V. Kovalenko
*V. N. Karazin KharkivNational University, Kharkiv, Ukraine*

**12:25-12:40 AN INFLUENCE OF DOPINGS ON THE GROUNG STATE SPIN OF NL ACCORDING TO T-J MODEL 132**

A. A. Kravchenko
*V. N. Karazin KharkivNational University, Kharkiv, Ukraine*

**12:40-12:55 OPTICAL AND ELECTROPHYSICAL PROPERTIES OF CARBON NANOTUBES DISPERSIONS IN NEMATIC LIQUID CRYSTALS WITH PHOTOACTIVE COMPONENTS 133**

O. M. Samoilov
*Institute for Scintillation Materials, Kharkiv, Ukraine*

**12:55-13:10 FUNCTIONALIZATION OF N(B)-DOPED SINGLE-WALLED CARBON NANOTUBES AND GRAPHENE BY THE $XO_4^{2-}$ (X = Cr, Mo, W) OXYANIONS 134**

V. Borysiuk[1], Yu. Hizhnyi[1], S. Nedilko[1], A. Shyichuk[2]
[1]*Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
[2]*Department of Rare Earth, Faculty of Chemistry, Adam Mickiewicz University, Poznań, Poland*


**13:30-14:00** **CLOSING**

**14:00-15:00**  ***Time for Lunch***

**15:00-16:00** **CONCERT OF CLASSICAL MUSIC**

**17:05-18:00**

# POSTER SESSION I
# MONDAY, 6 JUNE

## MAGNETISM AND MAGNETIC MATERIALS

## OPTICS, PHOTONICS AND OPTICAL SPECTROSCOPY

## QUANTUM LIQUIDS AND QUANTUM CRYSTALS, CRYOCRYSTALS

## THEORY OF CONDENSED MATTER PHYSICS



## TECHNOLOGIES AND INSTRUMENTATION FOR PHYSICAL EXPERIMENTS

K. V. Slipchenko
*V.N. Bakul Institute for Superhard Materials, Kyiv, Ukraine*

**16:55-18:00** **POSTER SESSION II**
**TUESDAY, 7 JUNE**

## ELECTRONIC PROPERTIES OF CONDUCTING AND SUPERCONDUCTING SYSTEMS

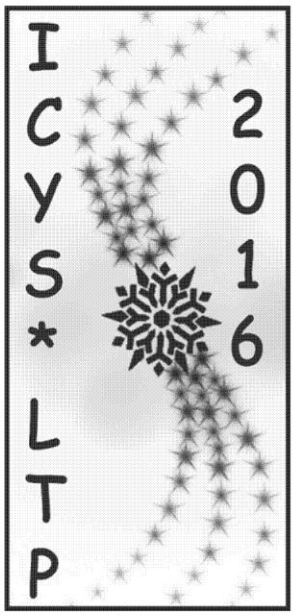
## NANOPHYSICS AND NANOTECHNOLOGIES

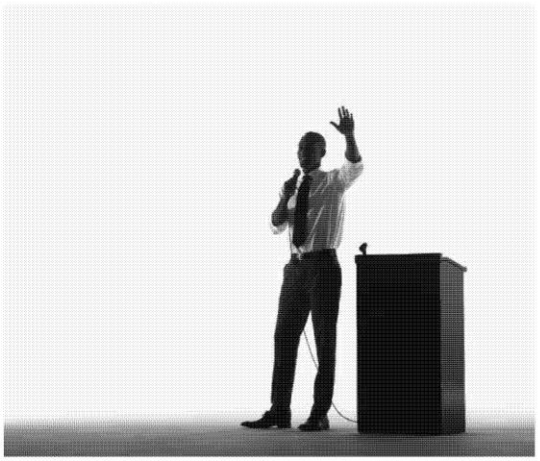
## BIOPHYSICS AND PHYSICS OF MACROMOLECULES

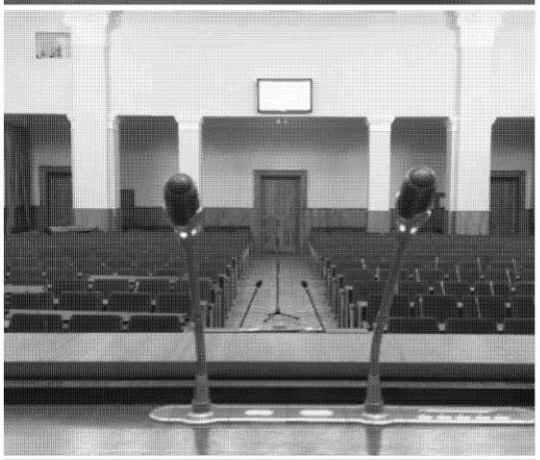


## MATERIALS SCIENCE

# Plenary Lectures of Invited Speakers





# TRANSPORT PROPERTIES IN SUPERCONDUCTING HYBRID NANOSYSTEMS

**A. Braggio[1,2]**

*[1]CNR-SPIN Dipartimento di Fisica, Via Dodecaneso 33, 16146, Genova (Italy)*
*[2]INFN, Sezione di Genova, Dipartimento di Fisica, , Via Dodecaneso 33, 16146, Genova (Italy)*
*e-mail: alessandro.braggio@spin.cnr.it*

The recent advancements nanotechnology has expanded considerably the possibility to create hybrid devices. At the same time the development of the topological materials[1] in the last decades has further extended the interest for hybrid devices which mix superconductors, normal metals, ferromagnetic and/or material with strong spin-orbit[2]. Hereafter we discuss three different examples. We firstly consider the thermal transport properties of a Josephson junction[3]. We review how the galvanic term depends on the phase difference, discussing the recent experimental advancements in the field[4]. We also compare those terms with other contributions such as the radiative ones, which are expected to be very small for Josephson junctions[5]. As second example we consider the thermo-electrical properties of a normal-metal-ferromagnetic-insulator-superconductor system[6]. We will discuss how those systems may present strong Seebeck coefficient, as recently measured[7], than can be used for high sensitivity thermometry up to 30nK $Hz^{-1/2}$. We discuss different configurations of the device in order to extract the information on temperatures and we discuss how the non-equilibrium conditions guarantees the maximal temperature sensitivity[8]. As a third example we investigate the Josephson current of a nanoring in the presence of a finite size topological superconductor[9]. Here we propose an alternative and complementary experimental recipe to detect topological phase transitions in these systems[10]. We show in fact that, for a finite-sized system with broken time-reversal symmetry, discontinuities in the Josephson current-phase relation correspond to the presence of zero-energy modes and to a change in the fermion parity of the groundstate[11]. Such discontinuities can be experimentally revealed by a characteristic temperature dependence of the current, and can be related to a finite anomalous current at zero phase in systems with broken phase-inversion symmetry.

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# ABRIKOSOV FLUXONICS IN WASHBOARD NANOLANDSCAPES

**O. V. Dobrovolskiy[1,2], M. Huth[1], V. A. Shklovskij [2]**

*[1] Physikalisches Institut, Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt/M, Germany*
*[2] Physics Department, V. N. Karazin National University, Svobody Sq. 4, 61077 Kharkiv, Ukraine*
*e-mail: Dobrovolskiy@Physik.uni-frankfurt.de*

Abrikosov fluxonics [1], a domain of science and engineering at the interface of superconductivity research and nanotechnology [2], is concerned with the study of the properties and dynamics of Abrikosov vortices in nanopatterned superconductors, with particular focus on their confinement, manipulation, and exploitation for emerging functionalities. Vortex pinning, guided vortex motion, and the ratchet effect are three main fluxonic "tools" which allow for the dynamical (pinned or moving), the directional (angle-dependent), and the orientational (current polarity-sensitive) control of the fluxons, respectively [3,4].

In this talk a set of original experimental results [5-10] on the vortex dynamics in the presence of periodic pinning potentials in Nb thin films is presented. The consideration is limited to one particular type of artificial pinning structures – directly written nanolandscapes of the washboard type, which are fabricated by focused ion beam milling and focused electron beam induced deposition. Thanks to the periodicity of the vortex lattice, several groups of effects emerge when the vortices move in a periodic pinning landscape: (i) Spatial commensurability of the location of vortices with the underlying pinning nanolandscape leads to a reduction of the dc resistance and the microwave loss at the so-called matching fields [5,6]. (ii) Temporal synchronization of the displacement of vortices with the number of pinning sites visited during one half ac cycle manifests itself as Shapiro steps in the current-voltage curves [7,8]. (iii) Delocalization of vortices oscillating under the action of a high-frequency ac drive can be tuned by a superimposed dc bias [9,10]. The reported results are, in particular, relevant for the development of novel fluxonic devices, the reduction of the microwave loss in superconducting planar transmission lines and the synthesis of quantized power absorption levels in fluxonic nano-metamaterials.

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# CLUSTERING PROCESSES IN HYDROGEN-BONDED LIQUIDS BY MATRIX-ISOLATION FTIR SPECTROSCOPY

**I. Doroshenko[1], V. Pogorelov[1], G. Pitsevich[2], V. Sablinskas[3] and V. Balevicius[3]**

*[1] Taras Shevchenko National University of Kyiv, Acad. Glushkov Ave., 4, 03187, Kyiv, Ukraine*
*[2] Belarusian State University, Independence Ave. 4, 220050, Minsk, Belarus*
*[3] Vilnius University, Sauletekio 9-3, LT-10222, Vilnius, Lithuania*
*e-mail: dori11@ukr.net*

Clusters, by definition, are aggregates of atoms/molecules with more or less regular and arbitrarily scalable repetition of basic building blocks. Their size is intermediate between that of atoms/molecules and the bulk. The growing interest to the clustering phenomena that produce partially ordered atomic or molecular structures is due to the recent developments and challenges in nanotechnologies, smart materials, heterogeneous systems, basic biochemical research, etc.

The processes of molecular cluster formation in hydrogen-bonded liquids were investigated using FTIR spectroscopy and a matrix isolation technique [1-3]. The methods of cluster isolation in low-temperature matrices provide the possibility to study individual clusters of different sizes. FTIR spectra of water and monohydric alcohols (from methanol to decanol) in argon and nitrogen matrices were registered in the frequency range from 500 $cm^{-1}$ to 4000 $cm^{-1}$. The gradual transformation of the spectral bands assigned to different vibrations was observed with matrix heating from 10 to 50 K, indicating a transformation of the structure of the isolated clusters. Main changes with the temperature increasing were observed in the spectral regions of stretch O-H and C-O vibrations.

Spectral data were processed with modern methods of data analysis – principal component analysis and 2D correlation spectroscopy. Experimental spectra were compared with results of quantum-chemical simulations.

The observed temperature dependence of the registered spectra may be considered as a model of structural transformations in the studied objects during the phase transition from gas to liquid state.

The work was partly supported by Swedish Research Council (grant no. 348-2013-6720).

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# FERROMAGNETIC RESONANCE: APPLICATION FOR STUDY OF MAGNETIC SHAPE MEMORY ALLOYS

**V. O. Golub**

*Institute of Magnetism NAS of Ukraine and MES of Ukraine,*
*36-B Vernadsky blvd., 03142 Kiev, Ukraine*
*e-mail: golub@imag.kiev.ua*

In spite of a big progress in modernization of conventional magnetic measurements techniques such as VSM and SQUID magnetometries ferromagnetic resonance (FMR) is widely used for investigation and characterization of different magnetic materials. This is connected with the following advantages of FMR technique: high sensitivity, possibility to separate contribution from different magnetic phases and magnetic structure units, absence of an influence of diamagnetic subsystems, possibility to obtain data about exchange interaction inside magnetic materials or between magnetic components of magnetic materials, power of FMR technique for a saturation magnetization, magnetic anisotropy and magnetostatic interaction investigation.

This presentation is devoted to show a power of FMR technique to study structural, magnetic and resonance properties of thin epitaxial films of ferromagnetic shape memory alloys (FSMA). The influence of the phase transitions on magnetic properties of FSMA films will be discussed. It will be also shown that the elastic interaction between film and substrate determines the microstructure of FSMA films resulting to the dramatic change of their structure and magnetic parameters. This interaction suppresses the martensitic transformation for thin films while for the thick films it leads to formation of periodic twin structures. A formation of stress induced two-fold and four-fold magnetic anisotropy will be discussed in detail.

A lot of attention will be paid to the influence mesoscale twin structure on magnetic parameters of FSMA films. Modification of magnetic properties in periodic mesoscale twin structures in the case of ferromagnetic and antiferromagnetic exchange on twin boundaries will be demonstrated for epitaxial Ni-Mn-Ga and Ni-Mn-Sn films.

Rare example of nanomesh surface self-patterning for the films deposited by conventional magnetron sputtering method on single-crystalline substrates will be presented here. Natural selforganized morphology being formed by the elongated bar-like shaped crystals will be demonstrated for epitaxial Ni-Mn-Ga thin films deposited on MgO (001) substrate and will be discussed in terms of surface stress relaxation. These films have well defined crystalline and magnetic structure. They show unusual magnetic properties properties to be considered as systems interesting for possible smart nanoscale applications.

Some new possible applications of FSMA films such as magnonic and photonic crystals fabrication will be discussed. The resent results on the observation of giant magnetoresistance in epitaxial films will be also shown.

# ELECTRON-PHONON COUPLING IN BINARY MOLIBDATES

**D. Kamenskyi[1], A. Pronin[2], K. Kutko[3], S. Poperezhai[3]**

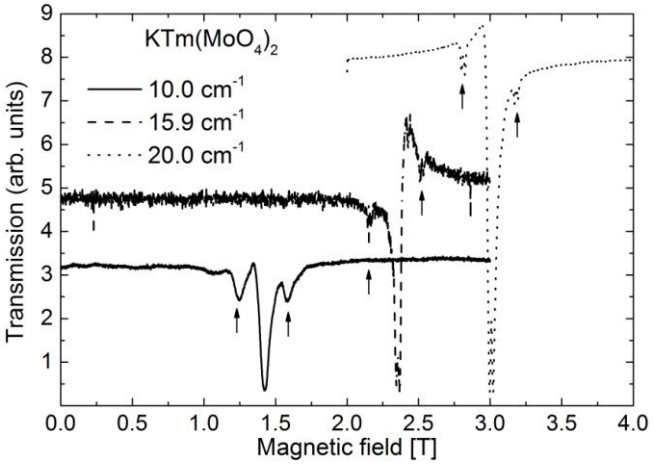
*[1]High Field Magnet Laboratory (HFML – EMFL), Radboud University, Toernooiveld 7, 6225ED Nijmegen, The Netherlands*
*[2]1. Physikalisches Institut,Universitat Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany*
*[3] B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, 61103 Kharkiv, Ukraine*
*e-mail: d.kamenskyi@science.ru.nl*

Dynamical non-linear systems are at the coalface of modern physics since most physical phenomena are inherently non-linear in nature. Non-linearity causes profound effects even in classical systems, the formation of solitons being one famous example.

Here we report the study of non-linear effects in binary molibdates. The characteristic feature of rare-earth compounds $MR(MoO_4)_2$ ($M^+$ is an alkali metal ion, $R^{3+}$ is a rare-earth ion) is the strong coupling between the electronic excitations of the $R^{3+}$ ions and phonons. Previous investigations show that the strength of electron-phonon coupling can be tuned by a magnetic field [1]. Such tunability is particularly important for the non-linear systems where a lack of control makes experimental investigations very challenging.

We investigate electron-phonon coupling by means of far infrared (FIR) and electron paramagnetic resonance (EPR) spectroscopies. FIR study performed in externally applied magnetic fields allowed us to determine energies of lattice vibrations and electronic excitations. We show that EPR spectra undergo significant modification when energies of microwave frequencies and lattice vibrations coincide. We argue that the effects observed are induced by strong coupling between electronic excitations and acoustic phonons.

Figure shows the EPR transmission spectra of the $KTm(MoO_4)_2$ at different frequencies. The magnetic field applied along the *c*-axis shifts the EPR transitions to high frequencies quite rapidly (g = 13.8) [2]. We show that EPR spectra undergo significant modification when energies of microwave frequencies change in respect to the energy of acoustic vibrations. The sidebands (shown by the arrows) are most developed at low frequencies and vanish when frequencies becomes higher than the limit frequency for the acoustic mode.




We show that such interaction between electronic excitation and acoustic phonon exhibit universal character and may significantly affect the magnetic properties of wide class of materials especially at high magnetic field.

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# ONE-MOLECULE SHOW: NOVEL APPLICATIONS OF METHYLENE BLUE DYE IN PHARMACOLOGY AND NANOBIOPHYSICS

**M. V. Kosevich**

*B.Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: mvkosevich@ilt.kharkov.ua*

Among a variety of stories of biologically active compounds, the one of Methylene Blue (MB) cationic redox-active dye is chosen for the present discussion due to the emergence of its new applications in pharmacology, biomedicine and nanosciences [1, 2].

Being used as antiseptic since its first preparation in 1876, nowadays MB is continuing to find novel applications. Popular in the middle of the last century use of MB as an antimalarial agent is currently revived in development of more efficient antimalarial drug compositions. One more promising pharmaceutical application of MB is connected with investigations of its potential activity in retardation of neurodegenerative Alzheimer's disease. Photophysical properties of MB are utilized in photodynamic therapy of cancer. In molecular biophysics research MB is used in investigations on interactions of intercalating agents with DNA.

MB applications in nanotechnology are based on its fluorescence, redox and aggregation properties [3]. Ability of MB to "shuttle" electrons provides its use as a mediator component in biosensors. In a new generation of electrochemical amperometric biosensors hybrids of MB and DNA are applied [4]. The principle of functioning of such nanodevices is as follows. DNA is attached to the surface of the sensor electrode by one end, and MB is tethered to its other end. The change of the DNA conformation in response to the target molecule recognition event changes the distance of the tethered MB to the electrode surface and correspondingly the efficiency of electron transfer (electric current) from the MB. Basing on this principle genosensors for detection of DNA hybridization, DNA damage, genetically modified organisms, oncomarkers, viruses, and *on-line* monitoring of polymerase chain reactions are developed.

Molecular mechanisms of action of MB and its redox transformations in various systems can be modeled and studied by means of mass spectrometric techniques [3]. In particular, mass spectrometric experiments permitted to reveal relationships between the monomer/dimer equilibrium and redox activity of MB [5]. Self-assembly and properties of composites incorporating MB and carbon nanomaterials [6], such as carbon nanotubes, graphene and fullerenes are disclosed.

In conclusion, this brief overview demonstrates how versatile physical and chemical properties of MB dye assure its diversified applications in pharmacology and nanotechnology.

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# OPPORTUNITIES AND TECHNIQUES IN THE NHMFL HIGH B/T FACILITY AT THE UNIVERSITY OF FLORIDA

**J. S. Xia, N. Masuhara, C. Huan, A. Serafin, M. W. Meisel, and N. S. Sullivan**

*Department of Physics and the National High Magnetic Field, University of Florida, Gainesville, FL 32611-8440, USA*
*e-mail: meisel@phys.ufl.edu and sullivan@phys.ufl.edu*

The scientific opportunities for research at ultra-low temperatures in high magnetic fields at the National High Magnetic Field Laboratory (NHMFL) High B/T Facility [1] at the University of Florida [2] are overviewed. The facility includes two nuclear demagnetization refrigerators for studies below 1 mK and up to 16.5 T. In addition, a fast turn-around dilution refrigerator is available for testing samples down to 10 mK and up to 10 T. One of the nuclear demagnetization stages employs a $PrNi_5$ refrigerant and has a cooling power of 10 nW down to 0.4 mK, Fig. 1. The second nuclear refrigerator uses Cu for the demagnetization material and can cool samples down to 0.1 mK. The facility employs electro-magnetic shielding and active vibration isolation to provide an ultra-quiet environment that is often critical for high sensitivity measurements at sub-milliKelvin temperatures.

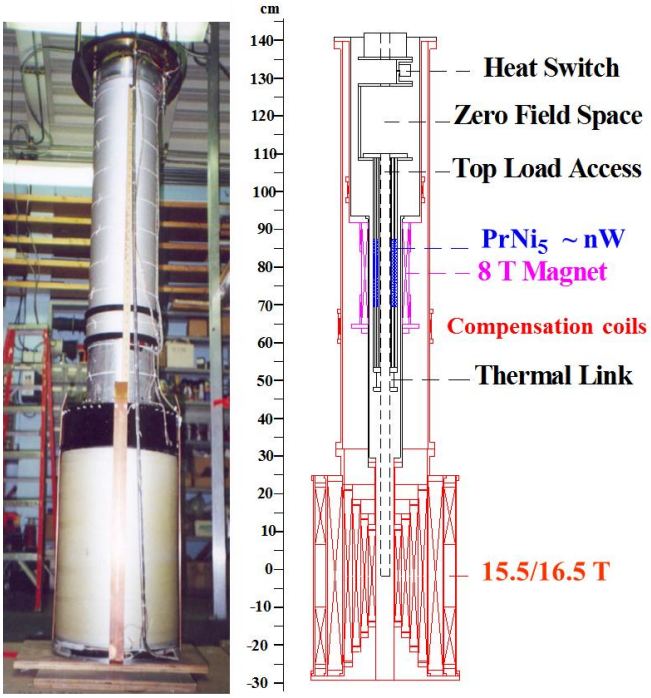


**Figure 1.** A photograph and a schematic drawing of the integral magnet system in Bay 3 of the NHMFL High B/T Facility.

Instrumentation is available for a wide variety of studies including ac magnetic and dielectric measurements, transport studies, nuclear magnetic resonance and nuclear quadrupole experiments, and ultrasound measurements. Some recent experiments include exploration of the Bose glass state in organic quantum magnets [3], properties of exotic quantum Hall states [4], dynamics and quantum plasticity in solid helium [5], and topological insulators.

The NHMFL High B/T Facility is supported by NSF Grant DMR-1157490 and by the State of Florida.

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# THERMODYNAMIC STUDIES ON THE SUPERCONDUCTIVITY AND THE SPIN LIQUID STATE IN ORGANIC CHARGE TRANSFER COMPOUNDS

**Y. Nakazawa, S. Yamashita, R. Yoshimoto, S. Imajo, H. Akutsu**

*Department of Chemistry, Graduate School of Science, Osaka University*
*Machikaneyama 1-1, Toyonaka, Osaka 560-0043, Japan*
*e-mail: nakazawa@chem.sci.osaka-u.ac.jp*

We discuss low-temperature thermodynamic properties studied by the single crytal calorimetry techanique for two-dimensional (2D) organic charge transfer compounds which show various quantum mechanical features dominated by charge and spin degrees of freedom.

At first, we show results of heat capacity measurements of κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$, EtMe$_3$Sb[Pd(dmit)$_2$]$_2$ and κ-H$_3$(Cat-EDT-TTF)$_2$, which are known as 2D dimer-Mott systems with triangle structure. Thermodynamic features characteristic of gapless liquid-like states produced by π-electron spins were obaserved as common aspects in these three compounds. We also discuss magnetic field effects for these low energy excitations from the analyses of heat capacity data under magnetic fields up to 10 T. Through detail studies of X[Pd(dmit)$_2$]$_2$ of which cation layers are chemically controlled by making solid-solution of different size of cations, we derived information on the systematic variation of electronic ground states. [1-3] We observed that the spin-liquid state exists as a distinct phase and kind of quantum phase transitions to AF and CO phases by changing chemical pressures. The relation with spin properties coupled with other degrees of freedoms is discussed in order to clairfy the electronic structrures in such organic compounds. The curious magnetic properties of dimer-Mott system of X[Ni(dmit)$_2$]$_2$ with non-symmetric counter cations X are also reported in relation to spin-liquid properties.

If the triangularity of spin-liquid system changes to square lattice, the system become antiferromagnetic insulators. In these materials, the application of pressure leads the system to conductive and superconductive phases. The thermodynamic measurements of the superconductors of these organic compounds show quadratic temperature dependences at low temperatures. The analyses of electronic heat capacity against magnetic fields both in magnitude and direction demonstrate that the superconductivity has d-wave with line-node characters.[4] Thermodynamic features for other organic superconductors with different structures are also discussed.

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# LOW-TEMPERATURE ACOUSTIC PROPERTIES OF NANOSTUCTURED Cu AND Cu-BASED NANOCOMPOSITES OBTAINED BY DIFFERENT METHODS OF SEVERE PLASTIC DEFORMATION

**P. P. Pal-Val**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: palval@ilt.kharkov.ua*

Study of physical-mechanical properties of nanostructured (NS) metals represents significant interest considering its importance both for the industrial applications and also from the point of view of fundamental physics. Transition of materials into NS-state changes the major physical characteristics, in particular, their elastic and inelastic properties, parameters of strength and plasticity. The NS-metals have high technological and operational characteristics and therefore are perspective for use as constructional materials working in extreme operational conditions.

Among various techniques of metals structure fragmentation, the methods using severe plastic deformation (SPD) are most accessible. These are equal channel angular pressing (ECAP), high pressure torsion (HPT), repeated drawing and extrusion, etc. They allow receiving practically pore-free bulk samples. However the materials received via SPD treatment have thermodynamically non-equilibrium structure because they contain a significant amount of deformation defects, first of all, dislocations and grain boundaries. Different methods of SPD structure fragmentation (ECAP, HPT, drawing and extrusion) may not only lead to creation of huge dislocation density or large number of grain boundaries but also to formation of different types of texture. It is the origin of instability of physical-mechanical properties of nanostructured metals, both at formation of the NS-state and during subsequent thermal and mechanical treatments.

Studying of elastic and inelastic properties may be regarded as a source of the valuable information on structural changes in nanostructured metals at different stages of their preparation and post-SPD processing. First, there the quantitative information on the elastic moduli may be received. Second, these experiments allow obtaining the data on dynamic properties of crystal imperfections of different nature (dislocations, impurity atoms, grain boundaries, etc.) and their interaction with excitations in electron and phonon subsystems. Non-destructive character is an additional advantage of the acoustic measurements and allows carrying out repeated measurements on the same specimen over the wide range of external parameters (e.g. temperature). It gives a possibility to establish the temperature boundaries and kinetics of structural instability of nanostructured materials.

In the present review, the results are summarized that were obtained in the range 5 − 340 K when studying the acoustic properties of nanostructured copper and Cu-Nb and Cu-Fe fiber nanocomposites prepared with the help of different SPD methods [1-3]. A number of low-temperature acoustic anomalies are revealed caused by generation of enormous dislocation density, formation of crystallographic texture, by introducing large number of grain boundaries. It is shown that the behavior of elastic moduli and inelastic characteristics of nanostructured metals of copper appears to be essentially different depending on the SPD techniques being used. It is established that this distinction is caused by formation of different substructures during preparation of the samples investigated and by the evolution of those during subsequent post-SPD treatment.

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# TERA-MIR RADIATION: MATERIALS, GENERATION, DETECTION AND APPLICATIONS III

**M. F. Pereira**

*Materials and Engineering Research Institute, Sheffield Hallam University, S1 1WB. Sheffield, United Kingdom*
*e-mail: m.pereira@shu.ac.uk*

In this talk, I start by summarizing the main goals and recent achievements of COST ACTION MP1204 [1], whose main objectives are to advance novel materials, concepts and device designs for generating and detecting THz and Mid Infrared radiation using semiconductor, superconductor, metamaterials and lasers and to beneficially exploit their common aspects within a synergetic approach. We use the unique networking and capacity-building capabilities provided by the COST framework to unify these two spectral domains from their common aspects of sources, detectors, materials and applications. We are creating a platform to investigate interdisciplinary topics in Physics, Electrical Engineering and Technology, Applied Chemistry, Materials Sciences and Biology and Radio Astronomy. The main emphasis is on new fundamental material properties, concepts and device designs that are likely to open the way to new products or to the exploitation of new technologies in the fields of sensing, healthcare, biology, and industrial applications. End users are: research centres, academic, well-established and start-up Companies and hospitals.

Results are presented along our main lines of research: Intersubband materials and devices with applications to fingerprint spectroscopy; Metamaterials, photonic crystals and new functionalities; Nonlinearities and interaction of radiation with matter including biomaterials; Generation and Detection based on Nitrides and Bismides.

Next I summarize research results in which I have been directly involved including: valence band THz polaritons and antipolaritons [2,3], a microscopic approach to dilute semiconductor optics [4], simulations of quantum cascade lasers and THz generation by frequency multiplication in semiconductor superlattices and a numerical study of high impedance T-match antennas for THz photomixers [5], harmonic generation in superlattices and quantum cascade laser simulations. The theoretical results outlined are intended to stimulate further cooperation between theory and experimental teams.

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# TUNEABLE LDHs

**A. N. Salak[1], D. E. L. Vieira[1], A. V. Fedorchenko[2,3], E. L. Fertman[3], A. B. Lopes[1], A. Feher[2], M. G. S. Ferreira[1]**

*[1]Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*
*[2]Institute of Physics, Faculty of Science, P.J. Šafárik University in Košice, 9 Park Angelinum, Košice 04154, Slovakia*
*[3]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: salak@ua.pt*

Layered Double Hydroxides (LDHs) are composed of alternating positively-charged mixed metal $M^{II}$-$M^{III}$ hydroxide layers and interlayers occupied by anions ($A^{y-}$) and water molecules. The metal cations in the layers are coordinated by six oxygen atoms forming 2-D structures of the face-linked oxygen octahedra. The general formula of the most common LDHs can be represented as $[M^{II}_{1-x}M^{III}_{x}(OH)_2]^{x+}(A^{y-})_{x/y}\cdot zH_2O$, where $z$ is an amount of crystal water per formula unit. The parameters $x$ and $z$ can vary over a rather wide range and thereby enable a flexibility of LDH structure allowing intercalation of anions of different nature (either inorganic or organic), size, configuration and charge. As a result, the characteristic layer-interlayer scale in LDHs can be from about 0.7 nm to several nanometers.

The general feature of LDHs is their unique anion exchange ability. The anions intercalated into interlayers can be substituted (in either *reversible* or *irreversible* way) by other anions or combinations of different anions. The exchange direction and rate depend on both the nature of the involved anions and the external factors, such as temperature, concentration, pH *etc*. The controllable exchange ability of LDHs finds use in sensing, corrosion protection, water treatment and other areas. In all these applications, the cation composition of the LDH hydroxide layers is usually unconsidered since it has no (or negligible) impact on the anion exchange. At the same time, particular cations in the oxygen-octahedra layers of the LDHs can offer additional functionality or even new properties.

We report on the systematic study of magnetic properties of LDHs containing cations Co(II), Fe(III) or Al(III). Layered double hydroxides intercalated with anions of different size, shape and charge (including paramagnetic anions) were prepared and investigated. Magnetic characteristics of these LDHs were measured and correlated to the chemical composition and the crystal structure. We show that although the magnetic properties of LDHs are mainly determined by the nature of the paramagnetic anions and their ratio, $(1-x)/x$, the magnetic characteristics can be reversibly tuned by variation of the interlayer distance through anion exchanges and control of the crystal water content.

The obtained LDHs are examples of *tuneable nanomagnets* and considered as promising models to study magnetic interactions in 2-D systems.

This work was supported by project TUMOCS – *Tuneable Multiferroics based on Oxygen Octahedral Structures*. This project has received funding from European Union Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 645660.

# EXOTIC MAGNETIC PHASES IN FRUSTRATED $J_1$-$J_2$ CHAIN MAGNET $LiCuVO_4$

**L. E. Svistov**

*P.L. Kapitza Institute for Physical Problems RAS, 119334 Moscow, Russia*
*e-mail:svistov@kapitza.ras.ru*

Quantum-spin chains with frustrated exchange interactions were among the most interesting issues for both experimental and theoretical research in condensed matter physics in the past decade [1-3] .

The enhanced effect of quantum fluctuations imposed upon a fine balance of exchange interactions leads to a variety of novel ground states and phase transformations in these systems [4-7]. $LiCuVO_4$ is an example of a quasi-1D magnet (S=1/2), which unconventional magnetic phases result from a competition of ferromagnetic and antiferromagnetic exchange interactions between nearest-neighbor ($J_1$) and next-nearest neighbor ($J_2$) in-chain magnetic moments.

As a result of this particular combination of exchange interactions a helical incommensurate structure is stabilized in this system below $T_N$~ 2.3K [8].

A strong reduction in the ordered spin component of Cu2+ ions in this state $\mu/\mu_B$~ 0.3 [8,9] provides evidence that the system partially retains properties of 1D chains.

Moderate applied magnetic fields 7-8 T induce a transformation of the spin helix into a collinear spin-modulated structure when all spins are parallel to the field, with their ordered components oscillating along the chain with an incommensurate period.

This transition may be related to the field evolution of short range chiral (transverse) and spin-density wave (longitudinal) correlations for the 1D, $J_1$-$J_2$ model [10].

In the field range just below the saturation field the theory predicts the presence of a long-range nematic ordering [7,11].

The experimental studies of magnetic structures of LiCuVO4 in fields up to saturation will be overviewed in the report.

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# LOW TEMPERATURE FTIR SPECTROSCOPY IN THE STUDIES OF SURFACE PHENOMENA

**A.A. Tsyganenko**

*V.A.Fock Institute of Physics, St.Petersburg State University, St.Petersburg, Russia*
*e-mail:atsyg@yandex.ru*

The paper deals with the advances in the application of IR spectroscopy for the studies of adsorption, mechanism of lateral interaction between the adsorbed molecules and linkage isomerism in the adsorbed state.

Spectroscopy at low and variable temperatures enable us to broaden the number of test molecules for surface sites and instead of ammonia, pyridine and nitriles, to use simple molecules that do not adsorb at 300 K, such as CO, NO, H2 to characterize acidic (electron-accepting) sites, while for basic (electron-donating) centers low-temperature adsorption of weak CH proton-donors like CHF3 can be used. Quantitative measurements reveal a correlation between the frequency shifts and absorption coefficients of adsorbed molecules.

The strength of surface sites is affected by lateral interactions between the adsorbed species, which can be repulsive or attractive. Static interaction changes the energies of adsorption and shifts the bands of test molecules. Dynamic interaction accounts for the changes in the bandshape and half-width and for splitting of the bands. It manifests itself even in the spectra of symmetric molecules weakly adsorbed on zeolites or amorphous adsorbents.

Some molecules, such as CO, reveal linkage isomerism and form with the cations in Y or ZSM-5 zeolites, besides the usual C-bonded species, the energetically unfavorable O-bonded complexes. Besides the frequencies, different geometry of isomeric species leads to dissimilarity in the isotopic shifts on 13C or 18O substitution. The linkage isomerism can be explained by electrostatic model, which also accounts for the absence of this phenomenon for oxides or X-zeolites, where formation of side-on complexes with surface anions or interaction with dual cationic sites is preferable. According to the model, isomerism is possible for halogenides or layered alumosilicates where negative charge of anions is lower or is delocalized over the polyanionic layers, that was recently confirmed by variable temperature FTIR measurements. Surface isomeric states were established for some other adsorbed species, such as cyanide ion CN- produced by HCN dissociation.

# MAGNETIC EXITATIONS IN SPIN-1/2 TRIANGULAR-LATTICE ANTIFERROMAGNETS: HIGH-FIELD ESR STUDIES

**S. A. Zvyagin**

*Dresden High Magnetic Field Laboratory (HLD)*
*Helmholtz-Zentrum Dresden-Rossendorf*
*Bautzner Landstr. 400, 01328 Dresden, Germany*
*e-mail: s.zvyagin@hzdr.de*

The spin-1/2 Heisenberg antiferromagnet (AF) on a triangular lattice is the paradigmatic model in quantum magnetism, which was intensively studied since several decades. In spite of numerous theoretical studies (which predict a rich variety of grounds states, ranging from a gapless spin liquid to Néel order), many important details of its phase diagram remain controversial or even missing. To test the theory experimentally, a precise information on the spin-Hamiltonian parameters for the materials of interest is highly demanded. Here, we present results of high-field electron spin resonance (ESR) studies of spin-1/2 Heisenberg AF $Cs_2CuCl_4$ and $Cs_2CuBr_4$ with distorted triangular-lattice structures. In the magnetically saturated phase, quantum fluctuations are fully suppressed, and the spin dynamics is defined by ordinary spin waves (magnons). This allows us to accurately describe the magnetic excitation spectra in both materials and to determine their exchange parameters using the harmonic spin-wave theory [1].

The viability of the proposed method was first proven by applying it to $Cs_2CuCl_4$, revealing good agreement with inelastic neutron-scattering results. For the isostructural $Cs_2CuBr_4$ we obtain $J/k_B$=14.9 K, $J'/k_B$=6.1 K, [$J'/J$~0.41], providing exact and conclusive information on the exchange coupling parameters in this frustrated spin system. We argue, that the proposed approach can have a broader impact, potentially used for *any* quantum AF with reduced (e.g., by the staggered Dzyaloshinskii-Moriya interaction) translational symmetry, resulting, as predicted, in emergence of a new exchange mode above the saturation field.

In addition, we show that the presence of a substantial zero-field gap, ~10 K, observed in the ESR spectrum of $Cs_2CuBr_4$ below as well as above $T_N$, can be interpreted in the frame of the triangular-lattice AF model, indicating good agreement with results of spin-wave calculations [2]. The peculiarities of the ESR spectrum will be discussed taking into account the effect of the Dzyaloshinskii-Moriya interaction present in both materials.

This work was supported by Deutsche Forschungsgemeinschaft (DFG, Germany). We acknowledge the support of the HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL). A portion of this work was performed at the NHMFL, Tallahassee, FL, which is supported by NSF Cooperative Agreement No. DMR-1157490, by the State of Florida, and by the DOE. S.A.Z. appreciates the support of the Visiting Professor Program at Osaka University, Japan.

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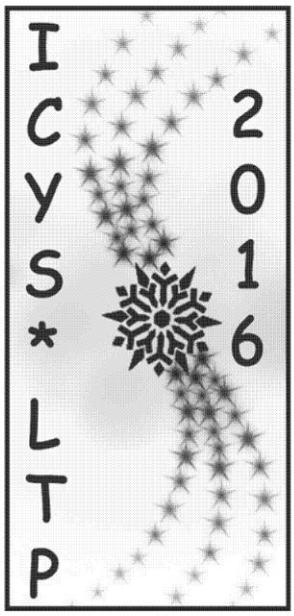
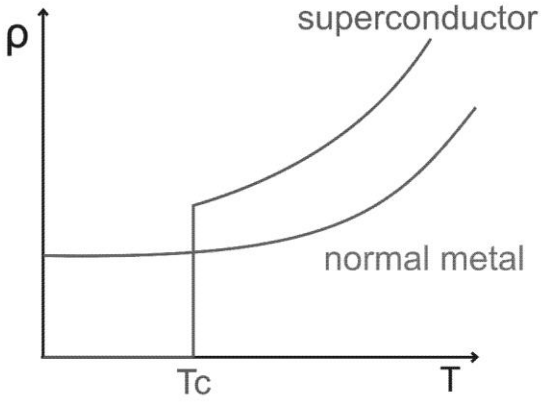
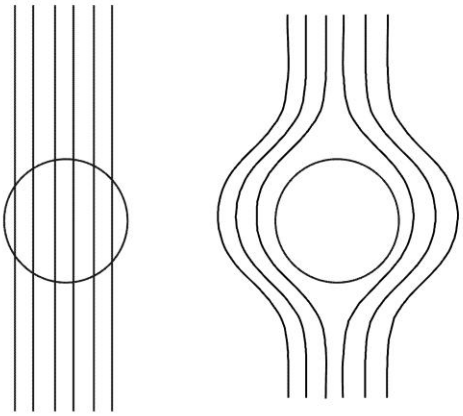
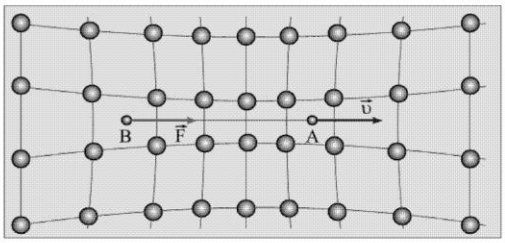
# Electronic Properties of Conducting and Superconducting Systems





# PSEUDOGAP AND FLUCTUATION CONDUCTIVITY IN $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ SINGLE CRYSTALS WITH DIFFERENT PRASEODYMIUM (Pr) CONTENT

**L. V. Omelchenko[1], A. V. Solovjov[1], R. V. Vovk[2]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2]Physics Department, V.N. Karazin Kharkiv National University, 4 Svoboda Sq., 61077 Kharkiv, Ukraine*

*e-mail: omelchenko@ilt.kharkov.ua*

Pseudogap (PG), which is opening in the excitation spectrum at the characteristic temperature $T^* >> T_c$, remains to be one of the most interesting and intriguing property of high-temperature superconductors (HTS's) with the active $CuO_2$ plane (cuprates) [1]. It is believed at present that the proper understanding of the PG physics has to give the possibility to decipher the basic pairing mechanism in the HTS's which is still uncertain. The conductivity characteristics of the HTS's compounds can be tailored through total or partial substitution of their components.

In this aspect, the $Y_{1-x}Ba_2Cu_3O_{7-\delta}$ compound has been studied more thoroughly and most rare-earth elements when substituted for yttrium (Y) yielded superconductors. Of particular interest in this aspect is the partial substitution of Y by praseodymium (Pr), which leads to the suppression of the superconductivity and allows the lattice parameters and oxygen stoichiometry of the compound to remain practically unaltered. The investigation of the impact of Pr impurities on the conditions and regimes of existence of the fluctuation conductivity state of such compounds plays an important role to elucidate the nature of HTS's but also for determining empirical ways of raising their critical parameters [2]. In the paper, effect of the Pr doping ($0.19<x<0.43$) on the magnitude and temperature dependence of the PG in $Y_{1-x}Pr_xB_2C_3O_{7-\delta}$ (YPrBCO) single crystals was studied for the first time over the temperature range from T* down to $T_c$.

Independently on effect of Pr, near $T_c$ the excess conductivity $\sigma'$ (T) is well described by the Aslamasov-Larkin and Hikami-Larkin fluctuation theories demonstrating 3D-2D crossover with increase of temperature. The result points out the presence of the fluctuating Cooper pairs in the samples, which are believed to be responsible for the PG formation.

In the basic sample ($x = 0$ $T_c = 91.67$ K) the PG temperature dependence $\Delta^*(T)$, shows the maximum $\Delta^*(T_{max}) \approx 175$ K at $T \approx 112$ K. With increasing of Pr concentration up to $x=0.19$, $\Delta^*(T_{max})$ increases and the maximum becomes wider. With further increase of the Pr concentration $\Delta^*(T_{max})$ decreases, and the maximum is noticeably smeared out and shift towards higher T. At the same time, $T_c$ monotonically decreases down to about 38.5 K whereas T* greatly increases up to ~ 238 K. According, for $x = 0.43$ the shape of the PG changes radically. Now the sharp peak of $\Delta^*(T)$ is observed at $\Delta^*(T_{max}) = 417$ K at $T_S \approx 229$ K, followed by a linear descanding region with a positive slope $\alpha \approx 7.2$ to $T_N = 210$K ($\Delta^*(T_N) \approx 292$K), below which the $\Delta^*(T)$ is a smooth curve with positive curvature down to $T_G = 40$K. Such dependence is typical for the magnetic superconductors of the $SmFeAsO_{0.85}$ type [3] and most likely is determined by the influence of the own magnetic moment of Pr ($\mu Pr = 4.6$ $\mu B$). The magnetic superconductors $T_S$ – corresponds to the structural transition and $T_N = T_{SDW}$ designates transition to the spin density wave mode (SDW) [3], which in our case can occur most likely due to antiferromagnetic spin ordering of Pr.

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# SPECIFIC FEATURES OF THE EXCESS CONDUCTIVITY AND PSEUDOGAP BEHAVIOR IN $FeSe_{0.94}$ IRON-BASED SUPERCONDUCTORS

**E. V. Petrenko[1], V. B. Stepanov[1], A. L. Solovjov[1], K. Buchkov[2], E. Nazarova[2]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2]Institute of Solid State Physics, Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria*

*e-mail: petrenkoyevgen@yandex.ua*

Pseudogap (PG), which opens at the T* >> T[1], where $T_c$ is the superconducting (SC) transition temperature, is one of the most intriguing properties of cuprate high-$T_c$ superconductors (HTSCs). However, the PG physics is still not completely clear. In resistivity measurements PG appears as a downturn of the longitudinal resistivity ρ(T) at T≤T* from its linear dependence $\rho_N(T)$ at higher T. This leads to excess conductivity $\sigma'(T) = [1/\rho(T) - 1/\rho_N(T)]$. Similar σ′(T) is observed in the iron-based superconductors, for example, in FeSe. However, the question as for the PG presence in such compounds, which is associated with a decrease in the density of states at the Fermi level, remains highly controversial.

For the first time, temperature dependences of σ′(T) measured on three $FeSe_{0.94}$ samples has been studied in detail. Two samples were prepared by partial melting method, and the sample, in which 4wt% Ag was added, had the least resistance. The third sample was produced by solid-state reaction method (SSR) [2]. It was shown that in the range from $T_c$ up to $T_{01}$ (~ 10 K above $T_c$) σ′(T) obeys the classical fluctuation theories of Aslamazov-Larkin (AL) and Maki-Thompson (MT), pointing to the existence of fluctuating Cooper pairs (FCPs) in FeSe in this temperature range. Like in cuprates, AL-MT crossover at $T_0<T_{01}$ is observed, which allows to determine the coherence length along the c-axis: $\xi_c(0) \sim 2.8$ Å, in good agreement with results of Ref. [2].

PG parameter Δ*(T) was calculated within the local pair (LP) model [1]. For all samples studied, Δ*(T) shows a narrow peak corresponding to the first structural transition at T ~ 245 K [3]. Then there is a minimum at $T_s$ ~ 90-100 K corresponding to a structural transition from the tetragonal to orthorombic phase, which is followed by the transition to AF state of SDW-type typical for Fe-pnictides [3]. It was shown that the second structural transition is accompanied by the sharp decrease of magnetization at T≤$T_s$, which can be considered as the evidence of the synchronous magnetic transition [2]. Simultaneously the parameter Δ*(T) of all samples was observed to increase. With a further temperature cooling, the values of Δ*(T) initially increases, but then undergoes a noticeable reduction below 50 K and 70 K for the SSR (sample 1) and the sample with silver (sample 2), respectively. At the same time no peculiarities of Δ*(T) were found for the third sample, in which the features of the hexagonal phase were indicated by X-ray analysis [2].

At $T_{01}$ the next minimum of Δ*(T) is observed (samples 1 and 2). Accordingly, below $T_{01}$, where the transition to SC fluctuations occurs, Δ*(T) gradually increases, showing all features being typical for cuprates as T approaches to $T_c$ [1]. The finding suggests the LP presence in $FeSe_{0.94}$ near $T_c$. Nevertheless, the question about the role of the local pairs in the possible PG state formation in Fe-pnictides, still remains open.

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# INFLUENCE OF ALTERNATING MAGNETIC FIELD ON PHYSICAL AND MECHANICAL PROPERTIES OF CRYSTALS

**V.I. Karas[1,2], E.V. Karasyova[1], A.V. Mats[1], V.I. Sokolenko[1], A.M. Vlasenko[1], V.E. Zakharov[3,4]**

*[1]National Science Center «Kharkov Institute of Physics and Technology» of the National Academy of Sciences of Ukraine, 1 Academicheskaya, str., Kharkiv, 61108, Ukraine*
*[2]V.N. Karazin Kharkiv National University, 4 Svoboda, sq., Kharkiv, 61022, Ukraine*
*[3]P.N. Lebedev Physical Institute of the Russian Academy of Sciences, 53 Leninskij Prospekt, 119991, Moscow, Russia*
*[4]L.D.Landau Institute for Theoretical Physics of the Russian Academy of Sciences, 142432, Moscow Region, Chernogolovka, Akademika Semenova av., 1-A, Russia*
*e-mail: karas@kipt.kharkov.ua*

The results of the investigation of the creep characteristics and activation parameters of polycrystalline nickel (of 99.996% purity) plastic flow at the temperature of 77 K will be presented. The influence of non-stationary magnetic field of strength of 500 oE (harmonic (50 Hz) [1] and monopolar pulses of the same frequency) upon the nickel creep characteristics was studied. We have deliberately conducted experimental researches of the influence of non-stationary magnetic field of alternating and constant sign at constant temperature in order to estimate the contribution to the dislocations mobility from the interaction of dislocations with the mobile domain boundaries and also from the heat effects connected with the induction electric field.

Experiments shown, that turning on of the stationary magnetic field of the strength of 500 oE during the creep of nickel specimens leads to the increase of strain, and turning off of the magnetic field is also accompanied by the growth of strain. Weakening takes place with the change of magnetic field from 0 to 500 oE and conversely. After turning on and off the magnetic field with different growth time the form of the creep curves changes essentially: the lesser the growth time the greater the strain rate jump for each investigated value of strength.

Weakening under the action of monopolar pluses and stationary field with the growth time of 1 s practically coincides in a wide range of creep strain stages. In case of harmonic pulses, the weakening grows essentially with the increase of strain.

To estimate the contribution of induction part of electric field generated by change of the monopolar magnetic field induction we have performed experimental research on the influence of pulse current density upon flow stress decrease. Comparative tests were conducted on similar samples of polycrystalline nickel of high purity (99.996 %). Electric current density parameters corresponded to the strength of electric field that emerged as a result of action of monopolar magnetic field pulses at creep study. At electric pulse conduction the flow stress decreases approximately on 1% that corresponds to 0.1% strain.

The proposed model of EPE suggests the following mechanism of weakening under the action of electric field [2]. Electric field gives energy to conductivity electron subsystem, making in thermodynamically nonequilibrium. Nonequilibrium electrons while interacting with acoustic phonons transfer more energy to short-wave part of the spectrum. Short-wave phonons due to large stress gradient effectively detach dislocations from stoppers.

Experimental results qualitatively match with the data obtained after numerical calculations.

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# PECULIARITIES OF AVALANCHES DYNAMICS OF MAGNETIC FLUX IN HARD SUPERCONDUCTORS

**E. I. Kuchuk**

*O.O. Galkin Donetsk Institute for Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 46, Kyiv, 03680, Ukraine*

*e-mail: elenkuchuk@gmail.com*

The results of investigations of magnetic flux dynamics at thermomagnetic avalanches in finite superconductors, obtained using integral and local measurements methods, are presented. The role of demagnetizing factor in the dynamic formation of a complex magnetic structure of the critical state of hard superconductors was determined.

New features in the behavior of the magnetic flux during and after the avalanche were discovered and changes of induction structures in area of avalanche spots are also explained. Two stages of the formation of the induction structures in the avalanche area were established, i.e. stages of homogeneous and heterogeneous filling with the magnetic flux. The mechanism of the inversion of the induction profile was considered. The oscillations of the flux front velocity at avalanches in Nb and NbZr discs were revealed. The frequencies of these oscillations for low temperature superconductors are within a few kHz and depend on the physical characteristics of material.

Transformation of the critical state near the edge of the sample was analyzed. The role of thermal effects and of demagnetizing factor in the dissipative flux dynamics was shown.

To understand the reasons of the essential restructuring of the induction profile the literature data on flux dynamics visualization during avalanches [1-6], which obtained by magneto-optical methods and the calculation results of field penetration into superconducting discs, were analyzed.

The transformation of Meissner hole cavities [7-8] during the destruction of critical state as a result of the thermomagnetic avalanches in trapping flux mode was found. Peculiarities of the Meissner hole behavior in various superconducting materials (Nb, single crystal $MgB_2$ [9]) are discussed.

The simple model of current transformation, explaining the local inversion of the magnetic induction profile inside the avalanche spots as a result of the avalanche magnetic flux input or output, was proposed.

In the framework of the Bean concept, the model of induction transformation of the critical state and of the superconducting currents of a finite superconductor as result of flux avalanches for regimes of screening and trapping of the magnetic flux was presented.

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# SPIN-CURRENT INDUCED SWITCHING BETWEEN STATES OF THE NONCOLLINEAR ANTIFERROMAGNET IrMn

**V. Kuchkin[1], O. Gomonay[1,2]**

*[1]National Technical University of Ukraine "KPI", 03056, Kyiv, Ukraine*
*[2]Institut fur Physik, Johannes Gutenberg Universitat at Mainz, D-55099 Mainz, Germany*
*e-mail: kychkinvladislav@gmail.com*

Antiferromagnets (AFs) – magnetically ordered materials with vanishingly small macroscopic magnetization, – are sensitive to spin currents and thus make an alternative to ferromagnetic spintronics. Magnetic memories based on AF would be robust against magnetic fields and fast compared to their ferromagnetic counterparts [1]. However, electrical reading of AF states is of great challenge. $IrMn_3$, metallic AF with triangular spin ordering [2], is a perspective candidate for spintronic applications as it shows large inverse spin Hall effect [3] which enables reliable read-out of states. In this paper we analyze spin-current induced magnetic dynamics of spins in IrMn3 and find the optimal parameters for reliable switching of localized spins.

We consider two states (logical "0" and "1") corresponding to spin ordering in (111) and (11-1) planes (Fig.1.A). Starting from the Landau-Lifshitz-Gilbert-Slonszuski equations for sublattice magnetizations we show that the spin current polarized in [001] direction induces rotation of localized spins around the fixed axis. In this case the magnetic dynamics can be effectively parametrized with the single variable – the rotation angle $\theta$, and conjugated generalized momentum – rotational frequency, $\Omega$.

Different switching scenarios for the case of ultra-short current pulses are analyzed in terms of phase trajectories (Fig.1.B). During short pulse the spin-polarized current transfers initial nonzero momentum to localized magnetizations which value depends upon the pulse amplitude and thus induces rotations. If corresponding "kinetic" energy is large enough for overcoming of the potential barrier between states 0 and 1, the switching will be successful. However, if the momentum is too large, the system will travel around the bathes of both states and can end up in the initial one. We calculate the range of the current amplitudes which allow reliable switching with account of damping effects during the current pulse. The results obtained could be used for tailoring all-electrically controlled spintronic devices based on AF materials.

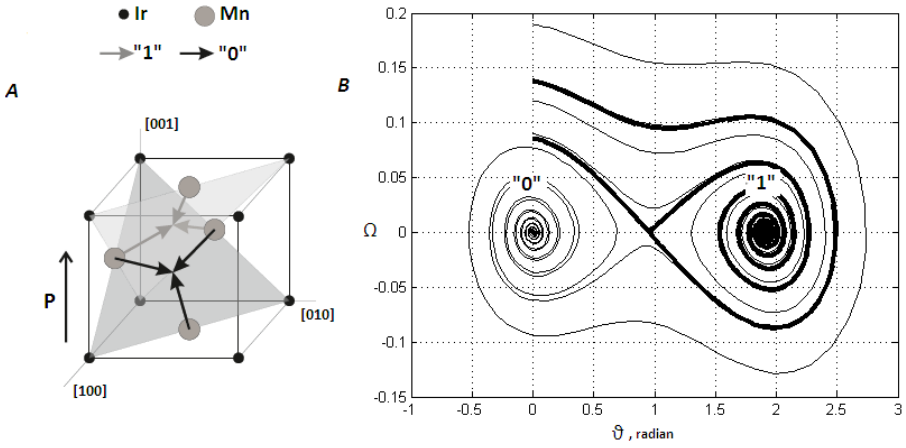


Fig. 1. (**A)** Structure of $IrMn_3$, two stable configurations and direction of spin polarization **P** are indicated. (**B)** Phase portrait in ($\theta$, $\Omega$) plane. Separatrices (bold lines) show the window for trajectories corresponding to switching between states 0 and 1.

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# SOLITON DYNAMICS IN AN ASYMMETRIC ARRAY OF JOSEPHSON JUNCTIONS

**I. O. Starodub, Ya. O. Zolotaryuk**

*Bogolyubov Institute for Theoretical Physics of NAS of Ukraine,*
*14-b, Metrolohichna Str., 03680 Kiev, Ukraine*

*e-mail: starodub@bitp.kiev.ua*

The Josephson vortices or fluxons have a physical meaning of magnetic flux quantum propagating in the dielectric layer of Josephson junction and described as solitary waves. These are the solutions of the sine-Gordon equation for the difference of the wave function phase of the superconducting condensate in both sides away from the dielectric layer of the junction [1]. The array of the Josephson junctions represents the superconducting quantum interference device (SQUID) [2]. Fluxon dynamics in the dc-biased array of asymmetric three-junction SQUID is investigated. This array is described by the discrete double sine-Gordon equation [3]. It appears that this equation in the Hamiltonian limit possesses a finite set of velocities (sliding velocities) at which the fluxon propagates with the constant shape and without radiation. The dependence of these velocities on the asymmetry parameter (the ratio of the critical currents of the left and right junctions of the SQUID) is shown. The signatures of sliding velocities appear on the respective current-voltage characteristics of the array as inaccessible voltage intervals (gaps). The value of this gap is depending on the asymmetry parameter and dissipation in the system. To confirm the mobility of the fluxon in such discrete system, the analysis of its motion modes for the different branches of the CVC is made with using the largest Lyapunov exponent method. The analysis confirmed the possibility of periodic motion of the fluxon around the array on the voltages lying closest to the value corresponding to the sliding velocity in the Hamiltonian limit. The critical depinning current has a clear minimum as a function of the asymmetry parameter, which coincides with the minimum of the well-known Peierls-Nabarro potential.

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# SUPERCONDUCTING VORTEX ORBITS VISUALIZED BY SCANNING TUNNELING MICROSCOPY

**T. Samuely[1], M. Timmermans[2], D. Lotnyk[1], B. Raes[2], J. Van de Vondel[2], V.V. Moshchalkov[2]**

*[1]Centre of Low Temperature Physics, Faculty of Science, P.J. Šafárik University in Košice, Slovakia*
*[2]Institute for Nanoscale Physics and Chemistry (INPAC), KU Leuven, Belgium*

*e-mail: tomas.samuely@upjs.sk*

Our innovative scanning probe microscopy technique [1] offers the possibility to visualize periodic motion at nanoscale with unprecedented temporal resolution. Hence, it allowed us to investigate in detail the behavior of superconducting vortices in $NbSe_2$ oscillating in ac magnetic field by scanning tunneling microscopy. We observed the hitherto well-known vortex motion along the so called "tin roof" potential. In this case, the vortex trajectory seemingly coincides with one of the primitive vectors of the Abrikosov lattice and the crystal lattice. However, with our approach, we were able to scrutinize this motion and reveal the unforeseen intricacy of the trajectory. On top of that, we observed a transverse trajectory at lower amplitudes of the ac field. We analyzed the differences of the observed trajectories and their time evolution.

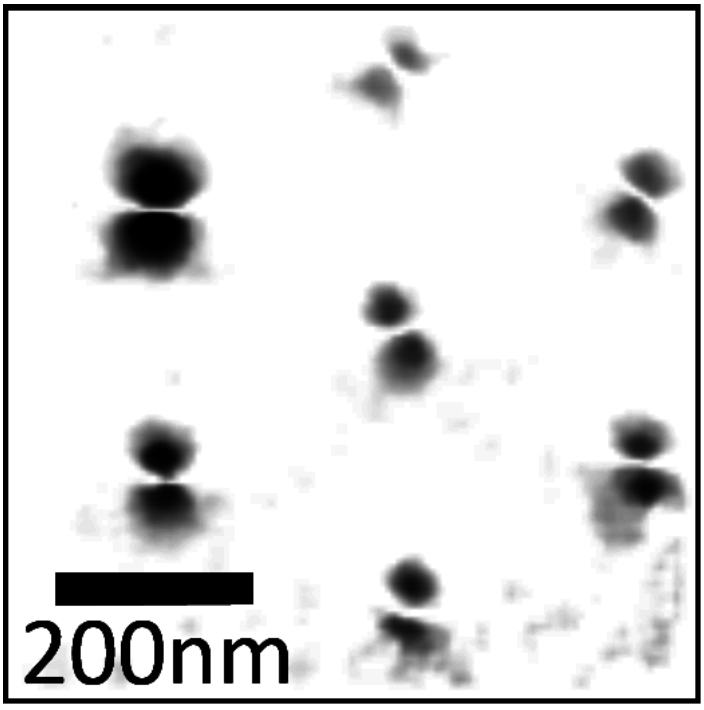


Figure: First harmonic of the differential conductance reveals vortices oscillating in ac magnetic field with varying direction and amplitude.

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# THE EFFECT OF SINTERING IN DIFFERENT ATMOSPHERE ON SUPERCONDUCTIVITY PARAMETERS OF YBCO

**M. Başoğlu[1], İ. Düzgün[2]**

[1]*Gümüşhane University, Department of Energy Systems Engineering, 29100, Gümüşhane, Turkey*
[2]*Gümüşhane University, Department of Physics Engineering, 29100, Gümüşhane, Turkey*

*e-mail: mehmetbasoglu@gumushane.edu.tr*

$YBa_2Cu_3O_7$ (Y123) is the first discovered superconductor with the transition temperature above the liquid nitrogen boiling temperature [1]. A lot of efforts have been dedicated to improve the superconducting properties of YBCO compound such as microstructure, critical current density, and transition temperature [2, 3]. One of these studies is about sintering in oxygen, air and argon atmosphere of Y-123, which shows that sintering in atmosphere, affects the critical current density of Y-123 superconductor prepared by a chemical pyrophoric reaction process. They found the highest value of critical current density of Y-123 when sintered in argon atmosphere [4].

In this study, Y123 superconductor was produced by solid-state reaction technique. During the production process, superconducting samples were sintered in argon and oxygen gas mixture in certain rations. XRD, M-T and M-H measurements of the samples were performed. The results of the measurements showed that the superconducting phases peaks were formed and Meissner effect observed in all samples. The critical temperature of samples was observed to be decreased relatively by a small amount with increasing rate of argon gas. The highest calculated critical current from M-H loops was observed in the sample that sintered in 50 % Ar- 50 % $O_2$ gases atmosphere.

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# EFFECT OF Dy SUBSTITUTION AT Ca SITES IN BSCCO CERAMIC SUPERCONDUCTORS

**İ. Düzgün[1], A. Öztürk[2] and S. Çelebi[2]**

[1]*Gümüşhane University, Department of Physics Engineering, 29100, Gümüşhane, Turkey*
[2]*Karadeniz Technical University, Department of Physics, 61080, Trabzon, Turkey*

*e-mail: ibrahimduzgun@gumushane.edu.tr*

We have investigated the effect of the partial substitution of Dy at Ca sites in the Bi-2212 superconducting samples with the nominal stoichiometry of $Bi_2Sr_2(Ca_{0.8}Dy_{0.2})Cu_2O_y$ prepared by standard solid-state reaction method. The sample was characterized by AC susceptibility and X-ray diffraction (XRD) measurements. AC susceptibility of Dy doped BSCCO superconducting sample was measured as a function of temperature at selected field amplitudes for $f$= 20 Hz and $f$=1000 Hz. Both XRD patterns and AC susceptibility data reveal that there exists both Bi-2212 and Bi-2223 phases. The possible reasons for the observed data on microstructural and superconducting properties due to Dy substitution were discussed.

# JOSEPHSON EFFECT IN GRAPHENE JUNCTIONS

**P. P. Shyhorin, I. P. Dmytruk and Yu. Datsiuk**

*Lesya Ukrainka East European National University,*
*Prospekt Voly, 13, Lutsk 43025, Ukraine*

*e-mail: pashyh@gmail.com*

We investigate the Josephson effect in the superconductor-graphene-superconductor junction (SGS-junction) with arbitrary barrier thickness and applied gate voltage across the barrier. We have shown that in the thin barrier limit the electronic transport properties in this junction are similar to the ones in a superconductor-isolator-normal metal-superconductor junction (SINS).

Using an equations for microscopic theory of superconductivity, we obtain the analytical expression for Josephson current through the SGS-junction. The Josephson current shows oscillatory behavior as a function of the barrier thickness and applied gate voltage. Such behavior can be understood in terms of resonant tunneling of Dirac-Bogoliubov quasiparticles in graphene.

We also study the energy dispersion of the subgap Andreev bound states.

# YANSON POINT-CONTACT SPECTROSCOPY OF TERNARY RARE-EARTH COPPER ANTIMONIDES $LaCuSb_2$

**N. V. Gamayunova, O. E. Kvitnitskaya, A. V. Terekhov, Yu. G. Naidyuk**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: gamayunova@ilt.kharkov.ua*

Ternary intermetallic compounds $RETSb_2$ (RE – rare-earth metals, T – transition metals) draw much attention because of their interesting low-temperature phenomena [1] and similarity of their crystal structure to that of the 112-type iron-based superconductors [2]. $LaCuSb_2$, belonging to this group of materials, shows a typical metallic behavior of the specific electrical resistivity temperature dependence and becomes superconducting below $T_C$=0.9 K [1].

We have investigated $LaCuSb_2$ in the normal state by the Yanson point-contact (PC) spectroscopy [3] to obtain the information about the electron-phonon interaction (EPI) function in this material. We have measured the 1st and 2nd derivatives of the current-voltage characteristics (CVC) for the homocontacts of $LaCuSb_2$ and heterocontacts $LaCuSb_2$–Ag. The 1st derivatives of CVC (or differential resistance) of PCs (Fig.1, inset) show the metallic behavior with a low value of $\Delta R/R$, that can be an evidence in favor of the spectral (ballistic or diffusive) regime of the current flow in the contact. Most of the 2nd derivatives of CVC (or point-contact spectra) display a pronounced maximum at about 20 mV (Fig.1), but there were other spectra which demonstrate features also at 11, 15 and 17-18 mV. Therefore, the obtained spectral features, which are located at the characteristic energies of the phonon frequencies in metals, can be associated with EPI in $LaCuSb_2$. It is the primary information to identify the obtained peaks with the EPI processes in the $LaCuSb_2$ compound.

The authors thank A.J. Zaleski for the providing of $LaCuSb_2$ samples.

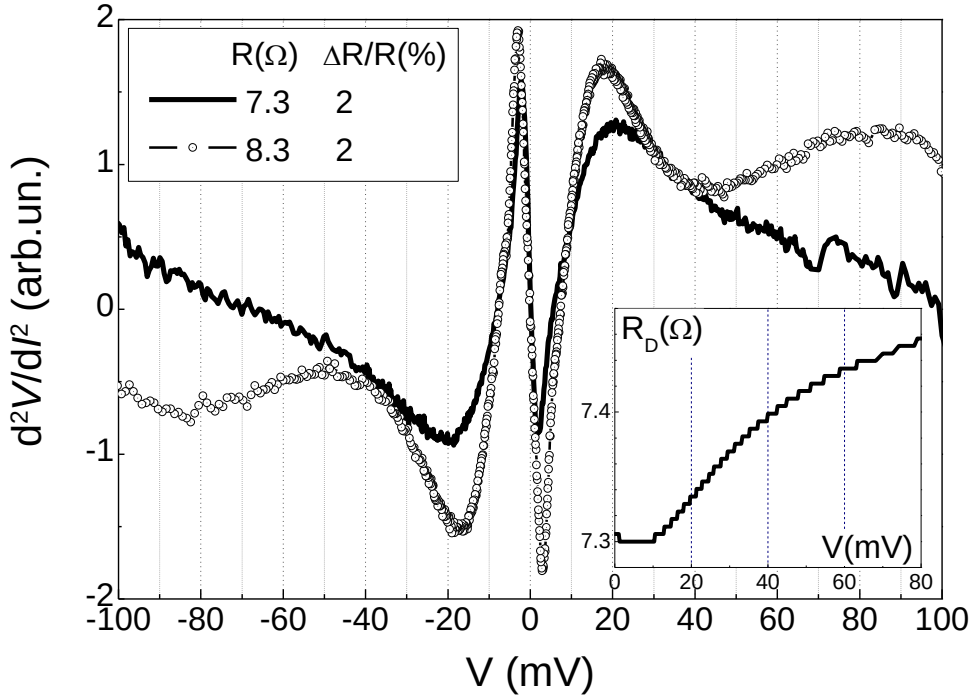


Fig.1 – PC spectra for two PCs of $LaCuSb_2$ measured at 4.2K. Inset: differential resistance $R_D=dV/dI$ for the corresponding curve in the main panel (solid line) with R=7.3Ω.

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# PHOTON TRANSPORT IN QUBIT-RESONATOR STRUCTURES

**D. S. Karpov[1], A. N. Sultanov[2], Ya. S. Greenberg[2], S. N. Shevchenko[1,3]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2]Novosibirsk State Technical University*
*20, Prospekt K. Marksa, Novosibirsk, 630073, Russia,*
*[3]V. N. Karazin Kharkiv National University,*
*Svobody Sq. 4, 61022, Kharkiv, Ukraine*

*e-mail: karpov@ilt.kharkov.ua*

A system composed of qubits coupled to the electromagnetic fields in resonators, represents a mesoscopic analogue of atoms coupled to light fields in optical cavities, and similar effects have been studied on atomic systems.

We study the real solid-state hybrid systems, which consist of two superconducting qubits and open line resonator. We considered the case, when the resonator is assumed to be driven by single photon. The detection of the output photon state allows describe qubits states. Such configuration can be realized experimentally.

We provide a full quantum-mechanical approach for description of this system behavior. The introduced approach sufficiently easy allows finding the information on the transport properties of the cavity mode and the two-level system. We propose to use non-Hermian Hamiltonian approach [1, 2, 3]. Also we calculate a quantum entanglement measure of the system.

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# EFFECT OF PRESSURE ON $MgB_2$-LCMO NANOCOMPOSITE

**V. V. Kononenko[1], V. Yu. Tarenkov[1], V. N. Krivoruchko[1], A. I. D'yachenko[2]**

*[1]O.O. Galkin Donetsk Institute for Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 46, Kyiv, 03028, Ukraine*
*[2]G.V. Kurdyumov Institute for Metal Physics of NAS of Ukraine, boulevard Vernadsky, 36, Kyiv, 03680, Ukraine,*

*e-mail: vkkononenko@gmail.com*

We investigated the possibility of current flow through a ferromagnetic manganite layers in superconductor-half-metal composite, which consists of the s-wave $MgB_2$ superconductor and $La_{0.7}Ca_{0.3}MnO_3$ (LCMO) ferromagnetic. The composite's specifity is significant difference in the size of the components: microgranules $MgB_2$ ($d$≈5μ) and nanogranules LCMO ($d$≈50nm). After thorough mixing, the composite was pressed under pressure 50 kbar without further heat treatment.

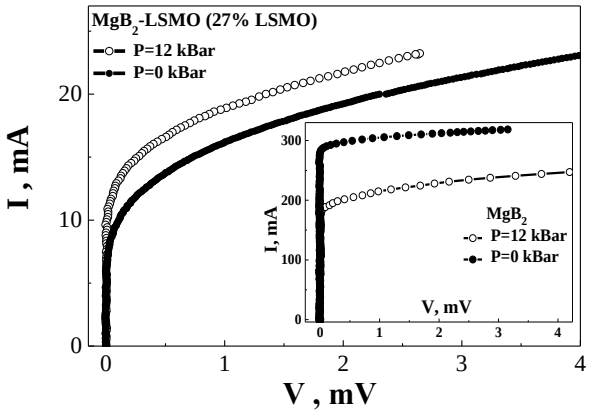


Fig. 1 Effect of high hydrostatic pressure on the CVC $MgB_2$-LCMO composite (27% LCMO). The inset shows the effect of pressure on the CVC $MgB_2$ pressed powder

The effect of high hydrostatic pressure on the current voltage characteristic (CVC) $MgB_2$-LCMO composite (27% LCMO) is shown in fig.1. Here the inset shows the effect of pressure on the CVC $MgB_2$ pressed powder. As it seeing from the figure, under the effect of hydrostatic pressure the composites critical current increases, whereas for the $MgB_2$ samples the critical current under pressure decreases. Such behavior of magnesium diboride is typical for conventional superconductors, in which the order parameter under hydrostatic pressure decreases. The critical current increase of the $MgB_2$-LCMO composite proves the manganite participation in supercurrent flowing. It means that through the LCMO half-metal layer superconducting current can flow. Flowing of a supercurrent through chains of superconductor-half-metal-superconductor points on the existence of the spin -active boundary [1, 2] on a surface of the manganite layer, which transforms the Cooper pairs with s-wave symmetry into pairs with p-wave symmetry.

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# CONDUCTIVE CHARACTERISTICS OF ANION-RADICAL TCNQ SALTS WITH COMPLEX CATIONS

**A. S. Bukrinev[1], A. S. Krasnyi[2], A. S. Mazitov[1], S. V. Vitushkina[1], A. V. Khotkevich[1,2]**

*[1] V.N. Karazin Kharkiv National University, Svobody Sq., 4, Kharkiv 61022, Ukraine*
*[2]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*

*e-mail: krasnyi@ilt.kharkov.ua*

Growing interest to organic conductors, and in particular to compounds based on 7,7',8,8'-tetracyanoquinodimethane (TCNQ), is due to their unusual electrical, magnetic and structural properties [1]. By the date a wide range of possible applications of such objects as functional materials with respect to requirements of modern technologies was demonstrated. Development of new synthetic conductors becomes topical and studying of their physical characteristics is dictated by interests of both fundamental and applied science.

In this work the electrical characteristics of a new class of TCNQ anion-radical salts with heterocyclic diamines based cations which were synthesized for the first time are studied.

Single crystals of the salts as well as formed at high pressure tablets were fabricated. The temperature dependencies of resistance were captured in the temperature interval 77-300K at the He exchange gas atmosphere. The DC electrical measurements were performed using the two-point connection scheme with electrical contacts made of graphite paste. At room temperature the value of specific electrical resistance was determined. In doing so the van der Pauw method [2] was employed for the tablet samples. For the salts containing cations $[M^{II}(bipy)_3]^{2+}$ (M – Fe, Ni or Zn, bypi – 2,2'-dipyridil) specific conductivity at room temperature equals to 7.7, $2.3\cdot10^{-2}$ and $2.5\cdot10^{-2}$ $Ohm^{-1}\cdot cm^{-1}$, respectively. The temperature dependencies of resistance provide evidence that the studied compounds are narrow-band semiconductors with thermo-activated character of conductivity. The experimental data enabled high-precision calculations of values of the prohibited band widths in the electron spectrum.

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# ABOUT AN INFLUENCE OF A HIGH DENSITY CURRENT ON A CRITICAL CURRENT OF NIOBIUM BRIDGES

**S. I. Link[1], V. P. Koverya[1], A. V. Krevsun[1], E. V. Ilichev[2], U. Hubner[2], S. I. Bondarenko[1]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2] Leibniz Institute of Photonic Technology, e. V. Albert-Einstein-Straße 9 (Beutenberg Campus) 07745, Jena,Germany*
*e-mail: link@ilt.kharkov.ua*

An influence of high density current (HDC) on mechanical properties of metallic materials is investigated widely in last time [1]. An influence of HDC on critical current ($I_{tc}$) of niobium thin film have been tested in distinction from this investigations. The bridges can have the properties of Josephson contacts and the investigation of their properties after an influence of different factors is actual problem. The bridges with sizes 0.2 x 0.3 x 0.1 microns were fabricated by electronic lithography method of a film deposited on a single crystal silicon substrate by electron beam evaporation. Impulse current ($I$) thought the bridge has been created by a charge of a capacitor with a capacity 4 x$10^{-5}$ F into a bridge current circuit placed into helium steam at temperature 20K. After the charge the bridge was immersed into liquid helium and a value of $I_{tc}$ was measured. Criterion of $I_{tc}$ value was an occurrence of voltage $10^{-7}$ V on the bridge at increase in a transport current ($I_t$) through it. Reduction of $I_{tc}$ after the capacity category is revealed. Dependence of $I_{tc}$ on peak value of density $j_m$ of a current $I$ is shown in a Fig. 1.

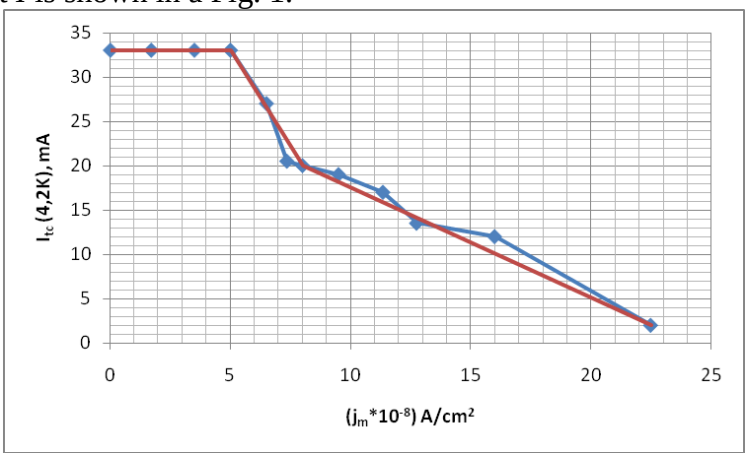


Fig.1 Dependence of a critical current of the bridge on amplitude of a density of a pulse current passed through it.

Work [1] contains data about local melting of a steel under the influence of a pulse current with $j = 10^6$ A/cm$^2$. In our case the amplitude of density of a pulse current is much more (Fig. 1). It can lead to short-term melting of the bridge and a substrate surface layer under it. There is possible a mixing niobium with silicon and transformation of the bridge after cooling in small dispersion structure of superconducting and not conducting clusters. Parity and links between them will define the $I_{tc}$ value of the bridge. From a Fig. 1 follows, that at increase $j_m$ value $I_{tc}$ decreases in tens times that it is possible to connect with reduction of a portion of superconducting links in the bridge. Possibility of a $I_{tc}$ control by means of HDC can make, in particular, manufacturing of quantum devices with bridges cheaper, than now [3].

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# SPECIFIC HEAT STUDY OF SUPERCONDUCTIVITY IN β-$Bi_2Pd$

**O. Mezhenska[1], J. Kačmarčík[2], Z. Pribulová[2], H. Suderow[3], D. Prabhakaran[4], P. Samuely[2]**

*[1]V. N. Karazin Kharkiv National University, Svobody sq., 4, Kharkiv, 61022, Ukraine*
*[2]Centre of Low Temperature Physics @ Institute of Experimental Physics, Slovak Academy of Sciences and P. J. Šafárik University, 04001 Košice, Slovakia*
*[3]Laboratorio de Bajas Temperaturas, Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center,Universidad Autónoma de Madrid, E-28049 Madrid, Spain*
*[4]Department of Physics, Clarendon Laboratory, University of Oxford, Park Road, Oxford OX1 3PU, UK*

*e-mail: elenamezhenskaya@mail.ru*

Recently it has been proposed that the $\beta$-$Bi_2Pd$ compound is another example of a multi-band/multi-gap superconductor [1]. The report was based on a bulk measurement of the specific heat using relaxation method, as well as by the surface sensitive transport measurements, though only in restricted temperature range down to 2 K.

Here we report the bulk calorimetric studies performed by very sensitive ac technique in the temperature range down to 0.6 K. We examined a single crystal of $\beta$-$Bi_2Pd$ with the critical temperature $T_c$ close to 5 K. All the measurements show sharp and well defined specific heat anomaly at the superconducting transition and exponential decrease at low temperatures as expected for an s-wave superconductor. Moreover, we inspected in details a shift of the anomaly with the angle between the applied magnetic field and the crystallographic structure of the sample at fixed field. Surprisingly, contrary to the previous results both, the overall temperature dependence of specific heat as well as the angular dependence of $T_c$, compared to the theory, indicate the existence of only single energy gap in the system.

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# SUPERCONDUCTING DENSITY OF STATES OF B-DOPED DIAMOND INVESTIGATED BY TYNNELING SPECTROSCOPY

**Oleksander Onufriienko[1], Tomas Samuely[1], Gufei Zhang[2], Pavol Szabó[1], Victor V. Moshchalkov[2] and Peter Samuely[1]**

*[1]Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences & Faculty of Science, P. J. Safarik University, 04001 Kosice, Slovakia*
*[2]INPAC-Insititute for Nanoscale Physics and Chemistry, KU Leuven, Celestijnenlaan 200D, B-3001 Heverlee, Belgium*

*e-mail: oleksandr.onufriienko@student.upjs.sk*

Utilizing the scanning tunneling spectroscopy with outstanding energy resolution at 0.5 K, available in our laboratory, we were able to acquire the local density of states of the superconducting boron doped diamond polycrystal prepared by chemical vapor deposition. The obtained differential conductance spectra (Fig. 1) exhibit features that differ substantially from the standard theoretical model of Bardeen, Cooper and Schrieffer. By employing more complex theoretical models, discussed in the presented work, we were able to reproduce the measured data with higher accuracy. This work was supported by the ERDF EU (European Union European regional development fond) grant, under the contract No. ITMS 26220120005, APVV 0605-14 and VEGA 1-0409-15.

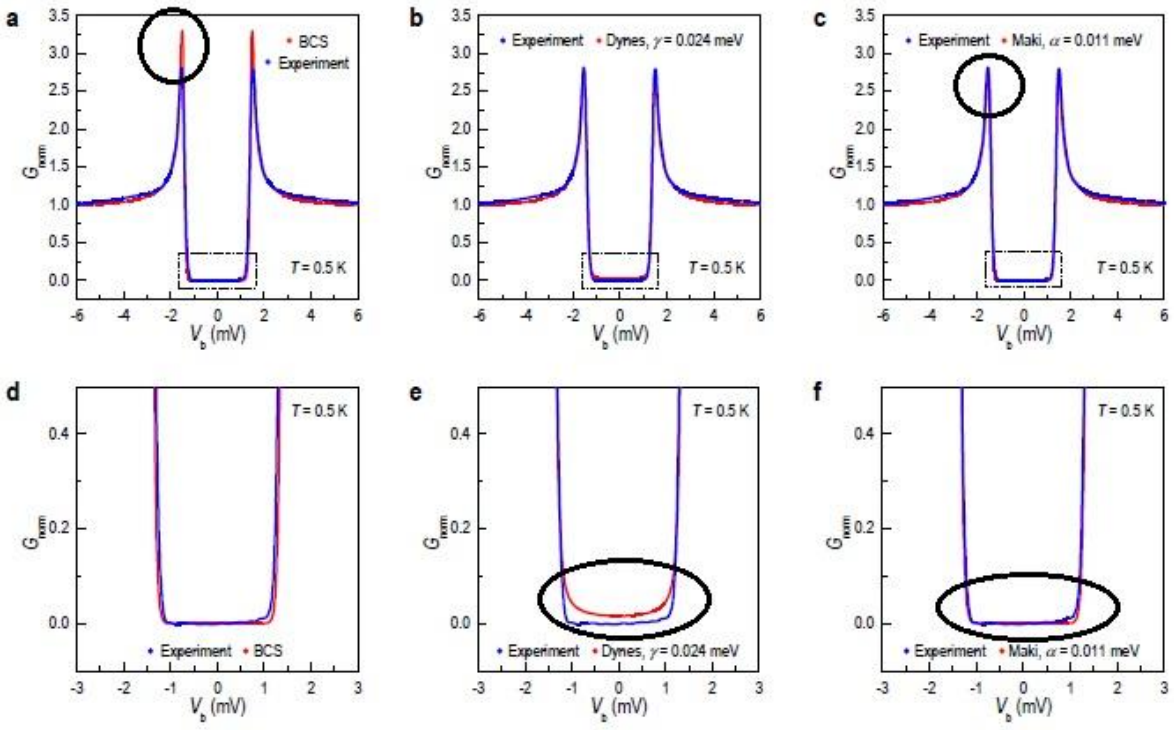


Fig. 1. Comparison the fitted parameters: a, d) BCS theory, b, e) Dynes modification with smeared parameter γ and c, f) Maki formalism with pair-braking parameter α.

# INFLUENCE OF THE DEPAIRING EFFECTS UPON THE CURRENT-PHASE RELATION IN SIS JUNCTION FOR ARBITRARY CONCENTRATIONS OF NONMAGNETIC IMPURITIES

**O. Y. Pastukh, A. M. Shutowskiy, V. Y. Sakhnyuk**

*Lesya Ukrainka Eastern European National University,*
*Potapov st., 9, Lutsk 43021, Ukraine*

*e-mail: pastukh.olexandr@gmail.com*

The equilibrium current states in superconducting junctions of SIS-type (S — superconductor, I — insulator) for an arbitrary dielectric layer transparency and in the presence of nonmagnetic impurities of arbitrary concentration are investigated. The similar analysis of the influence of dielectric layer transparency on the current-phase relation has been done for SIS junction in dirty limit in Refs. [1, 2] and in clean limit in Ref. [3].

The investigation has been done for temperatures close to the critical one, that is why the Ginzburg-Landau theory [4] has been used. The calculations have been made considering depairing effects, the presence of which in the system is reflected by the superfluid velocity term in Ginzburg-Landau equation. In case of small current values the depairing effects are insignificant, therefore this term can be neglected. If we consider bigger values of transmission coefficient, where the current can reach the magnitudes close to thermodynamic critical ones, these effects have to be taken into account, which has been done in the present research. Boundary conditions for Ginzburg-Landau equation have been received using the method of quasiorthogonality to asymptotics [5].

In addition to numerous results available in the present research, a new analytical formula for the current-phase relation for arbitrary electrons transmission values and for arbitrary electron free path has been obtained. Analytical formula for the dependence of critical current from barrier transparency and electron free path was also obtained. It is shown that the analytical result is consistent with numerical calculations very well.

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# PHASE SEPARATION IN IRON CHALCOGENIDE SUPERCONDUCTOR $Rb_yFe_{2-x}Se_2$ AS SEEN BY AB-INITIO CALCULATIONS AND RAMAN LIGHT SCATTERING

**T. Shevtsova[1], Yu. Pashkevich[1], V. Gnezdilov[2], P. Lemmens[3], S. Gnatchenko[2], E. Pomjakushina[4], and K. Conder[4]**

*[1]O.O. Galkin Donetsk Institute for Physics and Engineering of NAS of Ukraine, 03680 Kyiv, Ukraine*
*[2]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[3] Institute for Condensed Matter Physics, TU Braunschweig, D-38106, Germany*
*[4]Laboratory for Developments and Methods. PSI, CH-5232 Villigen PSI, Switzerland*

*e-mail: tatyana.shevetsova@gmail.com*

The recently discovered alkali metal intercalated iron selenide superconductors $A_xFe_{2-y}Se_2$ (A=K, Rb,Cs) has attracted great interest because they display a variety of properties unprecedented for the cuprates and iron pnictides [1, 2].

In this study we report Raman light scattering in the phase separated superconductive single crystal $Rb_{0.77}Fe_{1.61}Se_2$ with $T_c$ = 32 K. The spectra have been measured in the wide temperature region 3K -500 K. The observed phonon lines from the majority vacancy ordered antiferromagnetic phase demonstrate anomalies in frequency, intensity and halfwidth at the superconductive phase transition. The superconductive gap features are surely detected, whereas the two-magnon features that are expected for insulating antiferromagnetic phase were not detected in our spectra. Besides in the range 0-600 $cm^{-1}$ we observe highly polarized $B_{1g}$ type background which becomes well structured under cooling.

For interpretation of experimental results we have carried out ab-initio calculations. Our calculations have been performed within the density functional theory framework with a full-electron potential and an augmented plane-wave method – the program ELK [3]. We calculated the zone-center phonons and electronic structure of vacancy ordered $Rb_2Fe_4Se_5$ in both magnetic and superconductive phases. We identify phonon lines from the minority superconductive phase. Also we obtained the changes in band structure during the transformation from minority to majority phase. Furthermore, we calculated phonon spectra of vacancy free superconductive phase $RbFe_2Se_2$ [4].

The possible magnetic or orbital origin of highly polarized and well structured low intensive background has been discussed. We demonstrate that compressed vacancy ordered phase can be in the metallic state and therefore may serve as protective interface phase between the pure metallic 122 phase and insulating 245 phase providing the percolative superconductivity of the $Rb_{0.77}Fe_{1.61}Se_2$.

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# EFFECT OF PRESSURE ON PARACONDUCTIVITY IN $HoBa_2Cu_3O_{7-\delta}$ SINGLE CRYSTALS WITH OXYGEN DEFICIENCY

**K. V. Tiutierieva[1,2], R. V. Vovk[1,2]**

*[1]Ukrainian State University of Railway Transport*
*Feyerbaha Sq. 7, 61050 Kharkiv, Ukraine*
*[2]V.N. Karazin Kharkiv National University*
*Svobody Sq. 4, 61022 Kharkiv, Ukraine*

*e-mail: k.v.tiutierieva@gmail.com*

In this study, we investigated the effect of high pressure on the conductivity in the basal plane of the high temperature superconducting single crystals $HoBa_2Cu_3O_{7-\delta}$ with oxygen deficiency.

It was determined that the excess conductivity $\Delta\sigma(T)$ of the $HoBa_2Cu_3O_{7-\delta}$ single crystals in the temperature interval near the critical temperature $T_c$ is isfactorily described within the theoretical model of Aslamazov-Larkin. Also showed that the evolution of the transverse coherence length $\xi_c(0)$ in the case of application/removal of high pressure is largely determined by the "relaxation" pressure effect during prolonged exposure of the sample under load at room temperature.

# CONDUCTIVITY OF INHOMOGENEOUS TUNNEL MAGNETIC BARRIER

**N. R. Vovk[1,2], Yu. A. Kolesnichenko[2]**

*[1] V. N. Karazin Kharkiv National University, Svobody Sq. 4, 61022, Kharkiv, Ukraine*
*[2] B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*

*e-mail: nikolay_vovk@bk.ru*

Images obtained using STM display standing waves related to electron scattering by single defects. The physical origin of these patterns in the constant-current mode STM images is the same type of interference that leads to Friedel oscillations in the electron local density of states in the vicinity of a scatterer. The local magnetic defect produces a long-range spin polarization of the conduction electrons, which oscillates with the distance from the defect. This effect can be detected by using spin-polarized (SP) STM

One of the models that can be applied to describe STM experiments is the model of an inhomogeneous barrier of small transparency as a part of an infinitely thin interface between two conductors [1,2]. In this report we describe the electron tunneling from the quasi-two-dimensional (surface) states with the spin-orbit interaction into bulk-mode states and in the framework of a model of an infinitely thin inhomogeneous tunnel magnetic $\delta$-barrier [3]. This model may be used to describe SP-STM experiments. The influence of the scattering of quasi-two-dimensional electrons by a single magnetic defect on the tunnel current is analyzed.

We obtain analytic formula for the conductance of a tunnel point-contact as a function of its distance $\boldsymbol{\rho}_0$ from the defect

$$G = \frac{\pi e^2}{\hbar} T_{eff}\left(\varepsilon_F\right)\rho_{3D}\left(\varepsilon_F\right)\left[\rho_{2D}\left(\boldsymbol{\rho}_0\right) + \left(\mathbf{M}_0\mathbf{M}_S\left(\boldsymbol{\rho}_0\right)\right)\right].$$

Here $T_{eff}\left(\varepsilon_F\right)$ is depends on the effective area of the contact and plays the role of the tunneling matrix element, $\rho_{2D}\left(\boldsymbol{\rho}_0\right)$ is the local density of surface states scattered by a single defect, $\rho_{3D}\left(\varepsilon_F\right)$ the densities of states (for two spin directions) for defect free the three-dimensional (3D) electron system, $\mathbf{M}_S\left(\boldsymbol{\rho}_0\right)$the local magnetization density of states around the defect, $\mathbf{M}_0$ is a dimensionless magnetization of the tunnel barrier.

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# VORTEX LATTICE OF Mo/Si AND W/Si MULTILAYERS IN TILTED MAGNETIC FIELDS

**O. I. Yuzephovich[1,2], S. V. Bengus[1,2], M. Yu. Mikhailov[1], D. Gaida[2], K. Rogacki[2]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2]International Laboratory of High Magnetic Fields and Low Temperatures, Polish Academy of Sciences, Gajowicka 95, 53-421 Wroclaw, Poland*

*e-mail: yuzephovich@ilt.kharkov.ua*

The commensurability effects were discovered on Mo/Si and W/Si multilayers, which occur in parallel to the layers and slightly inclined magnetic fields [1, 2]. At some temperature corresponding to the fitting of the vortex cores within semiconducting interlayers a minimum (or a series of minima) appears on the dependences of the resistivity $R$ on magnetic field $H$. While temperature decreases the minimum becomes more pronounced and then transforms into a large zero resistance region (ZRR). In higher magnetic fields the resistance reappears. This effect can be explained in terms of the intrinsic pinning and the vortex lattice (VL) commensurability with the underlying layered structure. Locations of the zero resistance regions correspond to the stable VL configurations. The experimental data are in quantitative agreement with the Ivlev, Kopnin, Pokrovsky theory considering VL structure in the case of a strong intrinsic pinning [3]. We proposed the resistive method (based on commensurability effects) as a tool for the VL structure study in layered superconductors [1]. This method is applicable to all layered superconducting systems and can be used in strong magnetic fields.

The lock-in transition was observed on Mo/Si [2] which takes place in weakly tilted magnetic fields. Due to the anisotropy, at relatively small tilting angles the alignment of vortices in the parallel to the layers direction becomes more energetically favorable than the creation of tilted vortices. These experimental results are consistent with the theoretical predictions of Feinberg and Villard [4].

Here we present our new experimental investigations of the resistive transitions of Mo/Si multilayers with the number of bilayers more than 30 and the 10-bilayer W/Si structures in a wide angle range of magnetic field.

It is found that for Mo/Si samples at some larger angles than are required for the lock-in state, no minimum is observed on the $R(H)$ curves and vortices are tilted. But at much larger angles the pronounced minimum in the dependences $R(H)$ reappears. The existence of this anomaly in strongly inclined magnetic fields can be explained in terms of the combined vortex lattice predicted theoretically in a number of studies of layered superconductors [5].

The lock-in state is firstly observed in W/Si multilayers with the only 10 bilayers. But for this case there is no sign of the combined vortex lattice existence. We conclude that the number of bilayers play the important role in the combined vortex lattice formation.

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# ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF $RT_4AL_8$ (R =Sc, Y, La, Lu; T=Fe, Mn, Cr) COMPOUNDS. HYDROSTATIC PRESSURE EFFECT

**I. P. Zhuravleva, G. E. Grechnev, A. S. Panfilov, A. A. Lyogenkaya, O. V. Kotlyar, A. V. Fedorchenko**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky 47, Kharkiv 61103, Ukraine*

*e-mail: izhuravleva@ilt.kharkov.ua*

In this work we report on detailed investigations of the electronic structure and magnetic properties of $RT_4Al_8$ compounds (R = Sc, Y, La, Lu and T = Fe, Mn, Cr). These compounds crystallize in $ThMn_{12}$-type tetragonal crystal structure and possess a wide range of peculiar magnetic properties, which are governed by the 3*d*-metal sublattice.

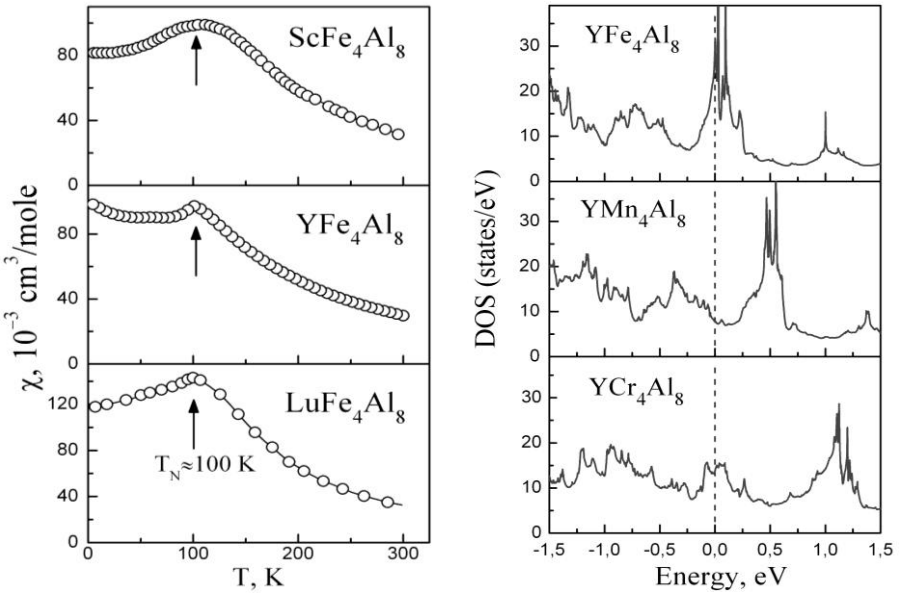



Fig.1. Temperature dependence of magnetic susceptibility (left) and density of electronic states (right) calculated for paramagnetic phase of $RFe_4Al_8$ compound.

For $RT_4Al_8$ compounds we carried out theoretical and experimental studies of magnetic susceptibility and its volume dependence.

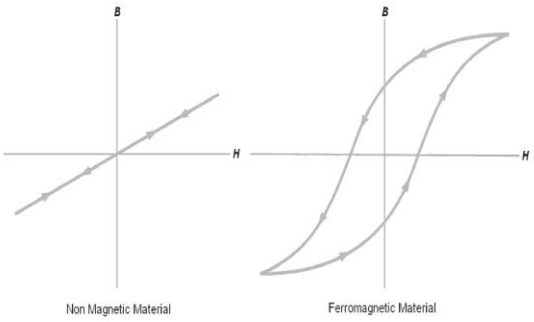
Measurements were performed for polycrystalline samples in the temperature range 2 – 300 K by using SQUID magnetometer. The temperature dependences of magnetic susceptibility $\chi$ of $RFe_4Al_8$ (see Fig.1, left) exhibit a peak at the Neel point $T_N$ ~100 K. The electronic structures of $RT_4Al_8$ in the paramagnetic state were calculated *ab initio* within local density approximation. The densities of electronic states $N(E)$(see Fig.1, right), bulk moduli $B$ and magnetic susceptibilities were systematically calculated for $RT_4Al_8$ systems for the first time. For $RFe_4Al_8$ there is a high narrow peak of $N(E)$ at the Fermi energy (e.g. for $YFe_4Al_8$ in Fig.1). This indicates the predominant role of Fe–subsystem in magnetism of $RFe_4Al_8$ (R=Sc, Y, Lu) compounds.

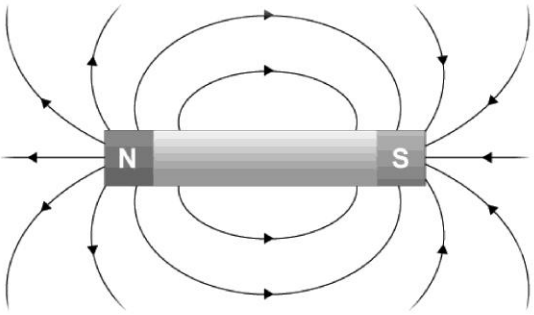
The calculations and experiments have revealed the anomalously large values of magneto-volume effect $d\ln\chi/d\ln V$ in $RMn_4Al_8$ and $RCr_4Al_8$ systems (see the Table), which can not be explained within the Stoner model for itinerant magnetism.

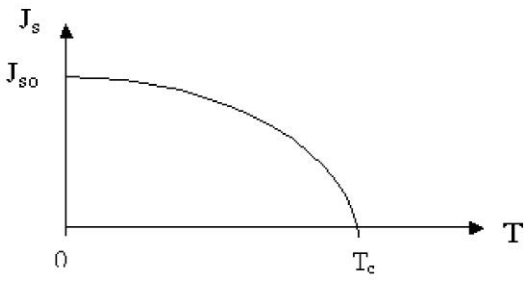
Table 1.

| | | $ScMn_4Al_8$ | $YMn_4Al_8$ | $La Mn_4Al_8$ | $Lu Mn_4Al_8$ | $LuCr_4Al_8$ | $CeCr_4Al_8$ |
|---|---|---|---|---|---|---|---|
| Theory | $\chi$ ($10^{-3}$ emu/mole) | 2,1 | 4,35 | 13,8 | 3,1 | 3,8 | 4,9 |
| | $d\ln\chi/d\ln V$(Mbar$^{-1}$) | 13 | 26 | 33 | 18 | 16,5 | 11 |
| Exp | $\chi$ ($10^{-3}$ emu/mole) | ~2,5 | 4 | ~12 | ~3,5 | 4,1 | ~4,58 |
| | $d\ln\chi/d\ln V$(Mbar$^{-1}$) | — | 20±2 | ~55 | — | — | 12 |

# Magnetism and Magnetic Materials

# MULTIFERROIC $PrFe_3(BO_3)_4$: STRONG ELECTRON-PHONON COUPLING IN AN EXTERNAL MAGNETIC FIELD PROBED BY TERAHERTZ SPECTROSCOPY

**K. N. Boldyrev[1], M. N. Popova[1], T. N. Stanislavchuk[2], D. Kamenskyi[3], L. N. Bezmaternykh[4]**

*[1] Institute of Spectroscopy, Russian Academy of Sciences,*
*Fizicheskaya st. 5, Troitsk, 142190 Moscow, Russia*
*[2] Department of Physics, New Jersey Institute of Technology,*
*Newark, 07102 New Jersey, USA*
*[3] High Field Magnet Laboratory (HFML-EMFL), Radboud University,*
*6525 ED Nijmegen, The Netherlands*
*[4] Kirensky Institute of Physics, Siberian Branch of the Russian Academy of Sciences,*
*Akademgorodok, 660036 Krasnoyarsk, Russia*
*e-mail: kn.boldyrev@gmail.com*

Recent studies of the rare-earth (RE) iron borates $RFe_3(BO_3)_4$ have shown that they belong to a new class of multiferroics. Their magnetic properties are governed by the presence of two interacting magnetic subsystems – $Fe^{3+}$ and $R^{3+}$. The magnetic structure of $RFe_3(BO_3)_4$ changes as a function of temperature, external magnetic field, and substitutions in the RE subsystem. Compounds belonging to this family display a considerable magnetoelectric effect and their electric (magnetic) properties can be controlled by the magnetic (electric) field. This is a promising finding in view of possible device applications.

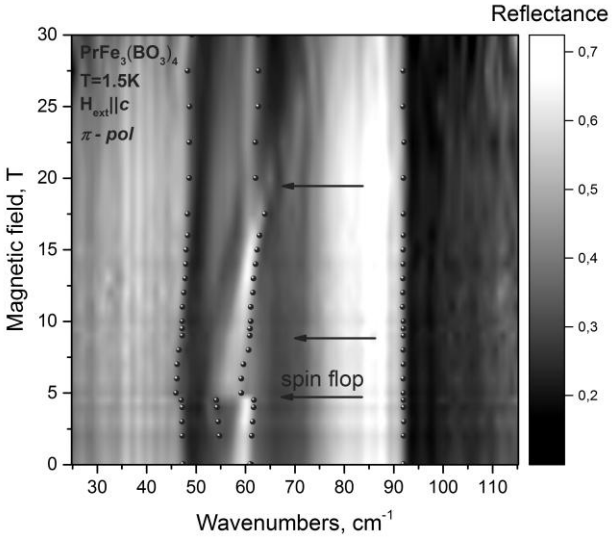



Fig.1. Color map of the reflection spectra.

We have shown that spectroscopy in the terahertz range allows investigating magnetoelastic interactions in RE iron borates [1]. The work [2] dedicated to the terahertz reflection spectroscopy of the $PrFe_3(BO_3)_4$ single crystal has revealed a spectral signature of the interaction of a low-frequency phonon with the lowest-frequency electronic excitation of the RE ion and of formation of the coupled electron-phonon mode. Modeling of the experimental data resulted in the value $W = 14.8$ cm$^{-1}$ of this interaction − a record value for such compounds [2].

Further studies of the reflection spectra in strong magnetic fields (up to 30 T) have revealed a number of effects (see Fig.1). Thus, a small increase of a magnetic field leads to an abrupt splitting of the coupled electron-phonon mode. Simulation has explained this phenomenon and has shown that the electron-phonon coupling constant does not depend on the magnetic field. We also succeeded in simulating a behavior of the coupled electron-phonon mode at $H > H_{SF}$ (the field of the spin-flop transition $H_{SF} = 4.2$ T at 1.5 K). Also we observe a number of effects in $H = 9$ T and $H = 17$ T with unknown nature.

Financial support by the Russian Science Foundation under Grant № 14-12-01033 is acknowledged.

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# CLASSIFICATION OF DEGENERATE EQUILIBRIUM STATES OF MAGNETS WITH THE SPIN S=1

**A. V. Glushchenko, M. Yu. Kovalevsky**

*Kharkov Institute of Physics and Technology*
*Academicheskaya, 1, Kharkov, 61108, Ukraine*
*e-mail: glushchenko.ant@gmail.com*

We have considered the problem of classification of equilibrium states of spin s=1 magnets with a spontaneously broken symmetry in the presence of vector and tensor order parameters. These order parameters, due to their transformation properties under time reversal, lead to different equilibrium states of magnetic systems in terms of their T-parity. The basis of the description of degenerate multiparticle states of these systems is the concept of quasi-averages [1] and the Gibbs distribution. In contrast to the well-known method [2], the proposed approach does not contain free energy models as an order parameter functional and does not use the requirement of the temperature proximity to the phase transition point. The cases of the SO(3) and SU(3) magnetic exchange interaction have been studied in the paper. The idea of the residual symmetry of the equilibrium state [3] and the requirement for the existence of a nonvanishing order parameter lead to restrictions on permissible values of the unbroken symmetry generator parameters and classify equilibrium states of degenerate condensed media. We have formulated classification equations and obtained the explicit form of vector and tensor order parameters for degenerate magnetic equilibrium states. We have also built graphic illustrations of the order parameter type.

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# SPECTRA OF COLLECTIVE EXCITATIONS AND LOW FREQUENCY ASYMPTOTICS OF GREEN'S FUNCTION FOR SPIN S=1 MAGNETICS

**A. V. Glushchenko[1], M. Y. Kovalevsky[1], L. V. Logvinova[2], V. T. Matskevych[1]**

*[1]National Science Center "Kharkov Institute for Physics and Technologies" of NAS of Ukraine, Akademicheskaya str., 1, Kharkov 61108, Ukraine*
*[2]Belgorod State University, Pobedy str., 85, Belgorod 308015, Russia*
*e-mail: matskevych.vt@gmail.com*

The report is devoted to describing of dynamic processes for the set of magnetic states with spin $s=1$ in an external alternating field. We consider ferromagnet and quadrupole magnetics with SU(3) symmetry, spin nematic, antiferromagnetic, easy-axis and easy-plane ferrimagnetics. Our investigation mainly based on approach of [1, 2]. For these magnetics closed algebras of Poisson brackets for all magnetic degrees of freedom are obtained. Explicit form of the exchange energy is established in terms of Casimir invariants. Nonlinear dynamic equations for these magnetics with sources due to the external field are derived.

An effective tool for studying magnetic systems is two-time Green's functions [3, 4], the knowledge of which allows us to understand both the state of equilibrium and peculiarities of non-equilibrium processes if the deviation from equilibrium is small. Low-frequency asymptotics of Green's functions for the above magnetics are found and their comparative analysis is carried out. The influence of unitary SO(3) or SU(3) symmetry on the structure of Green's functions characteristics are shown and analyzed. Along with the well-known analytical characteristics of Bogolyubov's type some magnetic states have non Bogolyubov's type features.

The pole of the obtained Green's functions determines the spectra of collective excitations of the respective magnetic states. For all considered magnetic states spectrum of collective excitations are obtained.

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# MAGNETIC PROPERTIES OF SUPERCONDUCTING NANOSTRUCTURES BASED ON INDIUM IN VARIOUS POROUS DIELECTRICS

**N. Yu. Mikhailin[1,2], V. I. Kozub[1], Yu. A. Kumzerov[1], R. V. Parfeniev[1], A. A. Sysoeva[1], A. V. Fokin[1], D. V. Shamshur[1]**

*[1]Ioffe Physical-Technical Institute , 194021, Politehnicheskaya, 26, Saint-Petersburg, Russia*
*[2]International Laboratory of High Magnetic Fields and Low Temperatures, Polish Academy of Sciences, Gajowicka 95, 53-421 Wroclaw, Poland*
*e-mail: mikhailin.nik@gmail.com*

We studied magnetic properties of indium nanostructured in pores of a dielectric matrix. Properties of the matrix were varied by using porous glass and opals; these dielectrics have a 3D network of nanopores, which is ordered in case of opal and random in porous glass. Pore size was also varied in case of opals. Structures were filled with In from melt under hydrostatic pressure; more than 95% of pore space was filled. This way, we obtained samples with 3D superconducting network of In particles with particle size from 7 nm in porous glass up to 100 nm in certain types of opals. Measurements of magnetization(m) were carried out using a VSM magnetometer at temperatures($T$) 4 – 1.5 K and magnetic fields(H) up to 30 KOe. m(H) dependencies show hysteresis in all samples and at all temperatures below critical. Critical temperature ($T_c$) and field ($H_c$) obtained from m(H) dependencies are bigger than in bulk In: in porous glass+In sample we obtained $T_c$ up to 4 K (3.2 K in bulk In) and $H_c$(T = 2 K) up to 15 KOe (for bulk In Hc (T=0) = 280 Oe). This correlates with the data obtained by resistivity measurements [1]. At temperatures lower than 3 K significant magnetization jumps were observed in m(H) dependencies (Fig.1). It was found, that properties of such jumps vary with temperature, field sweep rate and the structure of In network. Such jumps were observed earlier in a Pb+porous glass structure [2]. We assume that these jumps are caused by sample heating due to a thermomagnetic instability, which turns parts of the In network to normal state and allows field to penetrate it. It should be noted that at temperatures lower than 2 K two types of jumps are observed: small jumps at lower fields and bigger jumps at high fields. At temperatures between 2K and 3K only bigger jumps can be seen (fig.1).

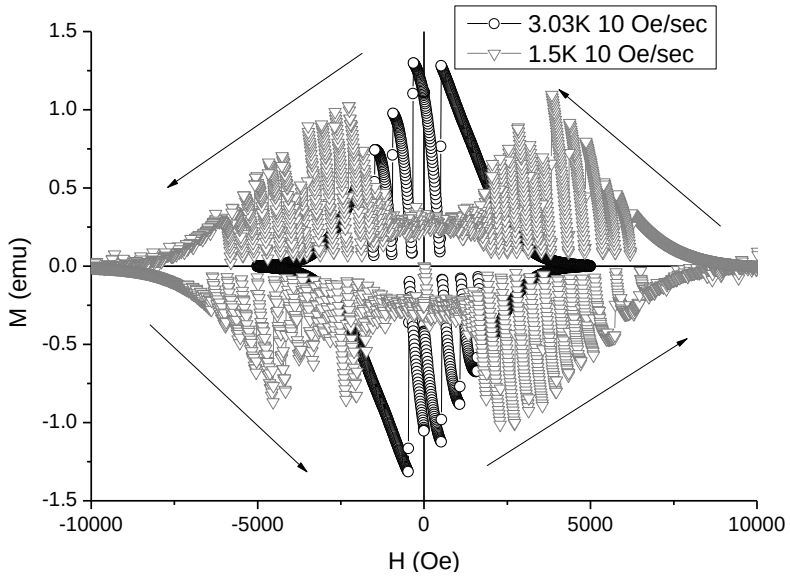


Fig.1. Magnetisation jumps in an opal+In sample at temperatures 3 K and 1.5 K.

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# DOMAIN WALL MOTION IN MAGNETIC HELICES UNDER ACTION OF RASBHA TORQUE

**O. V. Pylypovskyi[1], D. D. Sheka[1], V. P. Kravchuk[2], K. V. Yershov[2,3], D. Makarov[4], Y. Gaididei[2]**

*[1]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine*
*[2]Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, 03680 Kyiv, Ukraine*
*[3]National University of "Kyiv-Mohyla Academy", 04655 Kyiv, Ukraine*
*[4]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany*
*e-mail: engraver@univ.net.ua*

The manipulation of magnetization patterns in magnetic nanostructures by using spin-transfer torques is relevant for numerous applications including racetrack memory and magnetic logic. Here, we report on how the static and dynamic properties of domain walls are affected by the shape of a helical magnetic wire with easy-tangential anisotropy with the magnetic length $\ell$. Helical wires are considered as a prototypical example as this is the simplest geometry, which is characterized by the coordinate-independent nonzero curvature $\kappa$ and torsion $\tau$.

Shaping a uniaxial Heisenberg magnet in a helical wire results in the emergence of an effective anisotropy (easy-axis and easy-surface) and Dzyaloshinskii-Moriya interaction, which alter the magnetization state [1, 2]. The effective easy-axis anisotropy causes the tilt of the equilibrium magnetization with respect to the tangential direction by the angle $\psi \propto \kappa\tau$. The effective easy-surface anisotropy of the order of $\kappa^2$ orients the magnetization within the tangent-binormal surface. The structure of the static domain wall is mainly determined by the effective Dzyaloshinskii-Moriya interaction. The magnetization becomes a function of the coordinate along the wire with an amplitude of asymmetric deformation $\Upsilon$ proportional to $\tau$. The nonzero curvature results in the coupling of the domain wall type (head-to-head or tail-to-tail) and its magnetization chirality. The sign of $\tau$ (helix chirality) determines the magnetization direction in the centre of the domain wall: inside or outside the helix.

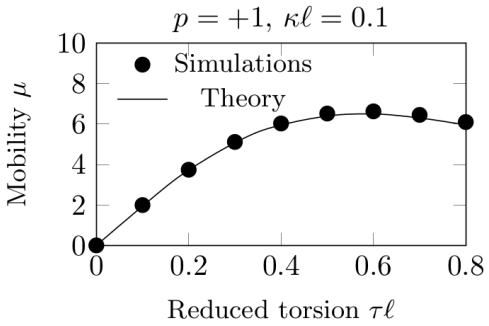

Fig.1. Mobility of the domain wall

In contrast to planar systems [3], in helix wires head-to-head domain walls can be efficiently moved under the action of the Rashba torque even in the case of the parallel electrical current injection. Due to $\psi \neq 0$, there exists a Rashba field component, parallel to the magnetization in one of the domains. Using a generalized $q-\Phi$ model far below the Walker limit we obtain the following expression for the domain wall velocity in dimensionless units [4] (see Fig. 1) $\mu = \frac{2p\delta}{\eta}\frac{\sin\psi}{1+\delta^2\Upsilon^2}$, where $p=+1$ for head-to-head and $p=-1$ for tail-to-tail domain walls, $h$ is the reduced Rashba field, $\eta$ is the Gilbert damping and $\delta$ is the domain wall width.

All analytical predictions are confirmed by micromagnetic [5] and spin-lattice simulations [6].

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# REORIENTATION PHASE TRANSITION IN PERMALOY SPHERICAL SHELL

**M. I. Sloika[1], D. D. Sheka[1], V. P. Kravchuk[2], Y. B. Gaididei[2]**

*[1]Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska str., Kyiv 01601, Ukraine*
*[2]Bogolyubov Institute for Theoretical Physics, 14-b, Metrologichna str., Kyiv, Ukraine*
*e-mail: sloika.m@gmail.com*

A competition between short-range exchange and long-range magnetostatic interactions results in nontrivial distribution of magnetization in a magnetic nanoparticle [1]. Such magnetic distributions as vortex and onion are widely explored for the case of planar structures [2]. In the current study we analyze the magnetic reorientation transition between the vortex phase and onion one for a thin spherical shell [3].

We provide the systematic study of the equilibrium magnetization distributions in the spherical shell. Namely, by combining analytical methods and micromagnetic simulations (MAGPAR code [4]) we determined phase diagram for Permaloy sphere with inner radius $R$ and thickness $h$: the vortex state, Fig.1(a), is realized for relatively large and thick shells, while the onion state, Fig.1(b), is typical for smaller ones. As opposed to the planar counterpart [5] and hemispherical caps [6] the spherical shell exhibits continuous magnetization transformation from the vortex state to the onion one, which is characterized by the magnetization rotation from the sphere parallel orientation to the meridian direction, Fig.1(c). The key moment of our study is the simple analytical approach, which gives a possibility to describe different magnetization states as well as the transition between them, see Fig. 1.

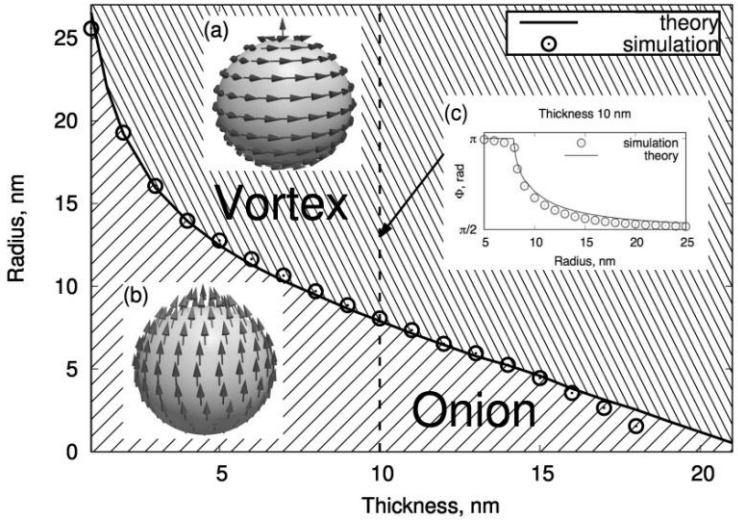


Fig.1. Phase diagram for the spherical shell with inner radius $R$ and thickness $h$.

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# CURRENT DRIVEN DOMAIN WALL MOTION IN MAGNETIC HELIX

**K. V. Yershov[1,2], V. P. Kravchuk[1], D. D. Sheka[3], Y. Gaididei[1]**

*[1]Bogolyubov Institute for Theoretical Physics of NAS of Ukraine,*
*Metrologichna Str. 14-b, Kyiv 03680, Ukraine*
*[2]National University of «Kyiv-Mohyla Academy»,*
*Skovorody Str. 2, Kyiv 04655, Ukraine*
*[3]Taras Shevchenko National University of Kyiv*
*Volodymyrska Str. 64/13, Kyiv 01601, Ukraine*
*e-mail: yershov@bitp.kiev.ua*

The controlled displacement of magnetic domain walls along ferromagnetic nanowires by means of electrical current is a key practical task for a number of devices including racetrack memory and magnetic logic.

We base our study on the phenomenological Landau-Lifshitz-Gilbert equation with additional Zhang-Li spin-torque terms [1,2]. To analyze the domain wall properties we use collective variable approach based on generalized $q$-$\Phi$ model. We show that the torsion effectively shifts the material parameter of nonadiabaticy $\beta \to \beta - \beta^*$, where $\beta^*=p\Delta_0\tau$, here $\tau$ is a torsion of the helix wire, $\Delta_0$ is the domain wall width, and $p$ is a topological charge of the domain wall. This effect can lead to a negative effective nonadiabaticity resulting in negative domain wall mobility [3]

$$\mu=(\beta - \beta^*)/\alpha, \quad (1)$$

where $\alpha$ is Gilbert damping constant. We also show that the curvature results in appearance of Walker limit even for the case of an uniaxial wire [3]

$$u_c \approx v_0 \pi \kappa \alpha l/(\alpha-\beta+\beta^*), \quad (2)$$

where $v_0=\omega_0 l$ with $l$ being exchange length and $\omega_0$ being characteristic time scale parameter, and $\kappa$ being the curvature of the helix wire.

In order to verify our analytical predictions we performed numerical simulations of the Landau-Lifshitz-Gilbert equation with additional Zhang-Li [1, 2] spin-current terms using the NMAG code [4]. The obtained results are in good agreement with the developed theory, see Fig. 1 [3].

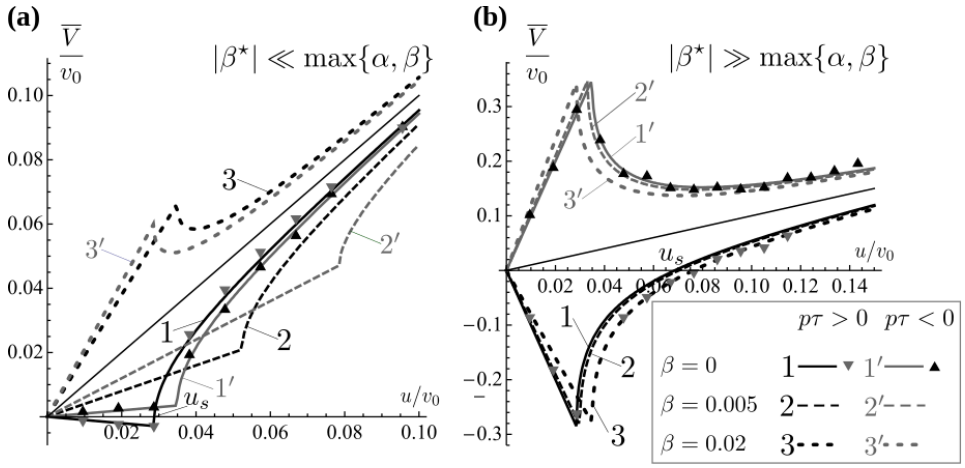


Fig. 1. Averaged domain wall velocity as a function of the applied current. Lines correspond to solutions of the collective variables equations, and markers show the results of NMAG micromagnetic simulations. Simulations as well as theoretical solutions are made for magnetically soft wire. All the other parameters are as follows: (a) $\kappa l$=0.01, $\tau l$=0.0005 ($\beta^*$=0.001); (b) $\kappa l$=0.1, $\tau l$=0.05 ($\beta^*$=0.1). In all cases $\alpha$=0.01. The thin solid line corresponds to the case of a rectilinear wire, where $V \approx u$.

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# MAGNETIC PROPERTIES AND H-T PHASE DIAGRAM OF $GdCr_3(BO_3)_4$

**O. Bludov[1], Yu. Savina[1], V. Pashchenko[1], S. Gnatchenko[1], T. Zajarniuk[2], M. U. Gutowska[2], A. Szewczyk[2]**

*[1]B. Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, 47 Nauky Ave., 61103 Kharkov, Ukraine*
*[2]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland*
*e-mail: bludov@ilt.kharkov.ua*

Gadolinium chromium borate $GdCr_3(BO_3)_4$ belongs to the vast family of compounds with general chemical formula $ReM_3(BO_3)_4$ (*Re*=rare earth or Y; *M*=Al, Ga, Sc, Fe, Cr). The crystal structure of majority of the family members, including $GdCr_3(BO_3)_4$, is similar to the huntite mineral, crystallizing in the *R*32 space group [1,2]. The structure consists of trigonal prisms $GdO_6$, octahedra $CrO_6$, and two slightly different planar triangular groups $BO_3$. The sharing edges $CrO_6$ octahedra form chains along the *c* axis. The $GdO_6$ prisms are separated from each other and each of them links three chains of $CrO_6$ octahedra.

The magnetic and thermal properties of $GdCr_3(BO_3)_4$ single crystal have been investigated. The temperature dependences of magnetic susceptibility $\chi(T)$, field dependences of magnetization $M(H)$, and the temperature dependences of specific heat $C_p(T)$ have been measured by using a SQUID magnetometer MPMS–XL5 QD (2–300 K, up to 5 T) and a PPMS QD (2–300 K, up to 9 T). The external magnetic field has been applied along and perpendicular to the crystallographic *c* axis.

Above 50 K, the temperature dependences of susceptibility $\chi(T)$ can be described by the Curie-Weiss law with the effective magnetic moment $10.6 \pm 0.1\ \mu_B$ per formula unit (the theoretical value is 10.4 $\mu_B$) and the paramagnetic Curie temperature $7.2 \pm 0.2$ K for both directions. The antiferromagnetic ordering at $T_N = 7.15 \pm 0.05$ K manifests itself by an abrupt drop on the $\chi(T)$ and by a λ-anomaly on the $C_p(T)$. It has to be mentioned that the behavior of the product $\chi(T)*T$ and sign of the paramagnetic Curie temperature show the predominance of ferromagnetic correlations in the high temperature region ($T > 50$ K). The maximum on $\chi(T)$ at around 8.5 K and the upturn below 20 K on $C_p(T,H=0)$ may indicate that this compound is a low-dimensional magnet. Previously, very similar behavior has been described in [3] for $NdCr_3(BO_3)_4$. The obtained data allowed us to build the *H-T* phase diagrams for $GdCr_3(BO_3)_4$ for $H \parallel c$ and $H \perp c$. For both field directions, the phase diagrams are almost identical and have only minor quantitative differences. The phase diagram is similar to the one typical for antiferromagnet with easy axis anisotropy, in the magnetic field applied along the easy axis.

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# MAGNETOPIEZOELECTRIC EFFECT AND MAGNETOCAPACITANCE IN NEODYMIUM FERROBORATE

**T. N. Gaydamak[1], I. A. Gudim[2], G. A. Zvyagina[1], I. V. Bilich[1], K. R. Zhekov[1], V. D. Fil[1]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2]L. V. Kirensky Institute for Physics, Siberian Branch of the Russian Academy of Sciences, Krasnoyarsk 660036, Russia*
*e-mail: gaydamak@ilt.kharkov.ua*

We have reported previously [1] about the revealing of a giant magnetopiezoelectric effect (MPE) in $SmFe_3(BO_3)_4$. The effective piezomodulus is increased more than twice in the antiferromagnetic phase and it is reduced by a high magnetic field. This effect, together with the study of the magnetocapacitance (MC) allowed to determine the parameters of magnetoelectric and magnetoelastic couplings. In [1] it was given also preliminary results related to Nd ferroborate, which revealed much smaller MPE and MC effects in this compound. At the same time it was known from the literature that both compounds show comparable values of electrical polarization induced by external magnetic field *H*. We were motivated in further researches of Nd ferroborate.

The following results were obtained:

1. Below the Neel temperature (~32K) permittivity $\varepsilon_{xx}$ starts to increase almost linearly with the slope of 6 times smaller than in $SmFe_3(BO_3)_4$. The growth of $\varepsilon$ turns to a slight decrease at $T_{cr}$=13÷20K. At $T_{cr}$, according to the neutron data, in $NdFe_3(BO_3)_4$ appears the helical phase. Piezomodulus $e_{xx}$ slightly changes above $T_{cr}$ but at low temperatures it notably increases.

2. In the external magnetic field $H_{cr}$, applied in basal plane, the helical phase transformed to a "spin-flop" phase. The $H_{cr}$ value doesn't depend on the magnetic field direction.

3. At $H > H_{cr}$ MPE and MC effects are qualitatively similar to those in Sm compound, but much smaller in magnitude.

Phenomenological description can be given in frame of model, used in [2] for the explaining the change the sign of polarization, induced by magnetic field. It is suggested that Nd ions are in the effective field $\mathbf{H_{eff}}=\pm\mathbf{H_{ex}}+\mathbf{H}$, where $\pm\mathbf{H_{ex}}$- exchange fields created by iron sublattices.

Due to $H_{ex}$ is comparable in magnitude with the external field, Nd and Fe magnetic moments are partly independent, and should be considered separately. In particular it should be used partial phenomenological magnetoelectric and magnetoelastic coefficients describing the interaction of the magnetic subsystem with external fields.

We used thermodynamics potential like in [1]. For the related variationss of ε (β=π/4) at $H > H_{ex}$ it was obtained: $\frac{\delta\varepsilon}{\varepsilon} \approx \frac{4\pi}{\chi\varepsilon}(a_{Fe}+a_{Nd})^2(-\frac{a_{Nd}}{a_{Fe}+a_{Nd}}\cdot\frac{6}{H_{ex}}+\frac{1}{H^2})$ Here $a_{Nd,Fe}$- magnetoelectrical coefficients, $\chi$- susceptibility. The related variations of piezomodulus are described by more complicated expression with "mixed" magnetoelectrical and magnetoelastic coefficients. The main features of these equations are the linear dependencies on $H^{-2}$ dislocated relative to the origin in the region of negative ordinates. These features are well confirmed experimentally. Using the known literature data on $H_{ex}$ (8.5±0.5 T), $\chi$ ($1.38\cdot 10^{-5}$ emu/cm$^3$) and ε ($\varepsilon_{xx}$=15) at $T$=1.7K it was found that $a_{Fe}+a_{Nd} \approx 450$ μC/m$^2$. Expected value of the electrical polarization at $H_{cr}$~ 225 μC/m$^2$, that is comparable with the measured one. We notice also that the magnetoelectric coefficients have different signs and their ratio is $a_{Fe}/a_{Nd} \sim -0.4$.

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# ANTIFERROMAGNETIC RESONANCE IN MESOTWINED NiMnCoSn FILMS

**Yu. Kharlan, D. Popadyuk**

*National Technical University of Ukraine «Kyiv Polytechnical Institute»,*
*37 Peremogy ave., 03056 Kyiv, Ukraine*
*e-mail: SEVA_2009@ukr.net*

Magnetic shape memory alloys (MSMA) are of great interest now both from fundamental point of view and for their possible application. A lot of new physical effects related to martensitic transformation have been discovered recently in these materials: giant change of their size under the action of magnetic field, magnetic superelasticity, ordinary and inverse magnetocaloric effect, giant magnetoresistance, bias exchange, etc. Such compounds can have one hundred percent polarization of conducting electrons, which makes them very attractive for spintronics applications. Narrow resonance line of Heisler MSMAs opens an opportunity to use them for all-metal magnonic crystals fabrication. From fundamental physics point of view the investigation of MSMAs are of interest due to the possibility to observe a complex chain or combination of phase transitions. In particular a combination of magnetic and structural transitions opens a way to control this transition using magnetic fields.

This work is devoted to the investigation of evolution of magnetic and magnetoresonance properties of epitaxial NiMnCoSn films deposited on MgO (001) substrates in 100-400 K temperature range.

It has been shown experimentally that these films undergo the martensitic transformation near the room temperature from cubic high temperature austenitic phase to orthorhombic low temperature martensitic one. The characteristic feature of ferromagnetic resonance spectra of this compound in martensitic state is the presence of well field separated three resonance lines (See Fig.1.). The analysis of structural, magnetic and magnetoresonance properties of the samples does not allow ascribing the appearance of these lines due to formation of phases with different magnetic parameters. It cannot be also explained in terms of spin wave modes formation. Meanwhile the analysis of magnetic data shows a presence of antiferromagnetic interaction in the system.

The appearance of three resonance lines was explained in the frame of following model: ferromagnetic exchange interactions inside martensite twins and antiferromagnetic on the twins boundaries. As a result of such interactions three resonance modes should be observed like it takes place in usual antiferromagnetics, but the modes splitting in our case is much less due to the localization of antiferromagnetic interaction.

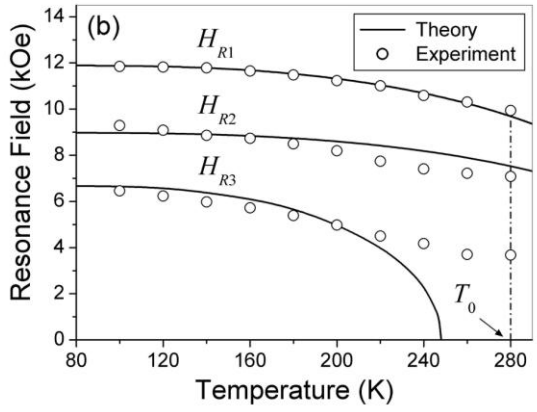


Fig.1. Theoretical and experimental temperature dependences of the resonance fields of main modes. $T_0$ is the temperature of martensite transformation start.

The proposed model allows quantitatively describe temperature dependence of the resonance fields for all three modes in martensitic phase using the following set of parameters: saturation magnetization at zero temperature $M_0$=500 emu/cm$^3$, exchange constant δ=2,92 and anisotropy parameter β=11.2. It is worth to be noted that this is the situation which is close to previously observed in so called "synthetic antiferromagnets".

# BEHAVIOR OF THE $Nd_{0.9}Dy_{0.1}Fe_3(BO_3)_4$ CRYSTAL IN THE MAGNETIC FIELD TILTED FROM THE CRYSTALLOGRAPHIC AXES

**M. P. Kolodyazhnaya[1], I. V. Bilych[1], K. R. Zhekov[1], G. A. Zvyagina[1], A. A. Zvyagin[1], A. N. Bludov[1], V. A. Pashchenko[1], I. A. Gudim[2]**

*[1] B. Verkin Institute for Low Temperature Physics and Engineering,*
*47 Lenin Ave., 61103 Kharkov, Ukraine*
*[2]L.V. Kirensky Institute for Physics, Siberian Branch of the Russian Academy of Sciences,*
*660036, Krasnoyarsk, Russia*
*e-mail: zvyagina@ilt.kharkov.ua*

Trigonal rare-earth (RE) ferroborates $ReFe_3(BO_3)_4$ (Re = Y; La-Nd; Sm-Er) are extensively studied last time because they have interesting magnetic, magneto-electric and magneto-elastic properties, which are mostly determined by the specific interaction between $Fe^{3+}$ and $Re^{3+}$ magnetic subsystems [1].

Below $T_N$=30-40 K antiferromagnetic ordering of iron subsystem appears in ferroborates, while RE ions bring the main contribution to the magnetic anisotropy and magneto-electric polarization. In ferroborates of Pr, Tb, Dy the easy-axis (EA) structure is realized, i.e., spins of iron are oriented along the trigonal $C_3$ axis (*c*-axis), and in compounds with Nd, Eu, Er, Sm the easy-plane (EP) structure is realized, i.e., spins of $Fe^{3+}$ are ordered in the basic *ab*-plane, perpendicular to the *c*-axis of the crystal.

In binary compounds $Nd_{1-x}Dy_xFe_3(BO3)_4$ the contributions of both $Nd^{3+}$ and $Dy^{3+}$ ions to the magnetic anisotropy can be competitive, and the spontaneous reorientation from the EP state to the EA one is possible. Our recent studies of magnetoelastic and magnetic properties of the $Nd_{0,9}Dy_{0,1}Fe_3(BO_3)_4$ have permitted to suggest that the spontaneous reorientation EP→EA took place in the crystal. This reorientation occurs in this compound in a composite way, via an intermediate phase [2-4]. It was shown that the magnetic field applied either along the trigonal *c*-axis or in the basal *ab* plane of the crystal induced different spin reorientation phase transitions (SRPT). Two following each other SRPTs have been registered in the EA phase in external field **H** || *c*, and only one SRPT has realized in the intermediate phase. The surprise was that the magnetic field applied in the *ab*-plane induced spin reorientation in all magnetic phases, even in the lowest-temperature one, which had supposed as EA phase.

Recently we have performed low-temperature magnetoacoustic investigations of single crystal $Nd_{0,9}Dy_{0,1}Fe_3(BO_3)_4$. We have observed how the features of the sound velocity and magnetization behavior in the magnetic field changed due to the tilting of the direction of the external magnetic field from the main crystallographic axes $C_3$ and $C_2$ in the *ac*, *bc* and *ab* planes in all magnetic ordering phases. Our observations show that SRPTs exist for large enough values of the tilting angle $\alpha$ of the external magnetic field from $C_3$ axis. There is a range of $\alpha$ ($30^0 \leq \alpha \leq 70^0$) where three following each other SRPTs registered in the lowest temperature phase. In this phase the behavior of magnetoelastic characteristics for tilting in the *ac* and *bc* plane is similar.

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# MAGNETO-OPTICAL PROPERTIES OF THIN FILM SYSTEMS BASED ON Fe AND Au

**D. V. Chereda, Yu. M. Shabelnyk, I. M. Pazukha, I. Yu. Protsenko**

*Sumy State University, 2, Rymskogo-Korsakova st., Sumy 40007, Ukraine*
*e-mail: i.protsenko@aph.sumdu.edu.ua*

The work deals with the analysis of experimental data of crystal structure, phase state and magneto-optical properties of film systems based on Fe and Au. The samples have been received by method of layer by layer thermal sputtering at room temperature with subsequent heat treatment to 700-900 K. The system refers to the nanostructured film materials where possible to implement the spin-dependent scattering and forming granular alloy during thermal annealing samples.

The diffraction and electron microscopy studies of investigated systems Fe/Au/Fe/S (S – substrate) indicate to two-phase state (fcc-Au and bcc-Fe with the lattice parameter 0.407 and 0.288 nm respectively), in comparison with samples received by simultaneous deposition of Au and Fe [1, 2]. According to [1, 2] the formation of Au-based or Fe-based solid solutions (s.s.) subject to film composition occurs at condensation stage. For our samples (cFe =30-65 at.%) formation of disordered Au-based solid solution are fixed at the electron-diffraction pattern after heart treatment to 700 K only. At the same time Fe-based solid solution have not be observed in investigated range of magnetic component concentration.

The method of magneto-optical Kerr effect (MOKE) is used to obtain an information of the magnetic properties of ferromagnetic thin film materials and nanostructures basis on them. From MOKE field dependences the information about such important parameters as coercivity $B_c$, saturation field $B_s$ and Kerr angle $Q_r$ can be received. In our work we study magneto-optical properties of the model Fe/Au/Fe/S three-layer films with different concentration of magnetic components. MOKE field dependences of the samples in as-deposited state characterized by rectangular form of the hysteresis loop ($B_c$ = 15 mT), which is typical for the system with individual layers. The analysis of concentration dependences of coercivity, saturation field and Kerr angle showed that at 60 at. % Fe the minimum on dependence of $Q_r$ and the maxima of $B_c$ and $B_s$ are observed. After heart treatment to $T_a$ = 700 K the modification of the MOKE hysteresis loop and increase the coercivity field in 3-4 times occur. It should be noted also that MOKE field dependences for annealed samples not reach saturation. This is causes not only a process of recrystallization during annealing and increase of the average grain size, which changes the domain structure of magnetic layers, but also with formation disordered solid solution.

In addition, in this work we investigated influence of changing of bottom magnetic layer thickness on magneto-optical properties in the whole system. For film systems with more thin bottom magnetic layers after annealing up to $T_a$ = 700 K noticeable shape change associated with solid solution formation process. But these changes are not significant because the thickness of the intermediate layers is thin and the magnetic layers remain relatively continuous.

The conclusion can be done that the process of Au-based solid solution formation during heat treated, as a result of diffusion processes, in film systems based on Fe and Au is accompanied by the formation of areas of inhomogeneous magnetic states leads to changes curve shape of MOKE field dependence and to increasing of coercivity $B_c$ and saturation field $B_s$.

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# LOW TEMPERATURE MAGNETORESISTANCE IN GRAPHITE INTERCALATION COMPOUNDS WITH COBALT

**V. Ya. Tkachuk[1], I. V. Ovsiienko[1], L. Yu. Matzui[1], I. B. Berkutov[2], I. G. Mirzoiev[2], G. E. Grechnev[2], Yu. A. Kolesnichenko[2]**

*[1]Taras Shevchenko National University of Kyiv, Volodymyrska Str., 64/13, 01601 Kyiv, Ukraine*
*[2]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*

The graphite intercalation compounds (GICs) with magnetic metals are layered structures consisting of the alternating magnetic and nonmagnetic layers. According to the data of theoretical simulation, the properties of charge carriers in such GICs are changed significantly, in particular, the degree of electron's polarization could reach even 100% due to the interaction between graphite layers enriched by the additional charge carriers with the layers of metal [1]. This determines the suitability of these materials for spintronics.

This work presents the results of low temperature investigations of magnetoresistance of GICs with cobalt. Anisotropic pyrolytic fine crystalline graphite (crystallite size $L_a$~20 nm, interplanar spacing $d_{002}$ = 0.34 nm) was used as the source material for GICs synthesis. The GICs were synthesized by two-stage method. At the first stage the GIC with potassium was obtained. At the second stage the reduction of cobalt chloride to cobalt metal with the subsequent substitution of potassium atoms by cobalt in the interplanar spacing was performed. As the result GICs of second and third stages were obtained. The measurements of magnetoresistance were carried out with use of standard four-probe method in the temperature range 1.6-300 K and magnetic fields up to 14 Tesla.

The investigations of low temperature magnetoresistance in the spesimens of GICs with cobalt revealed, first, asymmetry of magnetoresistance relative to magnetic field direction and, secondly, negative magnetoresistance in weak magnetic fields (Fig.1, curve 1). The asymmetric magnetoresistance was analyzed in terms of the Segal model [2]. Accordindg to Segal model the asymmetric magnetoresistance is observed for layered ferromagnetic systems with high degree of magnetic anisotropy.

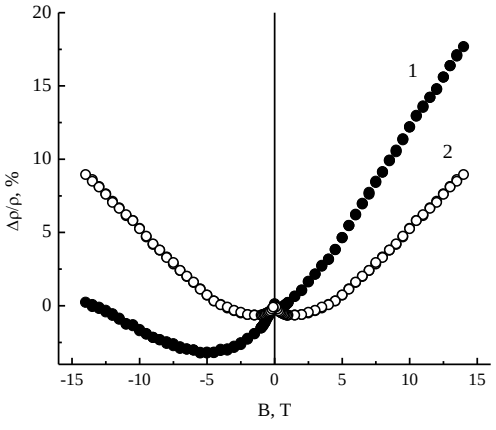


Fig.1. Dependence Δρ/ρ(B) for GIC-Co, T = 5K, 1 – experimental data, 2 – experimental data with account of linear term

For such systems resistivity in magnetic field can be written as $\rho(B) = \rho(B)_{ev} + bB$, where $\rho(B)_{ev}$ is even terms relative to magnetic field direction and bB is terms, that occurs when there are variations of clusters thickness and local Hall coefficient in specimen. Account of linear relative to magnetic field component completely removes asymmetry of magnetoresistance (curve 2).

It is also shown that negative magnetoresistance in specimens of GICs-Co is result of manifestation of quantum effects of weak localization and interaction of charge carriers, and that the dominant contribution due to the effect of electron-electron interaction causes the changes in the fields dependence of magnetoresistance.

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# ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF $BiFeO_3$, $SrFe_{12}O_{19}$ AND $SrCoTiFe_{10}O_{19}$ COMPOUNDS

**A. A. Lyogenkaya, G. E. Grechnev, A. S. Panfilov, O. V. Kotlyar, V. O. Pashchenko, A. N. Bludov**

*B. Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*

*e-mail: lyogenkaya@ilt.kharkov.ua*

The compound $BiFeO_3$ is a typical representative of materials known as multiferroics, in which magnetic and electric orderings coexist. Also hexaferrites $MFe_{12}O_{19}$ ($M$=Sr, Ba, Pb), which belong to strong permanent magnets are ferrimagnetic systems with expected manifestation of multiferroic properties. In these compounds a substitution of Fe or the cations with other metals can provide a mixed valence state and very unusual magnetic properties. A number of electronic structure calculations were carried out for these systems, however data on theirs electronic energy structure are still incomplete, inconsistent and controversial.

The aim of the present investigation was, firstly, to find a reliable approach of density functional theory DFT to describe properly electronic structure and magnetism of $BiFeO_3$, $SrFe_{12}O_{19}$, and then, using this approach, to explore electronic structure and magnetic properties of $SrFe_{12}O_{19}$-based systems where Fe is substituted with Ti and Co atoms. The calculations of electronic structures of these systems were performed using the generalized gradient approximation (GGA) for description of the exchange and correlation effects within DFT.

Our GGA DFT calculations of $BiFeO_3$ compound revealed that the chemical bonding is predominantly of an ionic character with partial covalent components of the Bi–O and Fe–O bonds. A covalent bonding facilitates stabilization of the structural distortions, which favours formation of a ferroelectric phase in $BiFeO_3$.

For $SrFe_{12}O_{19}$ and $SrCoTiFe_{10}O_{19}$ hexaferrites we have calculated electronic structure and magnetic properties by means of including the Coulomb parameter $U$ (GGA+$U$ method). It has been employed to deal with strongly correlated 3d-electrons.

As a result, the calculated magnetic moments of 3d-atoms are notably lower than the high spin values of the moments of free $Fe^{3+}$ and $Co^{2+}$ ions. It is revealed for the first time that the total magnetic moment is partly distributed among neighbouring oxygen ions. For ferrimagnetic $SrCoTiFe_{10}O_{19}$ the total magnetic moment depends on the particular sites occupancy with substitution of $Fe^{3+}$ ions by $Co^{2+}$ and $Ti^{4+}$.

As a whole, our calculations have revealed distinctive features of electronic structure of the investigated iron-based compounds with strongly correlated 3d-electrons, which are responsible for their peculiar structural and magnetic properties.

# STRUCTURAL AND MAGNETIC PROPERTIES OF THE NICKEL ORTHOBORATE $Ni_3(BO_3)_2$

**K. N. Boldyrev[1], A. D. Molchanova[1], M. A. Prosnikov[2], R. V. Pisarev[2]**

*[1] Institute of Spectroscopy, Russian Academy of Sciences,*
*Fizicheskaya st. 5, Troitsk, 142190 Moscow, Russia*
*[2] Ioffe Physical Technical Institute, Russian Academy of Sciences,*
*Polyteknicheskaya st. 26, 194021 St.-Petersburg, Russia*
*e-mail: kn.boldyrev@gmail.com*

Nickel orthoborate $Ni_3(BO_3)_2$ having a complex orthorhombic structure *Pnnm* (No. 58, Z = 2) of the kotoite type is known for quite a long time as an antiferromagnetic material below $T_N$ = 46 K [1-3], but up to now its physical properties including the lattice dynamics have not been explored. Six [$NiO_6$] units of 2*a* and 4*f* types are linked via rigid [$BO_3$] groups and these structural particularities impose restrictions on the lattice dynamics and spin-phonon interactions. We performed the symmetry analysis of the phonon modes at the center of the Brillouin zone. We report and analyze results of infrared and Raman studies of phonon spectra measured in all required polarizations. Clear evidence of the spin-phonon interaction was found for some particular phonons below $T_N$ (see Fig.1). An unexpected emergence of several very narrow and weak phonon lines was observed in the infrared absorption spectra exactly at the magnetic ordering temperature $T_N$. Moreover, anomalous behavior was found for some Raman phonons. The emergence of new phonon modes in the infrared and Raman spectra exactly at $T_N$ proves the existence of a magnetostructural phase transition of a new type in $Ni_3(BO_3)_2$. A possible nature of this transition is discussed [4]. Also the magnetic modes with interesting temperature dependence in the far infrared region were observed.

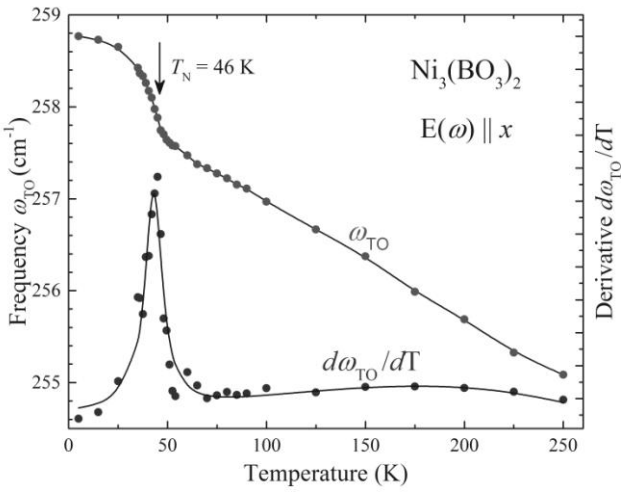


Fig.1. Frequency *vs* temperature dependence of the $B_{3u}$ mode near 255 cm$^{-1}$ active in the E($\omega$)||*x*-polarization and assigned to the $T_x$ translations of the Ni(2*a*) ions and [$BO_3$] groups, and the first derivative $d\omega/d$T of the phonon frequency, which emphasizes a frequency-shift anomaly at $T_N$.

This work was supported by the Russian Foundation for Basic Research (Projects No. 15-02-04222a and No. 15-32-20613) and the President of the Russian Federation for young scientists (Project No. MK-3521-2015.2).

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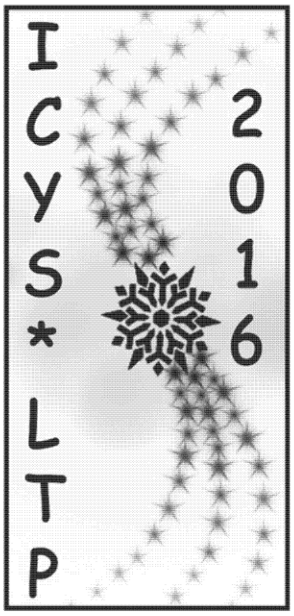
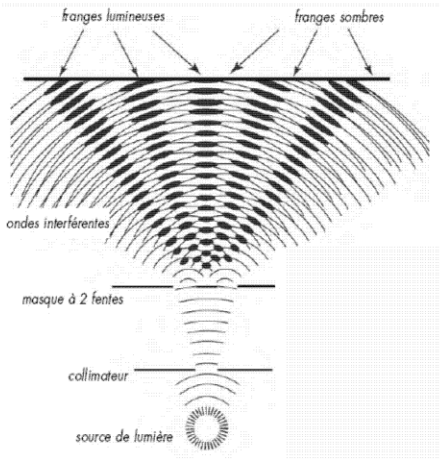
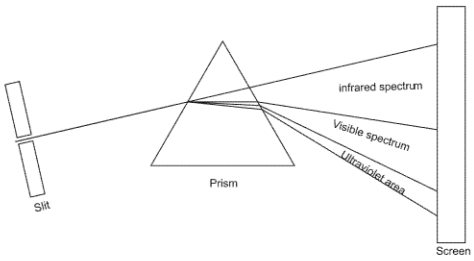
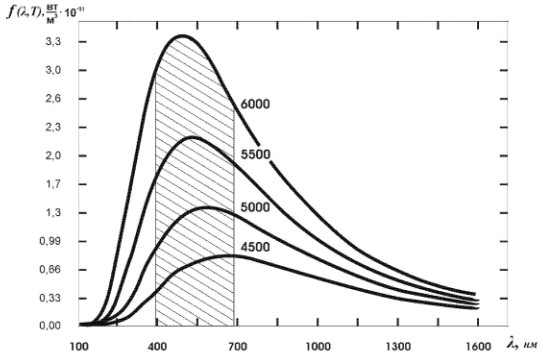
# Optics, Photonics and Optical Spectroscopy



# THz STUDY OF LOW ENERGY EXCITATIONS IN $KEr(MoO_4)_2$

**Sergii Poperezhai[1], Khrystyna Kutko[1], Papori Gogoi[2], Dmytro Kamenskyi[2]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, 47 Lenin ave., Kharkiv 61103, Ukraine*
*[2]Radboud University, Institute for Molecules and Materials, High Field Magnet Laboratory, 6525 ED, Nijmegen, the Netherlands*
*e-mail: Sergey.Poperedjay1986@gmail.com*

Here we report the systematic investigation of excitation spectra in the crystal $KEr(MoO_4)_2$. The characteristic feature of rare-earth compounds $KR(MoO_4)_2$ ($R^{3+}$ is a rare-earth ion) is the strong coupling between the electronic excitations of the $R^{3+}$ ions and phonons. Previous investigations show that the strength of electron-phonon coupling in $KR(MoO_4)_2$ can be tuned by a magnetic field [1, 2]. In $KEr(MoO_4)_2$ a magnetic field induced structural phase transition has been found at $H$~4T, $T$=1.4K.

We investigate $KEr(MoO_4)_2$ by means of far-infrared (FIR) spectroscopy using a commercial Fourier-transform infrared spectrometer (Bruker IFS113v) combined with a continuous-field 33-Tesla Bitter magnet. The low temperature FIR study performed in the magnetic fields allowed us to determine energies of electronic excitations as well as lattice vibrations. The obtained frequency-field dependences of electronic excitations show that in this material the phonon energies may coincide with electronic excitations in certain magnetic fields. Also we found complex structure of electronic spectrum in area of CJTE type phase transition.

Additionally in $KEr(MoO_4)_2$, the evidence of the non-linear effect induced by a strong coupling between electronic excitations and phonons has been observed in spectra obtained in Voigt configuration (**H** perpendicular to **k**).

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# FLUORESCENCE ENHANCEMENT BY J-AGGREGATES

**I. Yu. Ropakova, I. I. Grankina, A. V. Sorokin, Yu. V. Malyukin**

*Institute for Scintillation Materials, STC "Institute for Single Crystals", NAS of Ukraine,*
*60 Lenin ave., 61001 Kharkov, Ukraine*
*e-mail: adelma@ukr.net*

J-aggregates (Jelley aggregates or Scheibe polymers) are fluorescent organic well-ordered nanoassemblies formed by polymethine, porphyrine and some other dye molecules. Due to high order degree of molecular chain packing, electronic excitations are delocalized within some molecular chain fragments and Frenkel excitons appear. That results in the appearance of a new very narrow and intense absorption band (called J-band) bathochromically shifted with respect to the monomeric band and a near resonant luminescence band. In some cases, depending on mutual arrangement of molecules, excitonic band is hypsochromically shifted (H-band). Due to excitonic nature of electronic excitations, J-aggregates reveal a number of unique spectral properties, one of which is exciton migration over hundreds of monomers. Thus J-aggregates can be used as an optical antenna for energy delivery purpose. Indeed, exciton properties of J-aggregates are similar to those of light-harvesting complexes (LHC), which provide extremely fast and efficient energy transport of the absorbed sun light to the photochemical reaction center of plants and photosynthetic bacteria.

Recently we have reported the study of exciton migration for the case of J-aggregates formed in layered polymer films [1]. The feature of such film is a possibility to control distance between donors and acceptors of energy. This feature has been used to enhance J-aggregate fluorescence by metal nanoparticles [2]. In the case of energy acceptors embedded into the same polymer layer as the J-aggregates we found that the formers are strongly influenced to the aggregate optical properties [1]. So, the J-aggregates and the cyanine dyes which are playing role of energy acceptors were separated by polymer layer. Surprisingly, it caused an increase of the acceptor fluorescence intensity. Further studying the distance dependence of the acceptor fluorescence reveals it strong enhancement up to 7 times on the about 10 nm distance between the J-aggregates and the acceptors. Such dependence has been confirmed by fluorescence decay modification. Also changing the J-aggregate-acceptor pair leads to the same results. The results are explaining using an model of plasmon-like enhancement of the fluorescence.

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# PHOTOLUMINESCENCE PROPERTIES OF THE $Li_2O$-x$GeO_2$ GLASS-CERAMIC DOPED WITH SOME THREE CHARGED IONS

**Ya. Rybak[1], S. Nedilko[1], V. Scherbatskii[1], M.Trubitsyn[2], M. Volnianskii[2]**

*[1]Taras Shevchenko National University of Kyiv, 64 Volodymyrska st., 01601 Kyiv, Ukraine*
*[2]Oles Honchar Dnipropetrovsk National University, 72 Gagarin avenue, 49000, Dnipropetrovsk, Ukraine*
*e-mail: yar.rybak@gmail.com*

Various systems based on the germanate glasses were intensively studied last decades. One of the most popular substances of the family is lithium germanate of $Li_2O$-x$GeO_2$ composition.

The samples of the $Li_2O$-x$GeO_2$ (x=7; 11.5) glass-crystalline ceramics (LGO) were made from $Li_2CO_3$ and $GeO_2$ reagents of high purity [1]. Three types of the un-doped and doped with 3+ charged ions (Cr, Eu and Nd) were prepared using several stage of heat treatment: initial glasses, intermediate glass-crystalline samples, and polycrystals. Morphology of the sample's body and their surfaces as well as physical properties of the mentioned three types of the LGO samples were studied. Morphology of the samples surface was monitored using optical and electronic microscopy.

Photoluminescence (PL) emission and PL excitation spectra were studied at 4.2, 77 and 300 K. All of the samples under study are characterized with intensive PL in the visible region of the spectra. The PL spectra combine features of both own luminescence of the LGO matrix and emission of the three charged dopants. Composition and intensity of the PL bands depend on the dopant's concentration, type and morphology of the samples. By reference of the comparison between structure and properties some guess about electronic structure and peculiarities of the electronic transport as well as about luminescence origins were taken.

Obtained results were analyzed using known literature data about properties of the single crystals with $Li_2O$-7$GeO_2$ composition and glass-crystalline ceramics with $Li_2O$-x$GeO_2$ (x=7; 11.5) composition [2].

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# INTEGRATED QUANTUM CORRELATION COUNTER BASED ON MULTI-ELEMENT SUPERCONDUCTING NANOWIRE SINGLE PHOTON DETECTOR

**M. Yu. Mikhailov[1,2], V. Zwiller[1]**

*[1]Kavli Institute of Nanoscience Delft, Delft University of Technology*
*Delft 2628CJ, The Netherlands*
*[2]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: mikhail.mikhailov@gmail.com*

The development of efficient single photon sources and single photon detectors [1] for telecom wavelength bands (1310-1550 nm) are crucial for optical quantum information applications. Quantum correlation measurements are important diagnostic tool for characterization of such single photon sources [2]. Up to now, implementation of quantum correlation measurements (often in Hanbury Brown - Twiss interferometer geometry) required the use of bulky optical components such as beam splitters, lenses, discrete single photon detectors and measurements of quantum correlations higher than second order are very complicated due to increased amount of necessary equipment and possible artifacts due to misalignment. The detectors commonly used in such experiments are semiconducting avalanche photodiodes with low timing resolution and limited quantum efficiencies.

Here we present a new concept of integrated quantum correlation counter that requires neither alignment nor additional optical components. The developed counter is based on multi-element superconducting nanowire single photon detector made of ultrathin NbTiN film. The detector is self-aligned to single-mode optical fiber and each detector element is biased and readout independently. The detector has overall system quantum detection efficiency of 28 % at 1310 nm, a system dark count rate around 100 Hz and FWHM timing jitter of 32 ps when operated in closed-cycle refrigerator with a base temperature of 2.5 K. Using the developed integrated quantum correlation counter we measured the second-order intensity correlation function $g^2(\tau)$ of infrared nanowire quantum dot single photon source and observed characteristic photon antibunching statistics.

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# INFLUENCE OF ZINC CONCENTRATION ON STRUCTURAL AND OPTICAL PROPERTIES OF POLYCRYSTALLINE CZT THICK FILMS OBTAINED BY THE CLOSE SPACED SUBLIMATION

**Y. V. Znamenshchykov, V. V. Kosyak, A. S. Opanasyuk**

*Sumy State University, 2, Rymsky Korsakov Str., 40007 Sumy, Ukraine*
*e-mail: yaroslav.znamenshchykov@gmail.com*

The single crystals of $Cd_{1-x}Zn_xTe$ (CZT) ternary semiconductor are widely used for the X and gamma rays radiation detectors. It could be explained by the fact that band gap of this material can be adjusted over a wide range from 1.46 to 2.26 eV by the changing of Zn concentration. Introduction of zinc atoms may substantially increase resistivity of CZT and hence detector performance. On the other hand it may lead to decreasing in crystal quality due to deformation of crystal lattice. Also the nonuniformity in Zn volume distribution is one of the key problems of CZT crystal growth technology. The necessity of obtaining the low cost large-area uniform CZT wafers for X-ray imaging detectors lead to usage of thick films CZT instead of bulk crystals.

This paper reports results of studying of effect of zinc concentration on structural and optical properties of $Cd_{1-x}Zn_xTe$ thick films. Also the possibility of obtaining of high-quality thick polycrystalline CZT films with high Zn concentration ($x$>0.1) will be established.

The CZT films were deposited on Mo coated glass substrates by co-evaporation of the pure CdTe and ZnTe powders from independent sources using close spaced sublimation method (CSVS). Temperature of CdTe evaporator was $T_{e(CdTe)}$ =893 K, temperature of ZnTe evaporator was $T_{e(ZnTe)}$ = 993 K, substrate temperature was $T_s$=673 K. With the purpose to obtain CZT films with different Zn concentration the mass ratio of CdTe to ZnTe powder has been varied.

The X–ray diffraction (XRD), low temperature photoluminescence (PL) and Raman spectroscopy were used in order to study properties of CZT films.

XRD studies have shown that films were single-phase and contain a cubic phase of CdZnTe. Calculations of microstructural parameters, such as coherent scattering domains size and microstrains indicate decreasing of crystal quality with increasing in Zn concentration. In particular significant deterioration of crystal lattice was observed in films with zinc concentration higher than 30%.

The PL spectra of the samples show bound-exciton and donor-acceptor emission bands as well as broad band due to presence of dislocation. The clear observation of dominating $A^0X$ bands on PL spectra of the samples with zinc concentration up to 30% indicates fairly good crystal quality of the samples. The analysis of defect band of PL spectra confirms XRD results which reveal deterioration of the crystal lattice of CZT comparatively with CdTe.

Room-temperature Raman spectra of CZT films with different Zn concentration, obtained with a 785 nm laser excitation wavelength, include only CdTe and ZnTe-like longitudinal (LO) and transverse (TO) optical phonons modes. In order to carry out detailed phase analysis and hence to study spatial distribution of Zn atoms in samples we preformed surface Raman mapping of the ratio of $ZnTe(LO_1)$ to $CdTe(LO_1)$ modes intensities. As it was found, surface distribution of zinc atoms is rather uniform for all samples.

The in-depth study of CZT samples by XRD, PL and Raman show that CSVS method allow to obtain sufficiently uniform and high-quality thick films with Zn concentration up to 30%. Further increasing in $x$ value lead to non-uniform Zn distribution and monotonically decreasing of films crystal quality.

Our studies provide a way to obtain thick polycrystalline $Cd_{1-x}Zn_xTe$ films deposited on a Mo coated glass substrate by means of CSVS with large Zn concentration suitable for application in X-ray detectors.

# EFFECT OF THE STRUCTURE ON THE CHARACTERISTICS OF THE LANTHANUM-GALLIUM SILICATE GROUP CRYSTALS

**O. A. Buzanov[1], A. P. Kozlova[2], N. S. Kozlova[2], E. V. Zabelina[2], N. A. Siminel[2], D. A. Spassky[3]**

*[1] Fomos Materials Ltd., Buzheninova st., 16, Moscow 119049, Russia*
*[2]National University of Science and Technology "MISiS", Leninsky pr., 4, Moscow 119049, Russia*
*[3]Skobeltsyn Institute of Nuclear Physics, Moscow State University, Leninskie Gory, GSP-1, Moscow 119991, Russia*
*email: ane4kot@mail.ru*

Considerable improvement of the optical quality of crystals with the calcium – gallium germanate structure, the space group of symmetry is P321, in particular of langatate $La_3Ta_{0.5}Ga_{5.5}O_{14}$ (LGT) and langasite $La_3Ga_5SiO_{14}$ (LGS) attract enhanced attention because of their application perspectives in optics and opto-, piezoelectronics.

Crystals with this structure are neither pyro nor ferroelectrics, and non-hygroscopic. High values of piezoelectric coefficient and thermostable cuts allowed to apply the langasite for the creation of filters and resonators on surface and bulk acoustic waves. The drift of the piezoelectric coefficients is not observed in langatate in contrast to langasite and other piezomaterials therefore it is used for high-temperature sensors of different physical values. To use in different sensors these crystals are processed with different methods of machining (cutting, grinding, polishing). Therefore the study of their mechanical properties is necessary.

For this study the LGT and LGS crystals were grown from iridium crucibles by the Czochralski method at Fomos-Materials, in the atmospheres of argon (Ar) and argon with oxygen ($Ar+O_2$).

The main problem of application of these crystals is uncontrolled presence of point defects, and difficulties with determination of their origin. In LGS and LGT crystals point defects and their complexes influence its color and its characteristics (optical, mechanical properties) acting as color centers. Presence of color centers is connected with the growth atmosphere.

The complex investigation of luminescent and optical properties of the langatates grown in different atmospheres has been performed for the determination of the origin of defects.

Optical spectroscopy is a very sensitive tool to examine point defects. The influence of different growth atmospheres on optic transmission spectra of the crystals showed that decreasing of oxygen concentration in growth atmosphere of crystal lead to the considerable improvement of their optical characteristics. We observed the anisotropy of the transmission spectra of samples – this effect in crystals with Ca-gallogermanate crystals is well-known. However we also observed dichroism for the samples which were cut in parallel with axis Z. This effect occurs in some crystals with specific structure when naturally polarized and p-, s-polarized light pass along directions perpendicular to the optical axis, and may be caused by the symmetry of the crystals' structure or by the anisotropy of color centers.

The absorption spectra of crystals were measured in the temperature region 78–500 K. The luminescence characteristics were studied under excitation with X-rays and photons of UV and VUV energy regions at T=4.2–300 K.

LGT, LGS are known to demonstrate optical activity. The direction of polarization plane rotation was established from the changes in a conoscopic figure. It was found that all of the investigated samples were dextrorotatory regardless of the atmosphere of growth. In this work, we studied gyration coefficient φ of samples cut from crystals obtained in different atmospheres.

For the same samples microhardness anisotropy was found out. The microhardness of langatate crystals obtained in different growth atmospheres was studied.

# THE ELECTRIC FIELD INDUCED ROTATION OF POLARIZATION PLAN IN $HoAl_3(BO_3)_4$

**M. I. Pashchenko[1], V. A. Bedarev[1], D. N. Merenkov[1], L. N. Bezmaternykh[2], V. L. Temerov[2]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, 47 Nauky Ave., 61103 Kharkiv, Ukraine*
*[2] L.V. Kirenskii Institute of Physics, Siberian Branch of the Russian Academy of Sciences, Krasnoyarsk 660036, Russia*
*e-mail: pashchenko@ilt.kharkov.ua, p.maria1984@gmail.com*

The trigonal crystal of rare-earth borate $HoAl_3(BO_3)_4$ demonstrates a giant magnetoelectrical effect caused by the strong spin-lattice interaction [1]. This noncentrosymmetric crystal is transparent for visible range of light and can be interesting for studying of electro-optical effects [2].

The main purpose of this work was the investigation of electrogyration in a $HoAl_3(BO_3)_4$ The single crystal plate with dimensions 4x4 mm and thickness 230 μm was studied. Investigations were carried out with the wavelength of He-Ne laser (0.633 μm). In the experiments the light beam was directed along the crystal axis $C_3$ and the electric field E was directed along the $C_2$ axis.

The electric field dependences of polarization plane rotation were measured at room temperature. It was found that the value of electric-field-induced polarization plane rotation is ~ 0.1°at the $E = 4 \cdot 10^6$ V/m and linearly depends on electric field.

The phenomenological analysis showed that in such experimental geometry the rotation of polarization plane in $HoAl_3(BO_3)_4$ crystal is determined by electric-field-induced deformation only.

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# ANISOTROPY OF THE REFRACTIVE INDICES OF $Rb_2ZnCl_4$ CRYSTALS

**V. B. Stakhura, V. Yu. Kurlyak, V. Yo. Stadnyk, R. S. Brezvin, L. T. Karplyuk**

*Ivan Franko National University of Lviv, Lviv, 79005 Ukraine, Kyrylo and Mefodiy, 8, Str.*
*e-mail: stakhura2507volodymyr@gmail; vasylstadnyk@ukr.net*

Tetrachlorozincate of rubidium crystals (TCZR), $Rb_2ZnCl_4$, are a typical example belonging to the one dimensional modulated incommensurate system of $A_2BX_4$ type.

They are characterized by the following sequence of phases: a paraelectric (PP) ($T_i$ = 302 K) – incommensurate (IP) ($T_c$=192 K) – commensurate ferroelectric (CP). Despite the considerable interest, integrated research of refractive parameters in wide spectral and temperature ranges is not held. Also not examined the effects of uniaxial strain on refractive properties, and the position of points phase transitions (PT) PP-IP-CP. The purpose of this work is to study the refractive indices of $Rb_2ZnCl_4$ crystals in a broad spectral and temperature ranges under the influence of a uniaxial mechanical pressure along the main crystallophysic axes *a, b, c*.

It is established, that in the spectral range the dispersion of $n_i(\lambda)$ mechanically free crystals is normal ($dn_i/d\lambda < 0$) and when approaching the edge of absorption increases sharply. Uniaxial pressure does nor changes a nature of $n_i(\lambda)$curves, but only the magnitude of variance $dn_i/d\lambda$.

For nonlinear characteristic TCZR crystals change $n_i$(T), with the value of the nonlinearity increases with increasing temperature and PP it more than in CP. Phase transition IP-CP at T = 192 K to accompanied by minor changes in abrupt of refractive indices: $\delta n_a = 2{,}1\times10^{-4}$, $\delta n_b = 2{,}4\times10^{-4}$ and $\delta n_c = 1{,}9\times10^{-4}$. Uniaxial compression slightly reduces the magnitude of these jumps: $\delta n_a = 1{,}9\times10^{-4}$ and $1{,}8\times10^{-4}$ for $\sigma_b$ and $\sigma_c$=200 bar, respectively; $\delta n_b = 2{,}1\times10^{-4}$ and $2{,}0\times10^{-4}$ for $\sigma_a$ and $\sigma_c$=200 bar, respectively; $\delta n_c = 1{,}8\times10^{-4}$ and $1{,}7\times10^{-4}$ for $\sigma_a$ and $\sigma_b$=200 bar, respectively. At heating the temperature hysteresis are detected (PT~3 K).

It has been established that PP crystals studied enough sensitive to the effects of stress and in so doing discovered a significant offset points PT on the temperature scale in different directions depending on the direction of compression. So determined for pressures that $\sigma_m$=200 bar at PT PP-IP occurs when to $T_i^b = 306{,}2$ K, $T_i^c = 299{,}1$ K and $T_i^a = 297{,}4$ K, whereas mechanically free crystal $T_i = 302{,}0$ K. For the respective voltage PT from in commensurate to commensurate phase occurs when to $T_c^a = 188{,}4$ K, $T_c^b = 196{,}7$ K and $T_c^c = 190{,}1$ K, whereas mechanically free crystal to $T_c = 192{,}0$ K.

If we consider the total displacement ratios of PT points by the action of uniaxial pressure along the main crystallographic directions, we get :

$$dT_i/d\sigma_m = dT_i/d\sigma_a + dT_i/d\sigma_b + dT_i/d\sigma_c = -0{,}014 \text{ K}\cdot\text{bar}^{-1},$$
$$dT_c/d\sigma_m = dT_c/d\sigma_a + dT_c/d\sigma_b + dT_c/d\sigma_c = -0{,}003 \text{ K}\cdot\text{bar}^{-1}.$$

Since baric PT points offset coefficients differ ($dT_i/d\sigma_c = < dT_c/d\sigma_c$), it should be expected that under the influence of stress $\sigma_s$ the incommensurate phase of TCZR crystal will narrow. By extrapolating the curves $T_c(\sigma_c)$ and $T_i(\sigma_c)$ actually found that at pressures $\sigma_c \sim 18{,}3 \pm 0.5$ kbar and a temperature $T \sim 28{,}3 \pm 0{,}1$ K the IP of TCZR crystal are disappearing and there will be exist the para-ferroelectric phases, bypassing the incommensurate phase, that is, there will " triple point ".

# MODEL CALCULATIONS OF $Eu^{3+}$ LUMINESCENCE SPECTRA IN NANOSTRUCTURED CARBON NITRIDE FILMS.

**R. Yu. Babkin[1], O. G. Viagin[2], O. V. Gornostaeva[3], K. V. Lamonova[1], S. M. Orel[1], A. M. Prudnikov[1], Yu. V. Malyukin[2], Yu. G. Pashkevich[1]**

*[1]O. O. Galkin Donetsk Institute for Physics and Engineering, National Academy of Sciences of Ukraine, 03680 Kiev, Ukraine*
*[2]Institute for Single Crystals, National Academy of Sciences of Ukraine, 61001 Kharkov, Ukraine*
*[3]G. V. Kurdyumov Institute for Metal Physics, National Academy of Sciences of Ukraine, 03680 Kiev, Ukraine*
*e-mail: r.yu.babkin@gmail.com*

A wide range of prospective applications of carbon nitride films (hydrogen energy, electrochemical probes, functional sensory elements, tribological coatings, etc.) is explained by their wide phase diagram. In the work [1] it was shown that the carbon nitride can exist in different structural phases: amorphous, graphite-like, fullerene-like. However, we argue that in the carbon nitride films there are two more structural phases – diamond-like and nano-columnar ones. Nano-columnar films have a specific columnar structure: vertically oriented arrays of nano-columns that grow along the film thickness. Unfortunately, it impossible to describe the nano-columnar structure in terms of well-known fullerene-like structure model, and at the moment there is no an adequate model to describe the growth of this kind of objects. To study the nano-columnar structure the carbon nitride films were activated by europium chloride $EuCl_3$. The use of $Eu^{3+}$-based probes as the most studied lanthanide ions in submicron and nano-dispersion materials is provided to investigate the topology and structure of carbon nitride films.

In this work we study the luminescence spectra of trivalent europium, which acts as a probe in the carbon nitride films. The simulations of a luminescence spectra were carried out by MCFT-method [2, 3]. A series of calculations have been carried out: (i) the calculations of the free $Eu^{3+}$ spectra; (ii) the calculations of the crystal field energy levels of $Eu^{3+}$ ions in coordination complex $[EuCl_9]^{6-}$, which is the main structural units of compound $EuCl_3$; (iii) the simulation of the of the coordination complex deformation and changing set of ligands on the luminescence spectra.

The comparison of the luminescence spectra shows that a considerable part of europium (III) chloride enters into a chemical connection with the carbon nitride film matrix. It was shown that europium ions after annealing keep their place in chloride complexes, which means the ligand structure is substantially unchanged. The additional splitting of the electron levels, as well as changes in the intensities of the spectral lines can be connected to the low-symmetry distortion of the coordination complex $[EuCl_9]^{6-}$. Besides the general broadening of the spectra with increasing the dopant concentration indicates a loss of translational symmetry of the $EuCl_3$ nanoparticles and the loss of local symmetry in the first and second coordination spheres of the europium ions environment.

However, the film luminescence spectra contain quite a number of intensively weak lines, as well as characteristic changes in energy that do not fit into simple complexes distortions. These features are associated with partial destruction of the $[EuCl_9]^{6-}$ complexes, changes of the effective ligand charges, and the formation of chemical bonds with carbon nitride structures.

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# LUMINESCENCE PROPERTIES OF POLYCRYSTALLINE SYSTEM $Ca_{3-X}Cd_XGa_2Ge_3O_{12}$ DOPED WITH $Eu^{3+}$

**L. V. Kostyk, M. R. Panasyuk, A. P. Vas'kiv, M. S. Rudko, I. S. Novosad, S. S. Novosad**

*Ivan Franko Lviv National University, Ukraine,*
*1 Universytetska St., Lviv 79000, Ukraine*
*e-mail: rudko_mykola@ukr.net*

The peculiarities of spectral-luminescent properties of $Ca_{3-x}Cd_xGa_2Ge_3O_{12}$ (x=0–3) polycrystalline phosphors activated by $Eu^{3+}$ under X-ray and photo excitation in the temperature range 77-300 K were presented in this paper. $Eu^{3+}$ impurity concentration varied between 2 mol.% to 4 mol.%. Polycrystalline ceramic samples of stoichiometric composition in pallets form with a diameter of 8 mm and a thickness of 1-1.5 mm were obtained by solid phase synthesis at $1200^0$ C on standard ceramic technology, using high purity corresponding oxide powders. ***X-ray studies were*** carried out in "Interfaculty scientific-educational laboratory of X-ray structure analysis" of Ivan Franko National University of Lviv on diffractometer STOE STADI P (Cu $K_\alpha$-radiation). The analysis of obtained diffractograms shows the formation of a cubic garnet single phase (space group Ia3d). Introduction the $Cd^{2+}$ ions in the compound leads to lattice parameter changes between 12,248 Å (x=0) to 12,182 Å (x=3). We can assume that the $Cd^{2+}$ and $Eu^3$ ions occupy a lattice site with $D_2$ symmetry by replacing $Ca^{2+}$ ions in distorted dodecahedral positions [1].

Based on the analysis of data on research of spectral-luminescent properties of single crystals $Ca_3Ga_2Ge_3O_{12}$ doped by $Eu^{3+}$ ions [1,2] and experimental results obtained on ceramic samples, the groups of relatively narrow lines in the region between 570-800 nm were attributed to radiative f-f transitions in $Eu^{3+}$ ions. On the spectral range 585-630 nm, there are only two intense components of electro-dipole transition $^5D_0 \rightarrow {}^7F_2$, which is consistent with point symmetry $D_2$ (dodecahedral position in the garnet structure), and the lines near 700 nm can be attributed to $^5D_0 \rightarrow {}^7F_4$ transitions in $Eu^{3+}$ ions. With increasing Cd content in garnet the emission intensity near 700 nm increases. This may be connected with a greater probability of transition in Cd - garnets, caused by lower distortion in dodecahedral places in these garnets compared with $Ca_3Ga_2Ge_3O_{12}$ garnet composition.

Wide band luminescence with a maximum at 500 nm is observed only in Cd doped polycrystalline samples under UV or X-ray excitation. A significant increase in the intensity of this luminescence with increasing impurity contents can be evidence that defects, which associated with the introduction of Cd, are involved in radiative processes of $Ca_{3-x}Cd_xGa_2Ge_3O_{12}$: $Eu^{3+}$ ceramics.

The thermoluminescence (TL) glow curve obtained for $Ca_3Ga_2Ge_3O_{12}$ polycrystalline sample with 0,1mol. % $Eu^{3+}$ in the region80-450 K after X-ray irradiation during 5 min at T = 90 K consists a number of peaks appearing at about 150, 190, 337 and 390 K. The glow curve of $Ca_{1.5}Cd_{1.5}Ga_2Ge_3O_{12}$: $Eu^{3+}$ ceramics shows one wide composite intense peak with main maximum at 200 K due to strong broadening of low-temperature peaks. Photo stimulated luminescence (PSL) is exhibit in this material. IR-light irradiation of preliminary X-ray irradiated sample at 90 K significant reduces low-temperature peak near 150K, and slightly decreases of peak intensity at 190 K. We analyzed results on influence of IR-light irradiation on the TL glow curves with the aim to define the trapping level nature and features of recombination luminescence processes at low temperature.

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# LUMINESCENCE OF PAIR IODINE CENTERS IN AgBrI MICROCRYSTALS

**A. A. Akhmerov, A. V. Tyurin, S. A. Zhukov, A. A. Rimashevskii**

*Scientific Research Institute of Physics of Odessa I.I.Mechnikov National University*
*Pasteur str.,27, Odessa 65026, Ukraine*
*e-mail: oleksandr.akhmerov@onu.edu.ua*

As we have found earlier, the luminescence of pair iodine centers (λmax=540-570 нм) in microcrystals AgBrI reacts differently to additional infrared illumination, when being excited by the light from its own absorption area AgBrI (λ<470 nm) - depending on whether microcrystals are dispersed in water (sol), or are they in an isolated state in a synthetic binder (polyvinyl alcohol). Additional exposure to long-wavelength light with λ>1000 nm stimulates the luminescence "flash". But if AgBrI microcrystals are distributed in a gelatin, then in the luminescence band of pair iodine centers (λ max=540-570 nm) the influence of long wave light with λ>1000 nm produces the luminescence “quenching”. Regarding the reasons for such differences, some guesses were proposed but they were not confirmed experimentally.

In this work, the experimentally confirmed energy scheme of localized states in the AgBrI microcrystals is analyzed. It allows to produce a system of differential equations of the first order. Solution of this system allows to obtain the kinetics of luminescence for all the bands of low-temperature luminescence of AgBrI microcrystals under the influence of infrared (IR) illumination.

The following results were obtained for the band of luminescence of pair iodine centers in microcrystals AgBrI, upon photoexcitation (λ<470 nm) and at different wavelengths of additional infrared light:

a) the Schon-Klasens «flash» mechanism under IR light with λ=800-1000 nm;

b) the Lambe-Klick «quenching» mechanism under IR light with λ=900-1400 nm.

For the band of luminescence arising at the recombination of holes localized on the pair iodine centers with electrons located on the superficial silver centers of atomic and molecular degree of dispersion (λ max=750 nm):

c) the Williams-Prener «luminescence flare-up» mechanism, which is an increase of luminescence intensity under IR light with λ>1000 nm.

Analysis and experimental verification of the received results showed that the difference in the effects of IR light on the illumination of pair iodine centers in AgBrI microcrystals is caused by the appearance of additional centers of localization of electrons, when the microcrystals are placed into a gelatin medium.

# KINETICS OF LOW TEMPERATURE EXCITON PHOTOLUMINESCENCE IN $PbCdI_2$ CRYSTALS

**A. P. Bukivskii[1], Yu. P. Gnatenko[1], Yu. P. Piryatinski[1]**

*[1]Institute of Physics of National Academy of Sciences of Ukraine. Prospekt Nauky, 46, Kyiv 03028, Ukraine*
*e-mail: ap.bukivskii@gmail.com*

Earlier [1] we have shown the presence of $PbI_2$ nanoclusters (NC) which are naturally formed in $PbCdI_2$ layered semiconductor solid solutions. The presence of these NCs was first predicted based on analysis of low temperature photoluminescence spectra and then confirmed by scanning electron microscopy (SEM) methods. Presence of such different sized NCs gives layered $PbCdI_2$ semiconductor its unique PL properties, an example of which is an intense, wide PL band (about 600 nm). This PL band is observed at the wide range of temperatures, from liquid Helium temperatures to room temperatures and also appears after excitation not only by visible light, but also by high energy rays and particles such as X-Rays or Gamma particles. This gives a good opportunity to use $PbCdI_2$ solid solutions as detector material for X and Gamma rays.

In this particular study we investigate the photoluminescence at low temperature (4.5 K) and at room temperature of $PbCdI_2$ solid solutions and also the kinetic dependencies of PL bands at 493 and 510 nm at 4.5 K in particular. These bands are connected with photoluminescence of free excitons in pure $PbI_2$ captured inside $PbI_2$ NCs in $PbCdI_2$ solid solutions and recombination emission of donor-acceptor pairs (DAP), respectively. Investigated samples were $Pb_{1-X}Cd_XI_2$ solid solutions with concentration of composition components X = 0.7. PL kinetics data were obtained using Lifespec2 fluorescence lifetime spectrometer. PL excitation was carried out by 405 nm pulse laser with ~50 ps pulse width.

The mathematical analysis of experimental kinetics was made using the demo version of Edinburgh Instruments FAST software. This software uses a modified Maximum Entropy Method (MEM) to restore the shape of lifetime parameter distribution from kinetic PL data. This method is based on the fact that any observed kinetic dependency is a mathematical transformation of lifetime distribution function and can be presented as:

$$I(t) = \int_0^\infty \frac{1}{\tau} F(\tau) e^{-\frac{t}{\tau}} d\tau \quad (1)$$

where $\tau$ is the PL lifetime and $F(\tau)$ is its distribution function. Thus, using some mathematical simplifications such as discretization of time and transition from integration to taking a sum one can restore the shape of lifetime distribution function relatively easy:

$$t \to t_1, t_2, t_3 \ldots (2)$$
$$F(\tau) \to F_{\tau_1}, F_{\tau_2}, F_{\tau_3} \ldots (3)$$
$$I(t) = \int_0^\infty \frac{1}{\tau} F(\tau) e^{-\frac{t}{\tau}} d\tau \Rightarrow I(t) = \sum_{i=1}^{N} F_{\tau_i} e^{-\frac{t}{\tau_i}} \quad (4)$$

Using the right part of eq. 4 as a fitting function for the kinetic data $I(t)$ and choosing N for the best resolution/calculation complexity ratio (we used N = 200) we essentially get our desired lifetime distribution $F_i(\tau_i)$.

Also, we calculated the ensemble mean lifetimes of exciton and DAP photoluminescence at low (4.5 K) temperature. These calculations were made using the software created by us which gives one an opportunity to make this analysis with great accuracy and minimum difficulty.

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# PECULIARITIES OF GLASS FORMING OF THE FULLERITE $C_{60}$ SATURATED BY THE CARBON MONOOXIDE MOLECULES: PHOTOLUMINESCENCE STUDIES

**P. V. Zinoviev, V. N. Zoryansky, Yu. E. Stetsenko, V. V. Danchuk**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: zoryansky@gmail.com*

Low temperature (20–230 K) studies were carried out by the spectral-luminescent method of the fullerite $C_{60}$ saturated by carbon monooxide in the physsorption mode. Significant changes of the photoluminescent characteristics of the solutions $C_{60}$–CO with different concentration of the impurity were found even at small times of intercalation. Strong dependence of CO solubility on the saturation temperature was registered by analyzing the contribution to the luminescence of the "deep X-traps", and filling of octahedral voids by CO molecules occurs with smaller gradient of the impurity distribution in depth of $C_{60}$ crystals in comparison with $N_2$. Temperature dependences of the radiation integral intensity of the samples with different concentration of the carbon monooxide were studied. It was found for the first time that CO molecules have significant influence on the process of orientation glass formation and on the rotational dynamics of the $C_{60}$ molecules in contrast to $H_2$ and $N_2$. In the framework of the model of electron excitations transfer in $C_{60}$ crystals, there was explained the influence of the polar CO molecule on the processes of the $C_{60}$ molecules reorientations and changes of their rotations type in the concentrated $C_{60}$–CO solutions, which leads to observed strong temperature shift of the orientation $T_c$ and glass $T_g$ transitions to the region of low temperatures, which is accompanied by "blurring" of their boundaries.

# TEMPERATURE DEPENDENCE LUMINESCENCE OF $Ag_8SnSe_6$ ARGYRODITE

**I. V. Semkiv, H. A. Ilchuk, V. V. Kusnezh**

*Lviv Polytechnic National University, S.Bandera, 12, Lviv 79013, Ukraine*
*e-mail: Semkiv.Igor.5@gmail.com*

Ternary chalcogenide semiconductors, such as argyrodite with common formula $A_8^{I}B^{IV}X_6$ ($A^{I}$=Cu, Ag; $B^{IV}$=Si, Ge, Sn; X=S, Se, Te), have attracted attention as promising materials for thermoelectric, solar cell and resistive memory cells application. In particular $Ag_8SnSe_6$, which is a semiconductor with a direct band gap of 0.83 eV, high optical absorption coefficient and mixed ionic-electronic conductivity. $Ag_8SnSe_6$ crystallizes in either an orthorhombic structure (space group $Pmn2_1$) or in a cubic lattice (space group $F\bar{4}3m$).

In this work we report the results of studies of light emitting argyrodite crystals obtained by direct melting of the stoichiometric mixture of the Ag, Sn and Se of high purity grade (not less than 99.999%) in sealed ($10^{-5}$ Torr) silica ampoule.

The photoluminescence studies of $Ag_8SnSe_6$ were carried out in the cryostat. As the excitation source the 514 nm laser light was used.

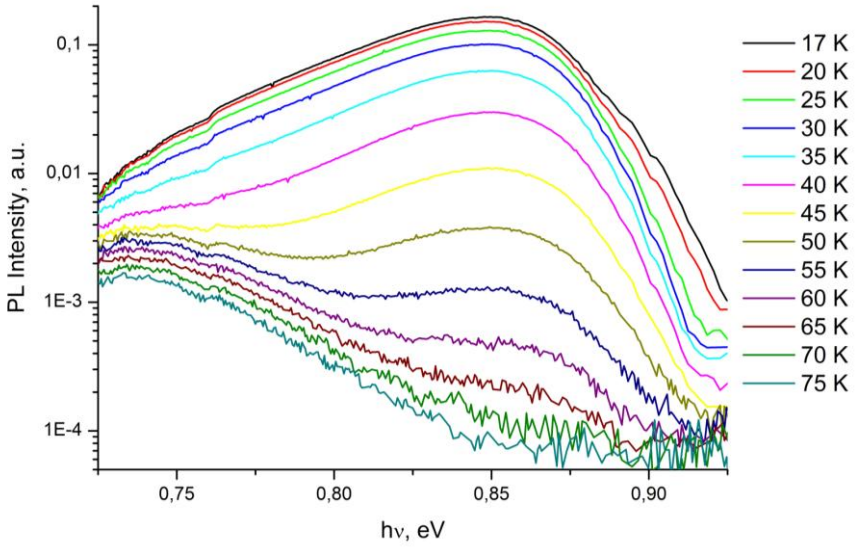


Fig.1. $Ag_8SnSe_6$ argyrodite photoluminescence spectra as a function of the temperature

The photoluminescence integrated intensity described by the equation $I_{PL} \sim P^m$ where $P$ is the excitation power and $m$ is fitted parameter. At the 17 K, photoluminescence occurs due to recombination involving defects ($m$ equal 0.76). Low temperature photoluminescence spectra show one broad asymmetric peak with maximum at 0.85 eV which is close to band gap value. The shape of the peak is typical for recombination which carried out between tails of conduction and valance band. But peak does not shift with increased excitation power. Thus the commonly observed effect of reducing potential fluctuations due to screening of charged defects by generated carriers is not observed. This can be explained by chemical or structural nonuniformity. With increasing temperature nonradiative recombination activates and above 70 K no signal can be detected. While photoluminescence quenches rapidly a new peak at 0.74 eV emerges. This recombination channel is associated with donor-acceptor transition.

# PHOTOCONDUCTIVITY KINETICS IN InGaAs QUANTUM WIRE HETEROSTRUCTURES

**S. A. Iliash, S. V. Kondratenko**

*Taras Shevchenko National University of Kyiv, Prospekt Hlushkov, 4, Kyiv 03022, Ukraine*
*e-mail: iliashsviatoslav@gmail.com*

Last decades the interest in the study of the physical properties of heterostructures InGaAs-GaAs, specifically centers with deep and shallow trap levels, has increased significantly[1, 3]. Heterostructure InGaAs-GaAs with quantum wires (QWRs) are known for their unique photo electrical properties that are perspective for the implementation of new phototransistors technologies, infrared photodetectors and solar cells. Deep defect states in the band gap of InGaAs are formed by doping a wide class of impurities [2, 3]. These states may be significantly complicated due to formation of dopants pairs or their interaction with their own lattice defects.

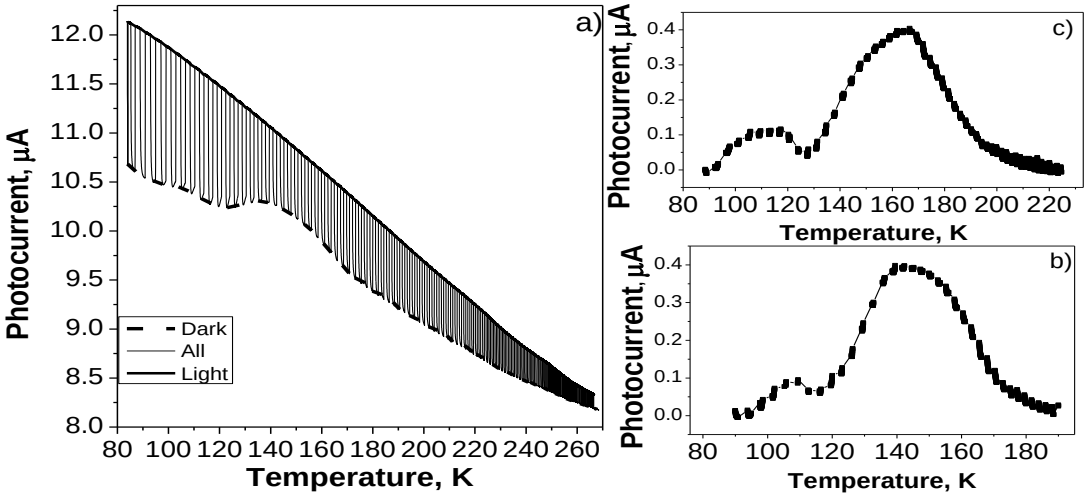


**Figure. 1.** (a) The dependence of the photocurrent(PC) spectra on the heating(excitation $h\upsilon_1$ = 1.35 eV). Thermally stimulated conductivity of sample 11ML InGaAs-GaAs for various excitation intensities, (b)for $h\upsilon_1$ = 1.35 eV, (c) for $h\upsilon_2$ = 1.65 eV.

Optical and electronic properties are studied by PC kinetics and thermal activation effects measurement. TSC spectra obtained for InGaAs-GaAs heterostructures. The spectrum of electronic states that determines recombination in 11ML InGaAs-GaAs heterostructures, obtained at different temperatures, using TSC method and kinetic method of periodic illumination of the sample. The structure of the TSC spectrum consist two peaks in the range 100-200K, which shifted relative to classical TSC in lower temperatures, for the kinetic method of periodic illumination of the sample. Obtained activation energy for potential wells of the band structure and studied temperature dependence of time constant τ show that the excitation of light with selective energy for subsystem $In_xGa_{1-x}As$ QWRs, leads to increase PC, caused electrons concentrated at QWRs. Contribution in conduction make electrons, which localized in potential well minimum when irradiation in the GaAs fundamental absorption.

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# DISPERSIVE READOUT OF A SUPERCONDUCTING QUBIT WITH A PHOTODETECTOR

**Andrii Sokolov**

*Institute of Physics of NAS of Ukraine,*
*Prospekt Nauky 46, Kyiv 03028, Ukraine*
*e-mail: andriy145@gmail.com*

A possibility for qubit readout is a basic requirement for quantum computation. [Physically, qubit readout is a measurement of a two-level system (quasi)spin projection.] Fast and robust readout is needed. Also, it is often required for the measurement to be quantum-non-demolition: i.e., a state which qubit wavefunction collapses to should not change during the readout.

Dispersive readout posseses those qualities [1]. It uses a cavity coupled off-resonantly to the qubit to infer its state. Depending on whether the qubit is in the excited or the ground state, the cavity resonance is shifted to the blue or to the red side. To probe this shift, it is common to measure a phase acquired by a radiation transited by the cavity.

However, this approach has disadvantages. Superconducting qubit and resonator are cooled to tens of millikelvins and are often placed on chip. To minimize added noise, output signal undergoes several amplififcation stages at different temperatures. The phase shift is then determined using a homodyne with a strong local oscillator. It is difficult to integrate this setup on chip. Also, sophisticated multiplexing and wiring are required for multiple qubit readout.

It was recently proposed to use a photodetector for the readout [2]. Microwave photodetectors suitable for integration were already demonstrated [3]. Detector provides a classical signal which is readily picked up by conventional electronics. Besides, lots of detectors may be integrated on chip hence simplifying the readout of multiple qubits.

This study [4] aims at improving readout that uses photodetector. Probability of the correct measurement result, i.e., fidelity, is maximized with respect to the system parameters. Strictly speaking, optimal parameters depend on the measurement duration. However, in some cases, for example, in a long measurement, it is sufficient to use a non-varying parameters. Also, it is shown that a photon-number-resolving detector provides shorter measurement time if one is to achieve a fidelity greater than 72%. Using the optimal readout parameters, it is possible to achieve a 99% fidelty in a single-shot measurement.

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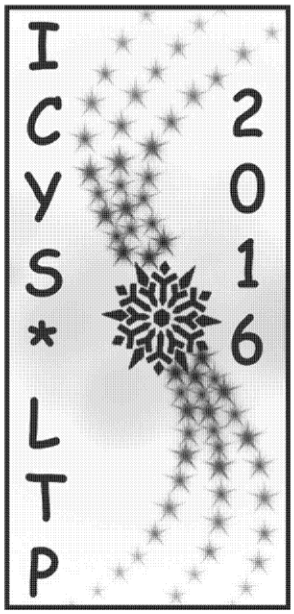
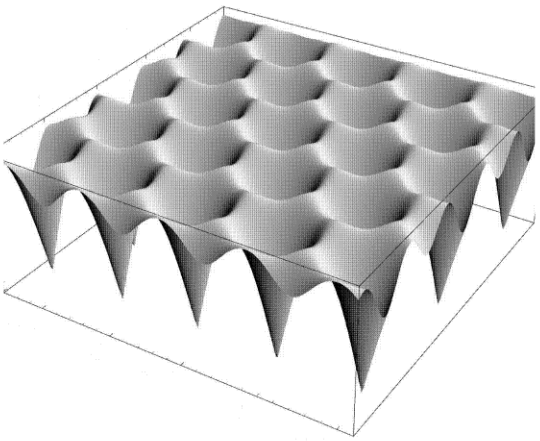
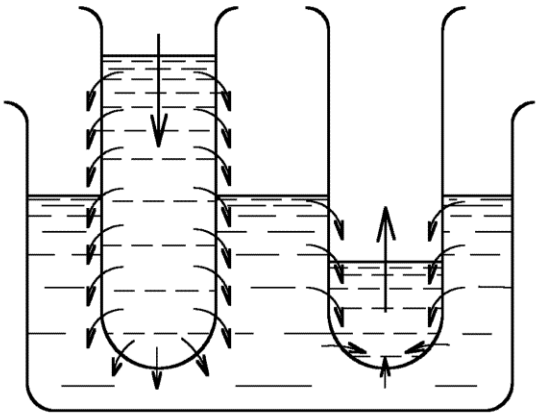
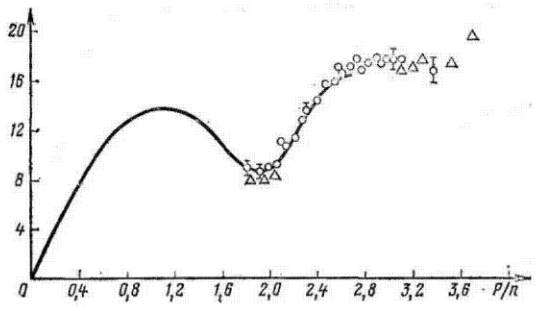
# Quantum Liquids and Quantum Crystals, Cryocrystals







# THE THERMAL CONDUCTIVITY OF POLYMORPHS 4-BROMOBENZOPHENONE CRYSTALS

**Yu. V. Horbatenko, O. O. Romantsova, A. I. Krivchikov, O. A. Korolyuk**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: horbatenko@ilt.kharkov.ua*

The thermal conductivity of two polymorphs of 4-bromobenzophenone crystals - monoclinic and triclinic was measured using the stationary heat flux method in a wide temperature range. The structure of these polymorphs is different by stacking order: the monoclinic structure has Z = 4 molecules per unit cell, and the triclinic has Z = 2 molecules. It has been shown that the thermal conductivity behavior of polymorphs 4-bromobenzophenone at temperature above 20 K can be described as a sum of two terms $\kappa = \kappa_1 + \kappa_{TA}$. The term $K_1$ of this expression has form $K_1 = A/T+B$, where $A/T$ describes the three-phonon scattering processes, and B is the contribution from short-wave excitations. The second term $\kappa_{TA} = \kappa_0 \exp(-E/kT)$ deals with some thermal activation process, which is characterized by activation energy parameter E at higher temperatures.

It has been shown the thermal conductivity of the monoclinic sample above 150 K behaves exactly the same way as in triclinic sample and also their activation energies have very close values. It was detected the thermal conductivity increases above 120 K for both bromine-containing polymorphs, while in the unsubstituted benzophenone it is no observed. Such behavior of the thermal conductivity is an experimental evidence of the new non-phonon mechanism of heat transfer due to the excitation of intramolecular crystal modes associated with C-Br stretch vibrations in the bromo-substituted compounds.

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# ON THE DIPOLE MOMENT OF QUANTIZED VORTICES IN THE PRESENCE OF FLOWS

**S. I. Shevchenko , A. M. Konstantinov**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: alexander.konstantinov2010@yandex.ua*

The recent researches [1-5] showed that the spatial inhomogeneity of any dielectric, including neutral superfluid liquid, should lead to the polarization of the system. In liquids the inhomogeneity of density can be created by the inhomogeneous velocity field. In the superfluid systems the velocity field of quantum vortices essentially depends on the coordinates near the vortex core, therefore we expect that induced by inhomogeneity dipole moment can be associated with the vortex line. The present report is devoted to the problem of the dipole moment at quantized vortices.

The consideration is performed in a model of a diluted Bose gas whose particles have internal degrees of freedom associated with motion of electrons relative to the nucleus [5]. The polarization charge $\rho_{pol}$ of an inhomogeneous superfluid system is expressed as a function of the order parameter $\Phi(\mathbf{r}_1, \mathbf{r}_2)$. It is shown that if the order parameter changes on macroscopic distances, the polarization charge $\rho_{pol}$ is proportional to $A\nabla^2 n$, and the polarization $\mathbf{P}$ is proportional to $A\nabla n$, where $n$ is the density of the system. For noninteracting atoms the proportionality coefficient $A$ is independent of density, but in the presence of interaction $A$ is proportional to $n$. It is shown that only in the presence of interaction between atoms the polarization $\mathbf{P}$ leads to the emergence of electric fields outside an inhomogeneous superfluid system.

In the presence of vortex line the motion of atoms in a quantum liquid and the distribution of density have axial symmetry. In the absence of flows the polarization has also this kind of symmetry (an axially symmetric polarization “hedgehog” appears around the vortex). Average dipole moment of vortex is zero and its observation is rather difficult. Therefore the problem of dipole moment of quantized vortices in the presence of flows arouses interest. The change of the bose gas density is found in the presence of a flow $\mathbf{w} = \mathbf{v}_n - \mathbf{v}_s$ passing the vortex. It is found that in the presence of a vortex in a superfluid film relative motion of normal and superfluid components causes appearance of an electric potential above the film. This potential has the form of a potential of a dipole, allowing to assign a dipole moment to the vortex. The dipole moment is a sum of two terms, the first one is proportional to the relative flow velocity $\mathbf{w}$ and the second one is proportional to $[\boldsymbol{\kappa} \times \mathbf{w}]$, where $\boldsymbol{\kappa}$ is the vortex circulation. The estimation of this dipole moment demonstrates that it would appear in a helium atom if one places it into an external electric field $E \sim 10^2$ V/cm (polarizability of helium is $\alpha = 2 \cdot 10^{-25}$ cm$^3$).

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# ANALYSIS OF INFLUENCE OF LIQUID DIELECTRIC FILM THICKNESS ON THE CHARACTERISTICS OF THE PHASE TRANSITION TO A SPATIALLY PERIODIC STRUCTURE IN A GAS OF CHARGED PARTICLES ABOVE IT

**D. M. Lytvynenko [1,2]**

*[1]Akhiezer Institute for Theoretical Physics NSC KIPT,*
*1 Akademichna Str., 61108, Kharkiv, Ukraine*
*[2]Kharkiv V.N. Karazin National University, High-Technology Institute,*
*31, Kurchatov Ave., 61108, Kharkiv, Ukraine*
*e-mail:d_m_litvinenko@kipt.kharkov.ua*

We develop a consistent theory of equilibrium states in the system of charged identical particles above liquid dielectric surface acted by an external constant electric clamping field. This system is considered to be quasi-neutral, i.e. the number of charges is exact as necessary to compensate the clamping electric field far from the dielectric surface. In terms of this theory we obtain the related self-consistency equations for the main parameters describing the system - the potential of electric field, the distribution function of charges and the surface profile of liquid dielectric.

These equations are used to study the phase transition of the system to a spatially periodic states. We obtain the parameters of the phase transition in the system to a spatially periodic structures of dimple crystal type and the dependency of these parameters on the thickness of liquid dielectric film is analyzed. The obtained results are in good agreement with the theoretical end experimental results of other researches [1-6].

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# BOSE-EINSTEIN CONDENSATION IN A MIXED FERMION-BOSON SYSTEM OF INTERACTING PARTICLES

**Yu. M. Poluektov , S. N. Shulga**

*Akhiezer Institute for Theoretical Physisc of the NSC "Kharkov Institute of Physics and Technology", 1, Akademichna str., Kharkiv 61108, Ukraine*
*e-mail: yuripoluektov@kipt.kharkov.ua, shulga.serge@gmail.com*

A model of Bose-Einstein condensation is constructed for a mixture of fermions and bosons with account of interaction between the particles of the same kind as well as between the particles of different kinds. We generalize to the case of fermion-boson mixture the model of Bose-Einstein condensation proposed in [1] for systems of interacting bosons. Taking into account the interparticle interaction permits one to avoid the difficulties inherent in the theory of Bose-Einstein condensation of ideal gas, that are connected with the executability of some thermodynamical relations and infinite fluctuation of particles number in the condensed phase. Thermodynamical functions of fermion-boson system are calculated above and below the condensation temperature. The behavior of thermodynamical functions near the critical temperature is studied and the influence of the admixture of Fermi particles on the character of the phase transition is considered.

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# THE ELECTRIC POLARIZATION OF He II WITH MOTION OF SUPERFLUID COMPONENT RELATIVE TO THE VORTICES

**I. N. Adamenko , E. K. Nemchenko**

*V. N. Karazin Kharkiv National University, Svobody Sq. 4, Kharkiv 61022, Ukraine*
*e-mail: i.n.adamenko@mail.ru*

In experiments [1, 2] the occurrence of an electric potential difference was firstly observed in the standing wave of second sound [1] and with torsional vibrations of superfluid helium (He II) [2]. The potential difference was absent both in a first sound wave and in normal helium (He I). This indicates a fact that the phenomena observed in [1, 2] are caused by the relative motion of the normal and superfluid components of HeII. The unusualness observed in [1, 2] phenomenon and the lack of satisfactory theoretical model initialized experiments [3], which confirmed the main result of work [1]. The purpose of this report is to present our theory, which explains experiments [1, 2, 3] result from a single point of view.

Phonons, rotons and quantized vortex rings are the quasiparticles of He II. These quasiparticles form normal component of He II, which can move with velocity $\mathbf{v}_n$, that differs from velocity of superfluid component $\mathbf{v}_s$. In the presence of relative motion velocity $\mathbf{w} = \mathbf{v}_n - \mathbf{v}_s$ quantized vortex rings are described by the Boltzmann distribution $n = \exp\left[-\left(\varepsilon - \mathbf{pw}\right)/k_B T\right]$. Here $\varepsilon$ is the energy of quantized vortex ring, which is an isotropic function of its momentum $p$.

In general case a dipole moment of quantized vortex ring (QVR) is $\mathbf{d}_V = \mathbf{d}_{in} + \mathbf{d}_{out}$, where $\mathbf{d}_{in} = d_{in}\mathbf{p}$ is intrinsic dipole moment of QVR and $\mathbf{d}_{out} = -d_{out}\mathbf{i}_F$ is dipole moment of QVR caused by external force $\mathbf{F} = F\mathbf{i}_F$, which polarizes $^4$He atoms. Expanding to a series with small parameter $\mathbf{w}$ the density of dipole moment $\mathbf{P} = \int \mathbf{d}_V n\left(\varepsilon - \mathbf{pw}\right) d^3p/\left(2\pi\hbar\right)^3$ up to quadratic terms we obtain

$$\mathbf{P} = \int \mathbf{d}_{out} n(\varepsilon) \frac{d^3p}{(2\pi\hbar)^3} - \int \mathbf{d}_{in} \frac{\partial n(\varepsilon)}{\partial \varepsilon} (\mathbf{pw}) \frac{d^3p}{(2\pi\hbar)^3} + \frac{1}{2}\int \mathbf{d}_{out} \frac{\partial^2 n(\varepsilon)}{\partial \varepsilon^2} (\mathbf{pw})^2 \frac{d^3p}{(2\pi\hbar)^3}. \quad (1)$$

In the experiments [1, 3] external force was absent and polarization of HeII was described by second integral in (1), which after solving gives $\mathbf{P}_{in} = d_{in} n_V \mathbf{w}/3v_T$. Here $n_V$ is the number density of quantized vortex rings, $v_T = k_B T/p_0$ is the temperature speed of QVR and $p_0$ is the momentum of QVR with minimal radius. Corresponding to $\mathbf{P}_{in}$ electric potential difference coincides with the experimental value [1] with $d_{in} = 4.9 \cdot 10^{-7} d_0$, where $d_0$ is the dipole momentum caused by interaction of two $^4$He atoms that are on an atomic distance from each other.

In He II film atoms of $^4$He are polarized by external Van der Waals force. In this case occurred dipole moment of QVR $d_{out}$ becomes much larger than $d_{in}$, so the second integral in (1) can be neglected. The first integral in (1) describes background, which won't be taken in account. Polarization of HeII caused by $\mathbf{w}$ is described by the third integral in (1), which after calculation gives $\mathbf{P}_{out} = w^2 n_V \mathbf{d}_{out}(z)/6v_T^2$, where z is a distance from the metal surface on which the HeII film is located. Corresponding to $\mathbf{P}_{out}$ electric potential difference coincides with the experimental values [2], if we assume that the vortices are realized in the film starting from the third atomic layer, which is known to be superfluid.

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# EFFECTS CAUSED BY ORIENTATIONAL DISORDER ON THERMAL CONDUCTIVITY OF MOLECULAR CRYSTALS

**G. A. Vdovychenko , A. I. Krivchikov, O. A. Korolyuk, O. O. Romantsova, Yu. V. Horbatenko**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*47 Lenin Ave., 61103 Kharkov, Ukraine*
*e-mail: georgiivdo@gmail.com*

Heat transfer in molecular solids is an actual question of modern physics. The situation is quiet clear in case of fully ordered crystal, and theoretical predictions using Debye-Pierlts model are well satisfying, but, low temperature properties of amorphous solids are still controversial question. But in ambient, cases of fully ordered dielectric solids are very rare. In real solids besides imperfections of crystal lattice persist different kinds of disorder and each of it makes contribution to mechanisms of heat transfer. Thermal conductivity has very high sensitivity to structure of molecular solid what makes it fine instrument for studying different dynamics features.

There are many phenomenological theories with was made to describe physical features of disorder solids, but there is still lack of experimental data which can describe influence of certain kind of disorder and will help to reveal the nature of amorphous behavior. Fortunately, there is variety of molecular substances which shows wide polymorphism at low temperatures. This makes possibility to study deviation of physical properties of same chemical substance depending on its structure.

The goal of this study was to experimentally investigate the thermal conductivity of oreintationally-disordered crystals at low temperatures. The objects were molecular substances with relatively simple chemical formula and compact molecular geometry: freon R-113, cyclohexene ($C_6H_{10}$), thiophene ($C_4H_8S$), tert-butanol ($C_4H_{10}O$) and halomethanes ($CBr_{4-n}Cl_n$ (n=0,1,2)).

It was found that anisotropy appearing in case of molecular crystal with compact geometry molecules induces the lack of amorphous behavior. Another important features are changing in behavior of thermal conductivity dependence solids with freezing dynamical orientational disorder and universal following $k(T) = T^2$ law in region of the lowest temperatures.

The data was analyzed in terms of time-relaxation Debye-Peirlts, Soft Potentials and Chahill-Pohl models.

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# SPONTANEOUS CURRENT OSCILLATIONS IN A PHOTO-EXCITED 2D ELECTRON SYSTEM ON LIQUID HELIUM

**K. Nasyedkin[1] , K. Kono[1,2,3]**

*[1]RIKEN Center for Emergent Matter Science,*
*2-1, Hirosawa, Wako, Saitama 351-0198, Japan*
*[2]Institute of Physics, National Chiao Tung University,*
*1001 Ta Hsueh rd, Hsinchu 30010, Taiwan*
*[3]Institute of Physics, Kazan Federal University,*
*16a Kremlyovskaya st., Kazan 420008, Russia*
*e-mail: kostyantyn.nasyedkin@riken.jp*

Microwave-induced resistance oscillations [1] and zero-resistance states [2] have been recently observed in a two dimensional (2D) electron system on liquid helium exposed to a resonant microwave irradiation and quantizing magnetic fields. The vanishing of magnetoresistance in the 2D electron system coincides with a number of striking nonequilibrium phenomena, such as the formation of an incompressible state in a photo-excited electron gas [3], nonequilibrium spatial redistribution of charge from the center to the edge of the electron pool (photovoltaic effect) [4] and spontaneously generated oscillations of the electron density [5].

In the present work we report the results of a further study of spontaneously generated current oscillations in surface state electrons on liquid helium in the zero-resistance state. We use a Corbino geometry cell with the outer ring electrode divided into four segments and record ac transient current signals from each segment simultaneously. Cross-correlation function analysis of the obtained data shows a phase shift between current oscillations for different segments that implies the existence of a charge flow in the azimuthal direction. The charge flow direction depends on the magnetic field polarity and coincides with the direction of edge magnetoplasmons propagation.

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# ELECTRON-STIMULATED DESORPTION OF EXCITED ATOMS FROM NITROGEN FILMS

**A. P. Barabashov, I. V. Khyzhniy, S. A. Uyutnov, E. V. Savchenko**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: apbarabashov@gmail.com*

Desorption or sputtering is among the most intensively studied radiation-induced phenomena. The term electron-stimulated desorption describes physical and chemical changes caused in the surface region of a solid by bombardment with low-energy electrons. Radiation effects in solid $N_2$ attract much attention in various areas of scientific researches including material and surface sciences, physical and chemical processes in interstellar space and solar system and also particle physics. Electronic desorption of solid nitrogen was studied under excitation with electrons, ions and photons [1]. Despite extensive studies the contribution of excited atoms into the desorption is still not well understood.

In the present paper radiation processes in the solid nitrogen irradiated with an electron beam were studied with special attention to the desorption of the excited atoms and its contribution to the electron-stimulated phenomena in general. The experiments were performed employing luminescence method and activation spectroscopy techniques – spectrally resolved thermally stimulated luminescence TSL and thermally stimulated exoelectron emission TSEE.

Atomic emissions were detected in the vacuum ultraviolet VUV range – the $^4P_{1/2\text{-}5/2} \rightarrow {}^4S_{3/2}$ transitions. They increased with respect to the bulk molecular emissions (the $a'^1\Sigma_u^- \rightarrow X^1\Sigma_g^+$ and the $A^3\Sigma_u^+ \rightarrow X^1\Sigma_g^+$) in thin films (< 100 nm) and under irradiation by slower electrons which have less penetration depth. Moreover, the observed atomic emissions coincided with the gas phase lines within the experimental error. These findings indicate the connection of the emissions observed with the desorbing excited atoms. Analysis of the spectrally resolved TSL and TSEE suggests connection of the atomic desorption with electron-ion recombination reaction. One can expect for the azide radical cation $N_3^+$ strong tendency to dissociate via $N_2$+N channel. Formation of N radicals in the bulk of solid $N_2$ by this reaction was assumed in [2]. Thereby analysis of the VUV luminescence and relaxation emissions allowed us to observe formation of defects, dissociation of molecules into the atoms and the desorption of the excited atoms from the surface of solid nitrogen and also to define the electronic states of these atoms.

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# RESEARCH OF QUALITY OF SURFACES BY ELECTRONS OVER A HELIUM FILM ON A SUBSTRATE

**Ya. Yu. Bezsmolnyy , V. A. Nikolaenko , S. S. Sokolov**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: bezsmolnyy@ilt.kharkov.ua*

The low-dimensional (LD) conducting systems form basis of modern nanoelectronics. As is known these systems are applied in receiving, radiating and digital computing devices. The surface quality and uniformity of the substrate in most cases are a critical factor in building a "clean" LD system. Contemporary nanotechnology needs to produce the homogeneous substrates with atomically smooth surface. Modern technologies allow to produce uniform substrate with a such surface. There are a number of nanometric and spectrometric methods for the analysis of the state of surface quality: the atomic force microscopy, the scanning tunneling microscopy, the scanning electron microscopy, the interference-phase method, X-ray structural, etc. The surface electrons (SE) located above substrates by the image force and the potential barrier on the border substrate – vacuum can serve as alternative tool under analysis of quality of dielectric substrate surfaces. SE over substrate with small dielectric constant have a “soft” hydrogen-like energy spectrum $E_n = Q_d^2 R / n^2$ (here $Q_d$ is effective electron charge modified by image force in dielectric and $R$ is Rydberg constant). The energy of electron ground state is about few meV. The mobility of SE over helium covering solid substrate is limited by interactions with the helium atoms in gas phase, ripplons and inhomogeneities [1, 2]. The mobility is $\mu^{-1} = \mu_c^{-1} + \mu_{im}^{-1}$, here $\mu_c$ and $\mu_{im}$ are mobilities of electrons for clean and non-clean substrate, correspondently. The values of $\mu_{im}$ and thermal activation energy $\Delta$ from expression $\mu_{im} = \mu_c e^{-\Delta/T}$ are parameters of transport process. The semiconductors covered helium and transformed into dielectric at low temperature can serve, in particular, as substrate.

The aim of the work is to identify a quality of substrate surface using SE transport characteristics over thin helium film on solid substrate. As in [3] we use the electron transport changing helium film thickness. In present work we increase the accuracy of method providing a uniformity of the film on substrate and fixing measuring contacts at experimental cell. This was provided by reliable positioning of the substrate using plumb method. The conductivity of SEs was measured by Sommer-Tanner method in standard experimental cell. The equipment for investigations includes measuring cell with substrate covered by liquid and plunger with electro-mechanic driver into a hermetic chamber. The moving plunger set helium level $H$ in the chamber and thickness of film was estimated as $d = 300/H^{1/3}$. The identification of electron transport characteristic depending on helium film thickness allowed us to identify the effective size of nanoroughness from several angstroms (for non-saturated helium film) to $10^2$ nm (for saturated one).

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# STUDY OF QUASI-LAMINAR FLOW IN SUPERFLUID HELIUM USING QUARTZ TUNING FORK

**I. A. Gritsenko, K. A. Klokol, S. S. Sokolov and G.A. Sheshin**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: gritsenko@ilt.kharkov.ua*

Experimental study is carried out of quasi-laminar flow in superfluid helium at temperature below 200 mK. Fluid flow was excited by a vibrating quartz tuning fork with a resonance frequency of about 24 kHz. It was found that at velocities of the tuning fork oscillations from 0.046 m/s till 0.4 m/s. The flow of He II can be both quasi-stable laminar and turbulent. Transitions between the flow regimes were observed (Fig. 1). The faster is increase of the velocity of vibrations of a tuning fork, the higher is the velocity at which the instability of quasi-stable flow appears and the flow instability occurs resulting into the transition to turbulent flow. The mechanisms are analyzed of energy dissipation of vibrating fork tines in the quasistable laminar flow [1]. It is established that there is an additional, compared with that caused by internal friction in the quartz, the mechanism of energy dissipation of the oscillating fork. This mechanism is associated with the mutual friction caused by the scattering of thermal excitations of He II on the quantized vortices leading to a cubic dependence of the exciting force of the fluid velocity.

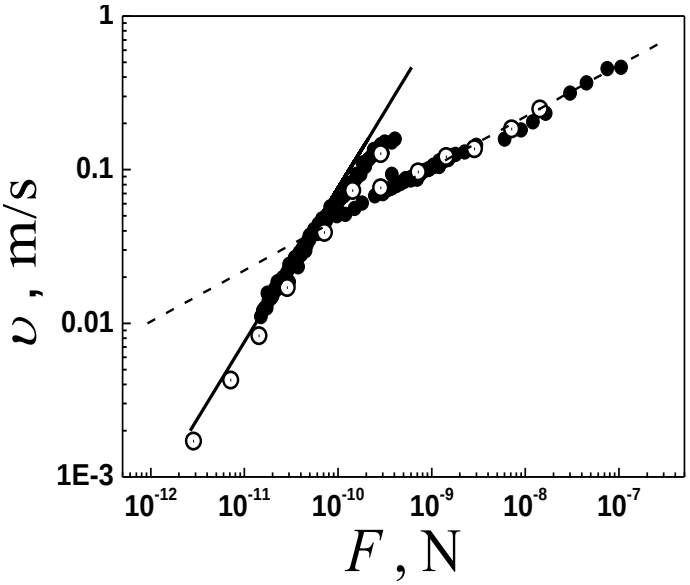


Fig.1. The experimental dependences of the oscillation speed of the fork tines of the excitation force at 150 mK (○) and 140 mK (●).
Dashed line – the linear dependence $F(\upsilon)$ (calculation by [2]), solid line – the power low $F \sim \upsilon^2$ (calculation by [3]),

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# ISOCHORIC THERMAL CONDUCTIVITY OF 1-PROPANOL IN ORDERED CRYSTAL PHASE

**A. V. Karachevtseva, V. A.Konstantinov, V. P. Revyakin, V. V. Sagan**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: zvonaryova@ilt.kharkov.ua*

This work presents the results of experimental study of the mechanisms of heat transfer in molecular crystals with hydrogen bonds – 1-propanol ($C_3H_7OH$). 1-propanol ($C_3H_7OH$) is the monoatomic alcohol and it can exist in different stable and long-lived metastable solid states (structural glass, orientational glass and completely orientationally-ordered crystal) at low temperatures.

Isochoric thermal conductivity of 1-propanol ($C_3H_7OH$) has been measured for samples of different densities in the temperature range from 110 K and up to melting by stationary radial heat flow method. It was shown, that the isochoric thermal conductivity in ordered crystal phase decreases with temperature weaker than $1/T$, which is predicted by the theory.

The experimental data are described in terms of the Debye model of thermal conductivity with allowance for heat transfer by both low-frequency phonons and "diffuse" modes.

# THE DESCRIPTION OF BEHAVIOR OF THE THERMAL CONDUCTIVITY OF SOLID $C_3H_7OH$

**V. A. Konstantinov , V. V. Sagan , V. P. Revyakin , A. V. Karachevtseva**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: zvonaryova@ilt.kharkov.ua*

In this work, based on experimental data for study of isochoric thermal conductivity of crystalline 1-propanol ($C_3H_7OH$), made an attempt to compare the two approaches in the description of heat conduction abnormalities dependence $\kappa \propto 1/T$. Both approaches are based on the fact that the thermal conductivity is determined by the sum of the contributions of the phonon and «diffuse» mode [1, 2-3]:

The first - the thermal conductivity is described by the equation $\kappa(T) = A/T+B$, where a member of the $A / T$ describes the three-phonon flipping processes and B - the contribution of the short-lived (diffuse) modes. The last contribution is assumed independent of temperature at $T \geq \Theta_D$.

The second - the integral of thermal conductivity is divided into two parts, describing the contributions to the thermal conductivity of the low-frequency and high-frequency phonons «diffuse» mode:

$$\kappa = \kappa_{ph}+\kappa_{dif} ,$$

$$\kappa_{\text{ph}}(T) = 3nk_B \text{v}\left(\frac{T}{\Theta_D}\right)^3 \cdot \left[\int_0^{\Theta_*/T} l(x) \cdot \frac{x^4 e^x}{\left(e^x-1\right)^2} dx\right]$$

$$\kappa_{\text{dif}}(T) = 3nk_B \text{v}\left(\frac{T}{\Theta_D}\right)^3 \cdot \left[\int_{\Theta_*/T}^{\Theta_D/T} \alpha \frac{\text{v}h}{2k_B xT} \cdot \frac{x^4 e^x}{\left(e^x-1\right)^2} dx\right]$$

It is shown that both of these models very well describe the temperature dependence of the isochoric thermal conductivity of 1-propanol, and it is difficult to give preference to any of them, as discussed in the case of tetrahydrofuran [2]. The first semi-empirical model suggests that «diffuse» the contribution is constant over the entire temperature. The second model with a moving boundary «diffuseness» $\Theta^*$ based on a more or less clear physical performances and requires a well-defined «crossover» between phonons and «diffusive» modes. Phonon contribution to the thermal conductivity varies in proportion to $T^{-3/2}$ as part of the phonon modes becomes «diffuse» is lowered $\Theta^*$. The final choice in favor of one or another model is difficult to do and requires more detailed theoretical analysis as well as the accumulation of experimental facts.

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# RADIATION-INDUCED SPECIES MONITORING IN NITROGEN SOLIDS

**I. V. Khyzhniy[1], E. V. Savchenko[1], S. A. Uyutnov[1], M. A. Bludov[1], A. P. Barabashov[1], G. B. Gumenchuk[2] and V. E. Bondybey[2]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2]Lehrstuhl für Physikalische Chemie II TUM, Lichtenbergstr. 4, Garching b. München 85747, Germany*
*e-mail: khyzhniy@ilt.kharkov.ua*

Nitrogen is one of the most abundant elements in the Universe. Solid nitrogen is of high interest for condensed matter physics and chemistry, material and surface sciences, dosimetry and astrophysics. Nitrogen solids are used as moderators, scintillators, systems for energy storage and components of interstellar and solar systems. In view of this radiation effects induced by ionizing radiation in solid nitrogen attract special attention.

Despite detailed investigations of electronic excitations the properties and dynamics of charge states as well as accumulation of uncompensated charge remained unexplored. It was believed that charge states do not play an essential role. Energy relaxation processes in subsystems of charged and neutral species were considered separately ignoring their interconnection. The first detection of thermally stimulated exoelectron emission from solid nitrogen [1] pointed to a key role of charge species in energy relaxation in preliminary irradiated samples.

We developed special techniques for studying charge states in cryocrystals and performed correlated in real time measurements of spectrally resolved thermally stimulated luminescence and exoelectron emission in combination with cathodoluminescence.

Analysis of the cathodoluminescence spectra indicated the formation of neutral $N_3$ centers. Simultaneous measurements of optical and current relaxation emissions revealed the formation and accumulation of radiation-induced ionic centers $N_3^+$ and $N_3^-$. The role of these species in energy relaxation cascades is discussed.

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# ADDED MASS OF THE OSCILLATING BODY IMMERSED IN SUPERFLUID HELIUM IN A TURBULENT FLOW

**I. A. Gritsenko, K. A. Klokol and G. A. Sheshin**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: klokol@ilt.kharkov.ua*

Both classical and quantum turbulence are studied intensively last years. The basic informational and highly sensitive method of research of the studies is research of oscillating characteristics of the body immersed in He II. Usually the current - voltage characteristics are studied, using which the basic mechanisms of dissipation of the kinetic energy are investigated of He II, being different for laminar and turbulent flows. In present work we applied a new method of study of turbulent flow, based on the behavior of the added mass ($m^*$) of the oscillating body. The $m^*$ behavior is rather different in laminar and turbulent flows. In laminar flow, $m^*$ does not depend on its velocity. However under increase of flow velocity and the beginning of a turbulent regime $m^*$ starts to increase due to the quantized vortices, which are on the surface of the oscillating body and drag He II. With further development of turbulence the density of quantized vortices starts to increase in proportion to the square of the flow velocity υ and, as a consequence, the $m^*$ increases. In the experiments, $m^*$ was determined by measuring the resonance frequency $f_0$ of the oscillating body, both in vacuum and in He II, as a function of υ.

Studies were carried out at ultralow temperatures where the density of the normal component is negligible. Oscillating quartz tuning forks were used in the experiments with resonance frequencies from 6 to 33 kHz. Under laminar flow $m^*$ is independent of υ, but inversely proportional to the oscillation frequency. It has been found that, for a turbulent flow, the $m^*$, as it expected, increases ~ $v^2$, being proportional to $f_0^{-3/2}$. The reason for observed dependence $m^*$ on $f_0$ is not clear at the moment. Probably it is connected with the features of the frequency dependence of the oscillating fork acceleration. The further experiments are planned for a more detailed analysis.

# ELECTRON DIFFRACTION STUDIES OF $N_2$ - $CH_4$ ALLOY FORMATION IN THE MOLECULAR MATRIX

**N. S. Mysko , A. A. Solodovnik and M. A. Strzhemechny**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: misko@ilt.kharkov.ua*

Structure investigations of binary mixtures of the simple molecular crystals are of considerable interest. Solidified methane and nitrogen are the fundamental solids for solving problems of the solid state [1]. Moreover methane is known to occur in the planetary environments [2]. Solid $N_2$ are the formed by the linear and $CH_4$ - tetrahedral molecules. In the lattice $CH_4$ molecules demonstrate a tendency to approximate to spheres. Both the crystal have cubic (fcc) lattice at the equilibrium vapor pressure, symmetry of $\alpha - N_2$ corresponds to the Pa3 space group [3 ] and methane is described Fm3c [4] below 20,4 K. The nitrogen – methane solid phase diagram has been determined using X-ray diffraction method in studies [5,6]. There are large discrepancies between results of these structural works. According to [5] a phase separation in $CH_4 - N_2$ system was not observed and solutions are cubic at all temperatures below $\alpha$- $\beta$ transitions of $\alpha - N_2$ at all concentrations. While authors [6] appointed that the mutual solubility of the components is practically absent in low temperature range despite the small difference in the lattice parameter of the components and their similarity of crystallographic structure. More experiments are required to resolve this controversy. Structure analyses of such solid solutions make it possible to obtain important information for a creation new theoretical approaches and a check of the existing models.

Structure of solid $CH_4 - N_2$ mixtures was studied with the transmission electron diffraction techniques equipped with a helium cryostat. The samples were grown “in situ” by condensation gaseous mixtures on Al or C substrate at $T$ = 20 and $T$ = 5 K. The deposition regime was chosen in order to obtain random distributions of impurity. The error in the lattice parameter measurements was usually 0.1 %.

Based on analysis of the obtained diffraction patterns and the concentration dependences of the lattice parameter and diffraction intensity the region of existence of solid solutions was determined. The limiting solubility of $CH_4$ in the nitrogen matrix approaches 10 % mol. The phase separation of the solutions is studied. The effect of dilution $CH_4$ in $N_2$ molecular crystal matrix on the orientation order has been investigated. At low enough impurity fractions obtained data were analyzed with using cluster model.

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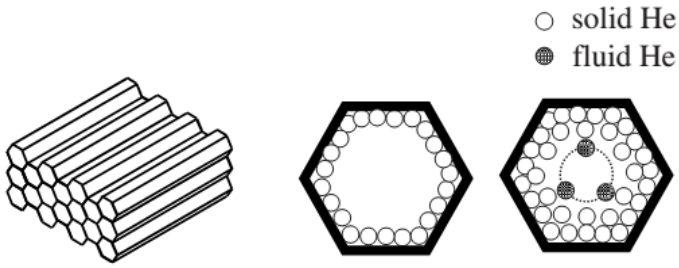
# NUCLEAR MAGNETIC RELAXATION OF $^3$He ADSORBED ON MCM-41 SUBSTRATE

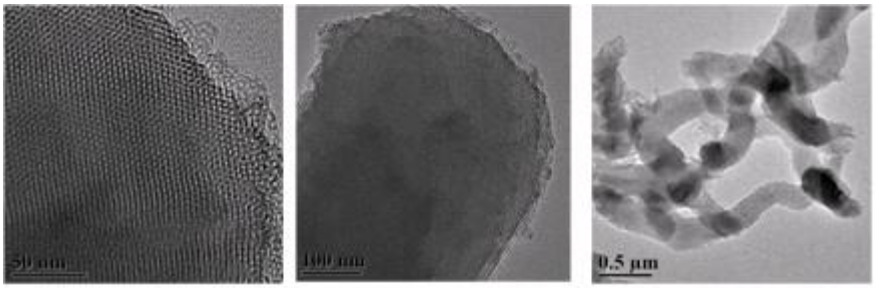
**A. P. Birchenko , Ya. Yu. Fysun, N. P. Mikhin**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: fysun@ilt.kharkov.ua*

Nuclear magnetic relaxation of a paramagnet helium-3, condensed into low-dimensional nanomaterial MCM-41 was studied by pulsed NMR (the resonance frequency $\omega_0$ = 9.15 MHz) in a temperature range of 1.3–7 K. MCM-41 is a bundle of parallel atomically smooth sintered tubes of $SiO_2$ with specific absorbing area ~300 $m^2/cm^3$. The inner diameter of each tube is about 2.5 nm, the length is about 0.3–0.5 micrometers. The outer surface of the nanotubes is hexahedron with the characteristic size of 4.5 nm. The transverse size of the nanotube's bundle is about 0.3 micrometers (See the figs. below).




It is known [1] that the first approximately 1.7 monolayers of adsorbed $^3$He is like a solid phase, because the attraction of $^3$He atoms by Van der Waals force is equivalent to excess pressure of ~ 40 bar.




The results of our measurements spin-lattice $T_1$ and spin-spin $T_2$ relaxation times are discussed in comparison with the data [3,4], obtained at other resonance frequencies. The rate of thermal relaxation in terms of compliance of the cell temperature and the real temperature of adsorbed helium-3 is also discussed.

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# MAGNETIC RELAXATION TIMES IN QUENCHED HCP $^3$He-$^4$He CRYSTALS

**A. P. Birchenko , N. P. Mikhin**

*B. Verkin Institute for Low Temperature Physics and Engineering,*
*47 Lenin Ave., 61103 Kharkov, Ukraine*
*e-mail: birchenko@ilt.kharkov.ua*

The aim of the work is the continuation of the research of the phase transition in non-equilibrium long-lived inclusions, which had been identified [1, 2] in quick-cooled hcp crystals of $^3$He - $^4$He.

The spin-lattice relaxation processes in 1% $^3$He in $^4$He solid mixture are studied by the pulse NMR technique. The measurements are performed over the temperature range 1.3 to 1.9 K and in pressure range 34 – 40 bar. All investigated hcp crystals have been grown fast (cooling rate 5 – 10 mK/s) from normal liquid by blocking capillary technique. Such procedure of crystal growing leads to formation metastable superfluid droplets in solid matrix [1-5].

Measurements of the spin-lattice relaxation time have been carried out by using two echoes method, which allowed to obtain reliable data for each of the coexisting phases in two-phase system: hcp matrix - superfluid inclusion. It is found that the spin-lattice relaxation in the superfluid droplets essentially different from appropriate values for the bulk superfluid. It is shown that in both cases the dominant relaxation mechanism is wall relaxation, which is orders of the magnitude faster than the bulk relaxation. However, in the case of bulk liquid, wall relaxation rate is limited by the diffusion of atoms to the cell walls, while in the liquid inclusions the basic role played the time of spin relaxation directly on the wall of solid helium. It is also observed a spontaneous dramatic change in the amplitude of the first echo signal associated with the solidification of the superfluid droplets and formation of long-lived metastable disordered (glassy) state of inclusions.

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# THE LINEAR DRAG COEFFICIENT OF QUARTZ TUNING FORK IN SUPERFLUID SOLUTIONS $^3$HE – $^4$HE

**V. A. Bakhvalova , V. K. Chagovets**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv* 61103, *Ukraine*
*e-mail: v.kovtun@ilt.kharkov.ua*

The work is dedicated to the study of the influence of impurity atoms $^3$He on the linear drag coefficient that occurs when the quartz tuning fork is placed in superfluid solutions of $^3$He in $^4$He and oscillate there. According to the Stokes equation for motions with a small Reynolds number, the linear drag coefficient that act on a slowly moving body in a medium is proportional to the linear velocity and the size of the body. The main mechanism of dissipation when the body moves, is the viscosity of the medium. When there are oscillatory, motions of the body (such as a quartz tuning fork) have additional dissipation mechanisms associated with the emission of the sound vibrating body. A feature of superfluid solutions of $^3$He in $^4$He, compared with pure $^4$He, is that at vibrational movement due to a strong coupling besides the usual emission of the sound emitting pressure waves, there is the second sound emitting heat wave. The contribution of the first and second sound in the dissipation of body oscillations in superfluid $^3$He in $^4$He solutions depends on the concentration of impurity atoms of $^3$He.

In the work, resonance curves of quartz tuning forks with a resonance frequency 32 kHz immersed in a solution of $^3$He in $^4$He were measured at temperatures 0.5-2.5 K. The measured values of the amplitude of the resonance curves at different excitation voltages and at constant temperature has made possible to plot the dependencies of velocities of fork tines against applied force and to determine the linear drag coefficient.

To determine the dissipation of oscillations of fork, the widths of resonances at half resonance height were measured in solution and the calculation of contributions of viscosity, first and second sounds in the resonance width were made. The results of the measured and calculated values were in good agreement.

# NEW FEATURES OF PLASTIC FLOW OF SOLID $^3$HE AT LOW TEMPERATURES

**A. A. Lisunov, V. A. Maidanov, V. Yu. Rubanskyi, S. P. Rubets, E. Ya. Rudavskii, S. N. Smirnov**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: rubets@ilt.kharkov.ua*

For the first time plastic flow of solid $^3$He was observed in the temperature range below 0.5 K. The flow occurs as a result of constant mechanical stress due to displacement of the porous membrane frozen into a crystal. Solid helium under stress flows through the holes in the membrane, that leads to a shift of the membrane and a change in capacitance of the measuring capacitor. The recorded time dependence of capacitance allowed one to find the average velocity of the membrane corresponding to the velocity of solid helium.

The typical inverse temperature dependence of the plastic flow velocity contains two areas with different temperature dependence. At temperature $T$ above ~ 0.2 K the velocity decreases exponentially with lowering temperature, which is typical for a thermally activated process. At $T <$ 0.2 K the helium flow velocity is almost independent on temperature, which can be treated as a manifestation of the quantum tunneling mechanism of mass transfer.

The analysis of dependences of the plastic flow velocity on and the stress $V(\sigma)$ showed that for fixed temperature it may be approximated by the expressions:

$$V(\sigma) = \tilde{V}\mathrm{sh}\left[\frac{\gamma}{kT}(\sigma - \sigma_i)\right] \quad (1)$$

$$\tilde{V} = V_0 \exp(-E_a / kT) \quad (2)$$

where $V_0$ is a constant depending on the properties of the crystal, $E_a$ is activation energy, $\gamma$ is activation volume, $\sigma_i$ is internal threshold stress.

According to Eq.2 we determined the activation energy $E_a$ of plastic flow, which is in good agreement with the data on the activation energy of vacancies obtained in x-ray experiment. It was found that the activation volume $\gamma$ 30-70 times exceeds the atomic volume, indicating that structural changes in the lattice during plastic flow deformation occur on a scale considerably exceeding the atomic size.

The results of the experiment can be explained within the vacancy model if the sources of vacancies are areas with high concentration of external stresses. The possible alternative explanation for the experimental data is based on the model of the motion of dislocations in the Peierls potential relief.

It should be emphasized that the quantum regime of plastic flow has been detected for the first time. The quantum plasticity is manifested only in solid $^3$He, in the case of solid $^4$He under the same conditions the plastic flow remains as a thermally activated.

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# MESURING LOW TEMPERATURE THERMAL CONDUCTIVITY OF EXTRA SMALL SOLID SAMLES WITH STEADY STATE METHOD

**G. A. Vdovychenko , A. I. Krivchikov, O. A. Korolyuk, O. O. Romantsova, Yu. V. Horbatenko**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: georgiivdo@gmail.com*

The thermal conductivity is very important physical property which is extremely useful both in science and technology. There are variety of steady-state [1,2] and dynamic methods allowing to perform measurements of different samples in different temperature ranges and at different pressures. The problem of measuring the low temperature thermal conductivity of solid macro samples [2-5] was resolved at a very high level. But recently our team faced problem of measuring samples that has dimensions about $1mm^3$. It was decided to make an attempt to resolve this problem using available equipement [5] and well known method.

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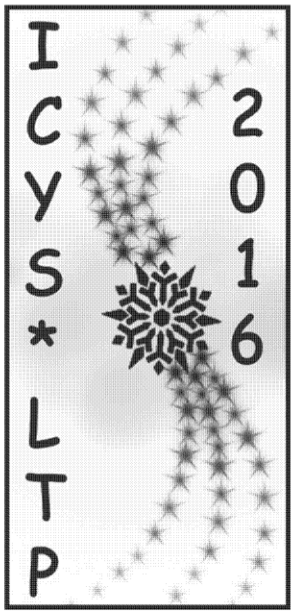
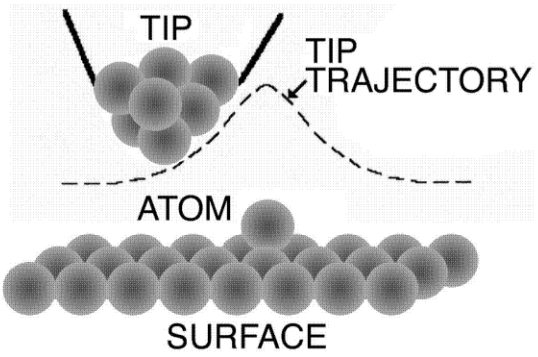
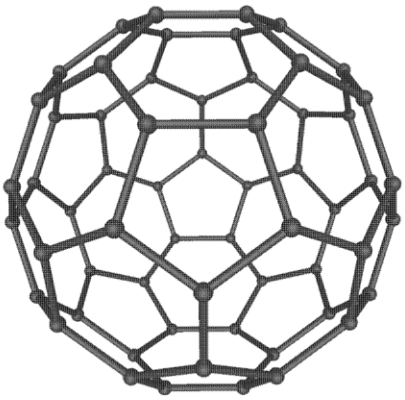
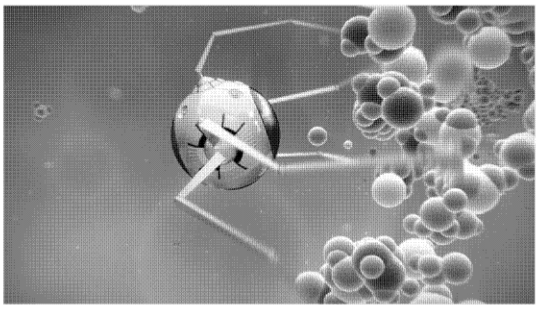
# Nanophysics and Nanotechnologies





# LOW TEMPERATURE HEAT CAPACITY OF THE 1D METHANE CHAINS

**M. S. Barabashko, M. I. Bagatskii, V. V. Sumarokov**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: barabaschko@ilt.kharkov.ua*

The heat capacity at constant pressure $C_{CH4}(T)$ of 1D chains of $CH_4$ molecules adsorbed in the outer grooves of bundles of single-walled carbon nanotubes (SWNTs) closed at their ends have been investigated in the interval 2 - 60 K. The ratio $n_{CH4}/n_C$=0.0034%, where $n_{CH4}$, $n_C$ – are the numbers of $CH_4$ molecules and C atoms, respectively, in the sample. According to the estimates, this concentration of methane could well suffice for the formation of one chain per groove when the $CH_4$ molecules occupy the grooves on the outer surface of SWNTs bundles.

The heat capacity of SWNTs bundles $C_{SWNT}(T)$ and of SWNTs bundles saturated by methane $C_{SWNT+CH4}(T)$ was measured using an adiabatic calorimeter [1]. The curve $C_{SWNT+CH4}(T)$ increases monotonically with a rising temperature. The heat capacity $C_{SWNT}(T)$ and $C_{SWNT+CH4}(T)$ were measured on the same SWNT sample before and after saturation with $CH_4$ gas.

It is found that filling SWNTs bundles with methane gas to the concentration 0.0034% enhances considerably the heat capacity in the whole interval of the temperatures investigated. The ratio $C_{SWNT+ CH4}/C_{SWNT}$ is equal to about 2.6 at 2 K and decreases with a growing temperature down to ~ 1.3 at 5.5 K, 1.14 at 20 K and 1.07 above 40 K, respectively. This large effect in the heat capacity is mainly due to the contributions of the translational and rotational degrees of freedom of the $CH_4$ molecules.

Character of the temperature dependence of $C_{CH4}(T)$ below 12 K indicates on the presence of Schottky anomaly caused by the tunneling between the lowest energy levels of rotational spectra of A, T, and E - nuclear spin modifications of the methane molecules. Special feature is observed in the area of 14 K, apparently, due to orientational phase transition, in which the nature of the rotational motion of the molecules varies from libration to hindered rotation. It is found that the value of the rotational heat capacity is close to the case of free rotation of the methane molecules in the temperature range of 30 - 40 K. The increase in derivative above 40 K and peculiarity in the $C_{CH4}(T)$ near 52 K are due to the processes of decay of 1D chains of $CH_4$ [2].

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# THE QUANTUM EFFECTS IN HYDROGEN SORPTION BY MESOPOROUS MATERIALS

**M. V. Khlistuck, A. V. Dolbin, V. B. Esel'son, V. G. Gavrilko, N. A. Vinnikov, R. M. Basnukaeva**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospect Nauky, 47, Kharkiv 61103, Ukraine*

The sorption and desorption of hydrogen by the mesoporous silicate MCM-41 [1, 2] material has been investigated in the temperature interval of 6,8–290 K. It is shown, that the mechanism of thermal activation is dominant in the kinetics of sorption of hydrogen molecules by the MCM-41 sample at T=60–290 K. The activation energy is estimated to be $E_a \approx$ 466 K. The diffusion of $H_2$ molecules to MCM-41 was practically temperature independent in the interval 17-60 K, which typically occurs when tunnel diffusion dominates over the thermal activation mechanism. The mobility of the $H_2$ molecules in the MCM-41 channels changes at T=8–17 K, which may be accounted for by the formation of a monolayer and subsequent $H_2$ layers on the inner surfaces of the channels on cooling (or their decomposition on heating). The activation energy of this process is $E_m \approx$ 21,2 K. Below 8 K the diffusion coefficients are only slightly dependent on temperature, which presumably corresponds to the behavior of a quantum $H_2$ in the MCM-41 channels covered with several layers of $H_2$ molecules. The results obtained are compared with the data for low temperature sorption of hydrogen by carbon nanotube bundles [3].

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# STRUCTURAL FEATURES OF SURFACE LAYERS THIN FILMS OF YTTRIUM IRON GARNET

**O. V. Kovalenko**

*V.N. Karazin Kharkiv National University, 4 Svobody Sq., 61022 Kharkiv, Ukraine*
*e-mail: kovalenkoolga87@mail.ru*

Feature of thin iron garnet films is the inhomogeneity of the magnetic properties in thickness due to the inhomogeneous distribution of the elements along the axis of the film growth [1]. On the other hand, the optical absorbance shows that the absorption coefficient α of wavelength essentially equal for all garnets [2]. In addition, thin YIG films are promising targets for creating magnetic chaos generators [3].

An important task is to shift the border transmission in the visible light region. YIG layer modification by ion implantation leads to the formation of planar components of the magnetization. Effect of implantation on uniaxial magnetic anisotropy associated with increase in the interplanar distances in the direction perpendicular to the surface. It is believed that the effects of ion implantation caused by elastic collisions of particles moving in the lattice atoms occupying regular positions. The thickness of implanted layer is chosen about 1/3 the thickness of the film usually.

YIG film was obtained in two ways: 1) by the method of ion-beam sputtering (IBS) of YIG target enriched to 25% $^{57}$Fe isotope by argon ions with a current density up to 10 mA/cm$^2$ and an energy of 1 ... 3 keV on gallium-gadolinium garnet (GGG) substrates and 2) by pulsed laser deposition on the substrate as GGG (111) orientation. In IBS method it is used several modes of film application differing in the degree of stabilization of the deposition process.

Elemental analysis of subsurface layer YIG films produced with the use of spectrometry of Rutherford backscattering (SRBS). Phase composition of the surface layers of YIG thin films was determined by Mossbauer spectroscopy on $^{57}$Fe nuclei in backscattering geometry of detection of internal conversion electrons (CEMS). To carry out the analysis of layered films the etching of films by phosphoric acid was produced. Film thickness was controlled by measuring the optical transparency of the film on substrates. Irradiation of thin film structures carried out by protons with energy E = 1.5 MeV and $He^+$ ions with an energy of 26 keV.

As a result of work the presence of the transition layers on the YIG films surfaces which based on experimental data obtained by the elemental composition of the YIG thin films deposited on substrates GGG been detected. Thickness of the transition layers up to 0.1 microns. The results obtained using the methods SRBS, CEMS and transparency measurements agree well with each other and show significant heterogeneity YIG films.

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# AN INFLUENCE OF DOPINGS ON THE GROUNG STATE SPIN OF NL ACCORDING TO T-J MODEL

**A. A. Kravchenko**

*V.N. Karazine Kharkiv National University, 4 Svobody Sq., 61022 Kharkiv, Ukraine*
*e-mail:alekseykravch@ukr.net*

Necklace ladder' (NL) is a lattice model with antiferromagnetic exchange interaction of neighbor spins, described magnetic and thermodynamic properties of organic salts and d-metal compounds. In the case, when one hole is in half-filled zone, lattice Hamiltonian for NL fragment has form

$$\mathbf{H} = t\,\mathbf{H}_1 + J\,\mathbf{H}_2\,,$$

$$\mathbf{H}_1 = \mathbf{a}_1^+\mathbf{a}_2 + \mathbf{a}_N^+\mathbf{a}_{N+1} + \sum_{n=1}^{N/3-1} \mathbf{a}_{3n+1}^+\left(\mathbf{a}_{3n} + \mathbf{a}_{3n+2}\right)$$

$$+\sum_{n=1}^{N/3}(\mathbf{a}_{3n-2}^+\mathbf{a}_{3n}\mathbf{Q}_{3n-2,3n-1} + \mathbf{a}_{3n-1}^+\mathbf{a}_{3n+1}\mathbf{Q}_{3n-1,3n}) + H.c.$$

$$\mathbf{H}_2 = \mathbf{a}_1^+\mathbf{a}_1\left[\sum_{n=1}^{N/3-1}\mathbf{A}_{1,3n} + \mathbf{S}_N\left(\mathbf{S}_{N-2} + \mathbf{S}_{N-1}\right)\right] + \mathbf{a}_{N+1}^+\mathbf{a}_{N+1}\left[\sum_{n=1}^{N/3-1}\mathbf{A}_{1,3n+1} + \mathbf{S}_1\left(\mathbf{S}_2 + \mathbf{S}_3\right)\right]$$

$$+ \sum_{n=1}^{N/3-1}\mathbf{a}_{3n+1}^+\mathbf{a}_{3n+1}\left[\sum_{k=1}^{n-1}\mathbf{A}_{1,3k+1} + \sum_{k=n+1}^{N/3-1}\mathbf{A}_{1,3k} + \mathbf{S}_1\left(\mathbf{S}_2 + \mathbf{S}_3\right) + \mathbf{S}_N\left(\mathbf{S}_{N-2} + \mathbf{S}_{N-1}\right)\right]$$

$$+ \sum_{n=1}^{N/3-1}\left(\mathbf{a}_{3n-1}^+\mathbf{a}_{3n-1} + \mathbf{a}_{3n}^+\mathbf{a}_{3n}\right)\left[\sum_{k=1}^{n-1}\mathbf{A}_{2,3k-2} + \sum_{k=1}^{n-1}\mathbf{A}_{2,3k-3} + \mathbf{S}_{3n-1}\left(\mathbf{S}_{3n-2} + \mathbf{S}_{3n}\right)\right],$$

$$\mathbf{A}_{1,k} = \mathbf{S}_k\left(\mathbf{S}_{k-2} + \mathbf{S}_{k-1} + \mathbf{S}_{k+1} + \mathbf{S}_{k+2}\right), \quad \mathbf{A}_{2,k} = \left(\mathbf{S}_k + \mathbf{S}_{k+3}\right)\left(\mathbf{S}_{k+1} + \mathbf{S}_{k+2}\right),$$

Where **t** is hopping parameter of Hubbard model,

**J** - coupling parameter,

$\mathbf{a}_n^+$ - the spin free creation operator for electron located on *n*-th site,

$\mathbf{Q}_{n,m}$ - operator of cyclic permutation of spin variables.

These Hamiltonian was used to calculate exact energy spectrum of 16 atomic clusters. The calculation results show that if J≠0 the basic state of fragment corresponded to minimal value of the total spin.

Also we show that an appearance of one 'hole" in the half-filled band leads to the destruction of ferromagnetic state. So, NL is very sensible for acceptors doping because of the fact can be user to construct new magnetic sensors.

The similar investigations were done for a model with cyclic boundary conditions. In this case we show that at change of parameter of the final repulsion ground state spin of the system at first decrease to minimal value, after it start to increase. Thus phase transfer from ferrimagnetic to ferromagnetic state occurs in nonmonotonic way via state with minimal spin.

# OPTICAL AND ELECTROPHYSICAL PROPERTIES OF CARBON NANOTUBES DISPERSIONS IN NEMATIC LIQUID CRYSTALS WITH PHOTOACTIVE COMPONENTS

**O. M. Samoilov**

*Institute for Scintillation Materials, STC "Institute for Single Crystals", NAS of Ukraine,*
*60 Nauky ave., 61001 Kharkov, Ukraine,*
*e-mail: samoilovisma@gmail.com*

This paper examines the optical and electrophysical properties of the liquid crystal matrix composed with a nematic liquid crystal 5CB and photoactive azoxy nematic ZhK-440, as well as their dispersions with carbon nanotubes.

We investigated the concentration dependence of these matrices both in the field of 1: 1, where certain effects due to the formation of complexes by charge transfer expected, and in the field of compensation dielectric anisotropy. We found some anomalous behavior of optical density, dielectric constant and conductivity near the compensation area. These anomalies may be associated with some of the local disorder on the fluctuations of the director. An interesting finding was that the addition of carbon nanotubes, even in small amounts, this effect is virtually eliminated, thus inhibit the growth of carbon nanotubes director fluctuations and stabilize matrix.

Fredericks transition for Zhk-440 + 5CB matrices was implemented. The opportunity for new "photoelectrooptical effects" in complex mixtures of nematic photoactive components and carbon nanotubes was shown.

# FUNCTIONALIZATION OF N(B)-DOPED SINGLE-WALLED CARBON NANOTUBES AND GRAPHENE BY THE $XO_4^{2-}$ (X = Cr, Mo, W) OXYANIONS

**V. Borysiuk[1], Yu. Hizhnyi[1], S. Nedilko[1], A. Shyichuk[2]**

*[1]Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska st.,01601 Kyiv, Ukraine*
*[2]Department of Rare Earth, Faculty of Chemistry, Adam Mickiewicz University, Umultowska 89b, 61-614 Poznań, Poland*
*e-mail: borysyukviktor@gmail.com*

Carbon nanotubes (CNTs) attract tremendous attention for last two decades due to their unique physical and chemical properties. In particular, chemical functionalization of CNTs can modify their physical and chemical properties, following improvement of their performance for specific applications. Some studies have already indicated that functionalized CNTs are a promising materials for removal of the toxic heavy metals from water waste [1]. This task is an important environmental issue because heavy metal oxyanions are toxic industrial pollutants and their removal from industrial wastes is a urgent technological problem [2].

That is why, theoretical modeling of molecular adsorption on the CNTs surfaces is a powerful tool what can predict some important physical and chemical properties of functionalized materials which possess macro-scaled practical applications.

In this work, adsorption of $XO_4^{2-}$ (X = Cr, Mo, W) molecular oxyanions on the surfaces of pristine and N(B)-doped single-walled CNTs and grapheme was studied. The DFT-based geometry-optimized calculations of the electronic structures of the SWCNTs and graphene molecular clusters including adsorbed oxyanions were carried out by Gaussian 03 program package [3]. Binding energies between oxyanions and adsorbents, relaxed geometries, energy barriers for desorption, electronic wavefunction contours were calculated and analyzed.

The influence of the B(N) doping on the type of chemical bonding between $XO_4^{2-}$ anions and CNTs was revealed. A possibility of the $XO_4^{2-}$ anions removing from industrial wastes using carbon nano-sized materials has been also outlined.

Perspectives of efficient of carbon nano-structured materials functionalization by oxide compounds are in the process of research.

Acknowledgement. The work are based on the research provided by the grant support of the State Fund For Fundamental Research of Ukraine (project F64/32-2015).

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# LOW-TEMPERATURE MAGNETIC ENTROPY CHANGE IN NOVEL $Gd_2O_3$@$SiO_2$ NANOCOMPOSITES

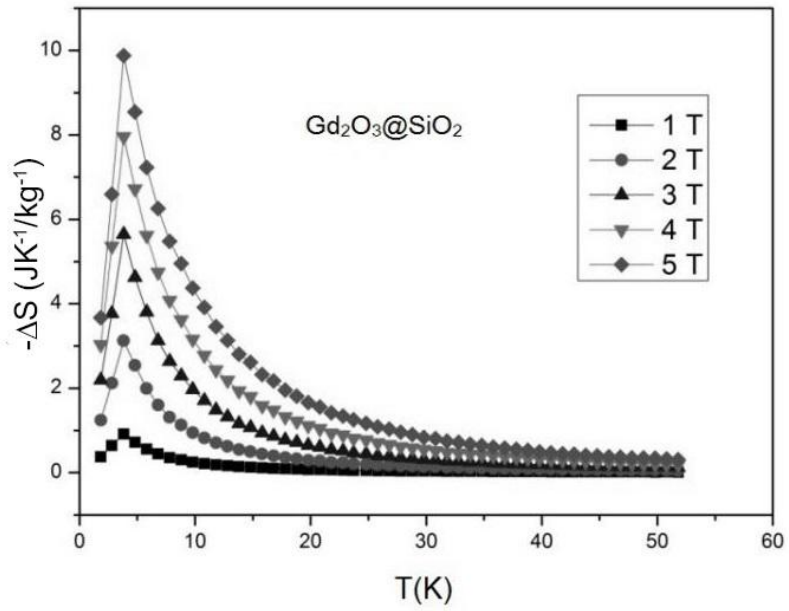
**A. Berkutova [1,2], A. Zeleňáková [1], P. Hrubovčák [1], O. Kapusta [1], V. Zeleňák [3]**

*[1]Department of Condensed Matter Physics, University of P.J. Šafárik, Park Angelinum 9, 040 01 Košice, Slovakia*
*[2]V. N. Karazin Kharkiv National University, Svobody sq., 4, Kharkov, 61022,Ukraine*
*[3]Department of Inorganic Chemistry, University of P.J. Šafárik, Moyzesova 11, 040 01 Košice, Slovakia*
*e-mail:anna.i.berkutova@gmail.com*

For the last years there is a big interest in lanthanide metals and their alloys because of their possible use in wide range of technological and biomedical applications (contrast media for MRI, therapeutic agents in tumor treatment and drug delivery). Also, Gd and its compounds shows good magnetocaloric properties (MCE) indicating them as promising magnetic materials for applications in refrigeration technologies.

In this work we studied MCE in $Gd_2O_3$@$SiO_2$ nanocomposite prepared by nanocasting of $Gd_2O_3$ nanoparticles in periodic nanoporous silica matrix with hexagonal symmetry. For measurements of magnetic properties we used commercial MPMS 5XL (Quantum Design) apparatus in external magnetic field up to 5 T and temperature range 1.8-300K. The values of entropy change was evaluated from magnetization curves using a Maxwell relation $\Delta S=\int(\partial M/\partial T)_H dH$.

Figure shows the peak of entropy change in studied material at very low temperature $T \sim 4$ K and the change in entropy with the change in applied magnetic field *(dS/dH)* is reasonably large $\Delta S(T) \sim 9.8$ J/K.kg for this type of nanocomposites. Results of our study confirm that $Gd_2O_3$@$SiO_2$ nanocomposites could be promising material for low temperature refrigeration technology.




Temperature dependence of the entropy change in $Gd_2O_3$@$SiO_2$ nanocomposite at different values of the applied magnetic field.

**Acknowledgement.** The author (A.B) would like to thank Visegrad Fund under contract No. 51501516 for financial support.

# MOLECULAR DYNAMICS OF ULTRATHIN FILM OF LIQUID ARGON COMPRESSED BETWEEN ATOMICALLY SMOOTH DIAMOND PLATES

**A. V. Khomenko, D. V. Boyko, M. V. Zakharov, K. P. Khomenko**

*Sumy State University, 2, Rimsky Korsakov Str., 40007 Sumy, Ukraine*
*e-mail: o.khomenko@mss.sumdu.edu.ua*

Friction plays a major role in diverse systems and phenomena that at first glance may not seem related, but which on closer examination revealed common features inherent in all tribological processes in the areas of technology, geology and biology [1-5]. Development of wear resistant surfaces with low friction and thin lubricant films has become an important factor in the miniaturization of moving parts in many technical devices. The latter include micro-electromechanical systems, computer storage devices, miniature motors. Simple empirical laws of friction do not always work in such systems. This occurs because they are characterized by a high ratio of surface to volume, and more important role of chemistry, adhesion and structure of surfaces. Conventional tribological methods used for macroscopic objects may be ineffective at the nanometer scale that requires new approaches to the study and control of such systems. The area of tribology that studies biosystems and also the lubrication mechanisms in joints is especially rapidly developing [6].

Using the method of classical molecular dynamics we investigate the properties of ultrathin film of liquid argon, which consists of one or two layers of molecules and is confined by two atomically smooth crystalline diamond surfaces [7]. The aim of research is validating the use of rigid surfaces and one of the available models of the argon molecule. We study the behavior of the equilibrium and dynamic characteristics of the system. It is revealed that at increasing external load the transition of film in the solid-like state occurs, which is indicated by the behavior of the velocity autocorrelation function of argon molecules, the descent of the magnitude of the diffusion coefficient and the shear viscosity increase. The organization of molecules in layers and the presence of their in-plane ordering are revealed. The dependences of the kinetic friction force on time and load are obtained. The results are compared with experimental data.

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# LOW-TEMPERATURE FEATURES OF TUNNELING MAGNETORESISTANCE HYSTERESIS IN $CrO_2$ PRESSED POWDER WITH AN ADMIXTURE OF IRON: THE EFFECT OF TEMPERATURE AND CURRENT.

**V. A. Horielyi, N. V. Dalakova, E. Yu. Beliayev**

*B. Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine,*
*47 Nauky Ave., Kharkiv, 61103, Ukraine*
*e-mail: horielyi@ilt.kharkov.ua*

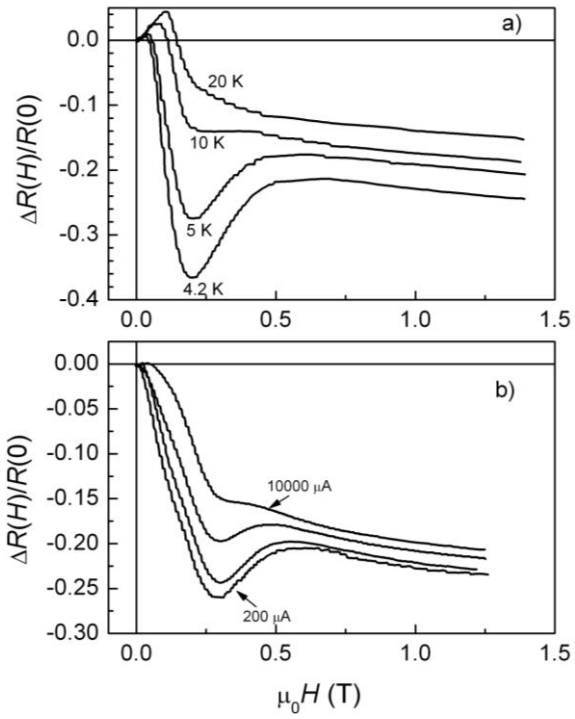


Fig.1 a) MR, recorded at different temperatures ($J$ = 100 μA, $\boldsymbol{H} \parallel \boldsymbol{J}$);

b) MR, recorded at different currents $J$ = 200 μA, 2000 μA, 5000μA, 10000 μA ($T$ = 4.93 K, $\boldsymbol{H} \parallel \boldsymbol{J}$). The rate of the magnetic field input d$H$/d$t$ = 0.021 T/s.

Resistive and magnetoresistive properties of compressed powder of ferromagnetic half-metal $CrO_2$ with an admixture of iron were studied. The Curie temperature of the powder $T_C \approx 390$ K. The powder was prepared by hydrothermal synthesis and consisted of needle-like nanoparticles of a solid solution of substitution $Cr_{1-x}Fe_xO_2$ with iron content 75 mmol per 1 mole of chromium. The average particles' diameter was ~34 nm, average length ~300 nm. Particles were coated by naturally degraded layer consisting of a mixture of amorphous dielectric $\beta$-CrOOH and some quantity of occluded chromic acid. At zero and non-zero magnetic field conductivity had tunneling character. The tunneling magnetoresistance (MR) $\Delta R(H)/R(0) = [R(H) - R(0)]/R(0)$. At temperatures $T < T_B$, where $T_B$ is the blocking temperature, in the area of magnetic fields $\mu_0 H$ <1.5 T. MR hysteresis loops were strongly dependent on the speed of the magnetic field change $dH/dt$, on the temperature and on the values of tunnel transport current. It is shown that the maximum negative MR values (≥ 30%) can be achieved in small magnetic fields (< 0.5 T) in conditions of low temperatures and high speeds of the input magnetic field.

Under these conditions, the magnetic subsystem is in a metastable state when $\tau > t$, where $\tau$ – relaxation time to equilibrium, $t$ – the time of observation, which depends on the speed of the magnetic field input. The form of hysteresis loop is defined by the relationship $t/\tau$. For given values of $dH/dt$ the MR hysteresis depends on transport current and temperature. With increased temperature or an electric current, electrons acquire additional energy from phonons or electric field. This strengthens activation processes, competing with orienting influence of the magnetic field. This in turn leads to additional fluctuations of the magnetic moments of particles and to reduction in the relaxation time $\tau$. This changes the ratio between the relaxation time and observation time ($\tau \to t$) and the system approaches equilibrium that corresponds to the curve of the field output. As a result, the value of MR decreases and the extremum on the $\Delta R(H)$ curve gradually smoothes out (Fig.1). Thus, to control the value of the tunnel MR at a fixed temperature one can change the value of transport current and the rate of the magnetic field input-output $dH/dt$.

# CATHODOLUMINESCENCE STUDY OF NEUTRAL AND CHARGED EXCIMER COMPLEXES IN ICOSAHEDRAL AND CRYSTALLINE NANOCLUSTERS OF XENON

**O. P. Konotop, O. G. Danylchenko, Yu. S. Doronin, G. V. Kamarchuk, A. A. Tkachenko, V. N. Samovarov, V. L. Vakula**

*B. Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, 47 Nauky Ave., Kharkiv, 61103, Ukraine*
*e-mail: konotop@ilt.kharkov.ua*

We studied cathodoluminescence spectra of substrate-free xenon nanoclusters produced in a supersonic jet adiabatically expanding into a vacuum. The cluster size was varied in a wide range from 100 to 18000 atoms per cluster which corresponds to quasicrystalline structures with a 5-fold axis of symmetry for small clusters and crystalline fcc structure for large ones. Clusters were excited by a 1-keV electron beam. The resulting luminescence spectra were measured in the 6-7.5-eV energy range containing emission bands of the neutral and charged excimer complexes $(Xe_2)^*$ and $(Xe_4^+)^*$ formed by vibronic transitions from vibrationally relaxed levels of the excited electronic states. We analyzed integrated intensities of the bands taking into account the fraction of jet substance condensed into clusters and demonstrated that in crystalline clusters the emission from neutral $(Xe_2)^*$ molecules comes from within the bulk of a cluster, while charged $(Xe_4^+)^*$ complexes radiate from its near-surface layers. We found the cluster size range in which the jet is dominated by quasicrystalline clusters as well as the size interval in which our spectra suggest transition to a crystalline structure.

# BIAS REGULATED PHOTOCURRENT IN A MOLECULAR DIOD

**V. O. Leonov, E. G. Petrov**

*Bogolyubov Institute for Theoretical Physics, Natl. Acad. Of Sci. of Ukraine,*
*Metrologichna str., 14-B,Kiev-03680, Ukraine*
*e-mail: leogluck@gmail.com*

Using the nonequilibrium density matrix approach the photocurrent formation in the nano-device "electrode–molecule-electrode" (molecular diode) is considered. In the framework of HOMO-LUMO model the kinetic equations for charge transmitting processes were obtained. It was shown that in case of such nano-device with an asymmetric coupling of the molecule to the attached electrodes, the tuning of photocurrent is made possible with alteration of a bias voltage transmission gaps. The transmission gaps determine energy differences between the device quantum states associated with the charged and uncharged molecule [1,2]. It is shown theoretically that the molecular diode is able to exhibit the photochromic effect (shift of illumination frequency). The effect is especially noticeable in the case of different space distribution of an electron density over the molecular orbitals.

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# INVESTIGATION OF THE GAS-SENSITIVE POINT CONTACTS' NONMONOTONIC RESPONSE UNDER HUMAN BREATH GAS

**A. S. Klimkin[1], M. A. Maslivets[2], V. A. Gudimenko[1], A. P. Pospelov[3], G. V. Kamarchuk[1]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2]V. N. Karazin Kharkiv National University, Svobody Sq. 4, 61022, Kharkiv, Ukraine*
*[3]National Technical University "Kharkov Polytechnic Institute", 21 Bagaliya Str., Kharkov, 61002, Ukraine*
*e-mail: klimkin@ilt.kharkov.ua*

Nowadays the point-contact gas-sensitive effect which was discovered in 2006 [2] and has already gained a wide progress and application represents a new unique trend in the classical Yanson point-contact spectroscopy [1]. In the framework of this trend the gas-sensitive point contact is considered as the basic element and the object under investigations manifested itself as a nanostructured element sensitive to variation of chemical composition of liquid or gaseous environment [3]. This object is conceptually the most sophisticated technological development which is able, due to its performance and simple technical solution, to replace today's gas-sensitive elements which were developed on the basis of film or nanostructured conductors.

We investigated point contacts formed between tungsten electrodes. The point contacts were prepared by the Fisun twist method using a specially designed holder. As with the twist technology, the contacts prepared were highly stable to external mechanical factors and retained their properties for a long time. The investigation was performed in a specially designed cell allowing gas feed control. The time dependences of the electrical resistance of the point contacts (response signal) exposed to human breath gas were obtained.

We found that the behavior of point contacts in their electric conductivity is essentially nonmonotonic upon breath action. The time dependence of the electrical resistance has a distinct spectral character. The point contacts respond to the gas medium immediately or with a short delay after feeding the gas to the contact, i.e., the response time of the contacts is small. Response signal is quite nonmonotonic and contains a number of maxima and minima varying in both intensity and reactivity rise rate. This behavior of the tungsten point contacts is unusual for conventional gas sensors, and was observed for the first time in this study. This finding opens wide possibilities to develop advanced tools allowing comprehensive analysis of complex gas media. The results obtained testify about prospect to continue the presented research in the course of obtaining additional information required to estimate individual contributions of the gas mixture components to the total nonmonotonic response of a point contact.

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# X-RAY STUDIES THE PHYSICAL AND CHEMICAL SORPTION OF CO MOLECULES BY FULLERITE $C_{60}$

**V. V. Meleshko, I. V. Legchenkova, Yu. E. Stetsenko, A. I. Prokhvatilov**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: meleshko@ilt.kharkov.ua*

The influence of CO gas sorptions on structural characteristics of the mono- and polycrystalline fullerite $C_{60}$ investigated by X-ray diffraction method in temperature range 150-600$^{o}$C under pressure 30 atm.

Sorption kinetics was studied by definition of $C_{60}$ lattice parameter dependences of fullerite saturation by CO molecules time. Carbon monoxide dissociation at a temperature T > 300$^{o}$C found. That dissociation is accompanied by carbon powder deposition and chemical interaction of atomic oxygen with $C_{60}$, CO and, probably, with condensate of carbon. These processes affect the structural characteristics of fullerite, which lead to non-monotonic saturation temperature dependence of the matrix lattice parameter and volume.

Explanations for observed peculiarities are proposed.

# THE STEP-EDGE EFFECTS ON SPECTRAL PROPERTIES AND PLANAR STABILITY OF METALLIC BIGRAPHENE

**K. A. Minakova[1], I. S. Bondar[2]**

*[1]National Technical University "Kharkiv Polytechnic Institute", 21 Bagalija Str., Kharkiv 61002, Ukraine*
*[2]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: kseniatrushina@list.ru*

In the structures of coherently stacked graphene monolayers (graphite as the end family-member) a honeycomb layers packing is remained, but Dirac singularity in electron spectrum is lost due to weak, van der Waalse, coupling of the layers. The latter gives rise to normal-metal conductivity in such systems instead of zero-gap semiconducting (semimetal) behavior of monolayer graphene [1, 2]. A growing interest to these systems is caused by their direct relevance to manufacturing the advanced, closed nano-arrangements of carbon (see e.g. [3-6]), and moreover, of transition-metal dichalcogenides [7, 8].

The phonon and electron spectra of metallic bigraphene are analyzed in the presence of step-edge crystal imperfection. Different geometries of step-edge are considered. The dynamic planar stability of the considered structure is proved for temperatures above the ambient. The number of phonon states is shown to grow near the K-point of first Brillouien zone, compared to pristine graphene. It is found, that this type of defects causes substantially non-uniform distribution of electron states and the pronounced increase in the number of states with energies close to Fermi energy can be expected in electron spectrum of the graphene-based compounds.

The performed calculations are in good agreement with inelastic neutron, X-ray and Raman measurements. Each of the bigraphene layers is considered as 2D-superstructure arranged by metallic and semiconducting triangular lattices.

The numerical calculations compared with spectral measurements have shown, that

1) Spatial distribution of electron states on the step atoms with dangling bonds and their neighbors is non-uniform and depends on step-edge chirality.

2) The integral DOS of clean bigraphene and that with step-edge differ near Fermi level, mainly: semiconducting gap opens for "zig-zag" configuration and the density of state increases for the "arm-chair".

3) The phonon spectral density grows at $\omega = \omega(K)$ for "arm-chair", similar to interstitials, which facilitate a rather high-temperature superconductivity. The dynamical planar stability still remains up to temperatures about $300 \div 400$ K.

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# THE PART OF ACOUSTIC PHONONS IN THE NEGATIVE THERMAL EXPANSION OF THE LAYERED STRUCTURES AND NANOTUBES BASED ON THEM

**K. A. Minakova[1], I. S. Bondar[2]**

*[1]National Technical University "Kharkiv Polytechnic Institute", 21 Bagalija Str., Kharkov 61002, Ukraine*
*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: kseniatrushina@list.ru*

The determination of the interatomic interactions is the key problem of the dynamics of the crystal lattice and many other sections of the solid-state physics [1]. In recent years, great progress has been made in this area, through to the development and widespread use of methods of calculation from first principles (see., eg, [2 - 4]), as well as quantum-chemical calculations. However, theoretical and experimental investigations of the phonon spectra and vibrational characteristics are still relevant to solve this problem. Information obtained on the basis of these studies, is particularly important for structures that combine different types of interatomic interactions. Such compounds usually have a complex array with unit cells polyhydric appreciable anisotropy and different interactions between the atoms. The anisotropy of the interatomic interactions can either be stored in the far right and lead to a strong anisotropy of the elastic characteristics and a local character, when the direction of the strong and weak ties vary from atom to atom. One of the most informative methods of studying the phonon spectrum of the connections with both the above-mentioned types of anisotropy is the identification and analysis of the temperature dependences of the vibrational thermodynamic characteristics, particularly tensor, such as coefficients of linear thermal expansion (the LTEC) along different crystallographic directions.

Thus, we have shown that the negative thermal expansion (or more generally, the nonmonotonic temperature dependence of the LTEC) peculiar structures, which are characterized by strong anisotropy of the interatomic interaction. This anisotropy may be stored in a long-range order and lead to a noticeable anisotropy of elastic modules and sound velocities, and wearing a purely local character, changing its direction from atom to atom.

At the microscopic level, the methods of the lattice dynamics explained a nature of the force compressing crystal with increasing temperature and caused by the rapid expansion its orthogonal direction. A connection of this force with the temperature derived from the mean square atomic displacements along different directions. On the basis of the microscopic calculations for specified structures demonstrated a good correlation between minima in the experimental temperature dependence of the LTE and maxima on the calculated ratio of the corresponding derivative of the mean-square displacements by the temperature. Moreover, such a correlation is shown as in structures with strong anisotropy of elastic modules (graphite and niobium diselenide), and in crystals, where the anisotropy of the interatomic interaction is local (type 1-2-3 of the HTS).

It has been established that the cause of the negative expansion graphene nanotubes is high amplitudes of their torsional vibrations, in which is most pronounced the quasi-one crystal structure of such systems. The contact of the minima of the temperature dependence of LTEC, which are actively studied in the experiment, and the maxima on current dependences of relations derivatives of mean-square displacements can extract (or verify) the information on the interatomic interactions in complex, highly anisotropic crystal structures.

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# CONVERSION OF ELECTRON BEAM ENERGY INTO VACUUM ULTRAVIOLET RADIATION OF ARGON CLUSTERS

**O. Y. Tkachenko[1], Yu. S. Doronin[2], A. A. Tkachenko[2], V. L. Vakula[2]**

*[1] V. Karazin Kharkiv National University,*
*4 Svobody sq., Kharkiv 61077, Ukraine*
*[2] B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail:doronin@ilt.kharkov.ua*

Liquid argon is traditionally used as scintillator in dark matter detectors and various elementary particle studies, including neutrino astrophysics. Performing absolute measurements with such detectors is a difficult task which requires the knowledge of fluorescence yields [1].

Clusters produced in the process of argon condensation in a supersonic jet can be liquid or solid depending on their size. Figure shows cathodoluminescence spectra from solid clusters with an icosahedral structure (average cluster size $\overline{N} \approx 1000$ atoms per cluster) and fcc structure ($\overline{N} \approx 8900$ at/cl) excited by a 20-mA beam of 1-keV electrons. The spectra display two emission bands of molecular states of argon. The continuum at 9.6 eV corresponds to transitions from vibrationally relaxed levels of neutral excimers $(Ar_2)^*$ and is analogous to the so-called «second» excimer continuum observed in liquid argon excited by ionizing particles [2]. The 8.90-eV band reflects transitions in charged complexes $(Ar_4^+)^*$[3].

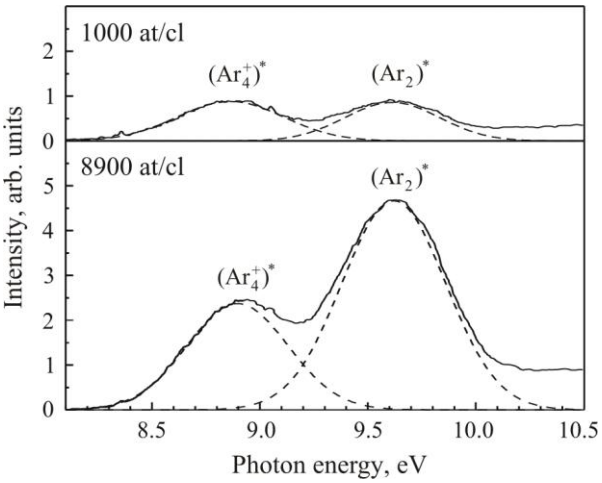


Fig. Cathodoluminescence spectra from solid clusters of argon.

In this work we estimate the efficiency of the electron beam energy conversion into the integrated intensity of 8.9-eV and 9.6-eV continua for clusters having on the average 1000 and 8900 atoms per cluster. To do this we measured with a calibrated AXUV-100 photodiode the absolute integral intensity of argon cluster supersonic jet radiation in the vacuum ultraviolet and ultrasoft X-ray spectral ranges.

The obtained results demonstrate the possibility of using rare-gas cluster beams to simulate processes occurring in liquid rare-gas detectors.

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# FEATURES OF THERMAL EXPANSION OF QUASI-TWO-DIMENSIONAL ORGANIC CONDUCTOR κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl

**R. M. Basnukaeva[1], A. V. Dolbin[1], M. V. Khlistuck[1], V. B. Eselson[1], V. G. Gavrilko[1], N. A. Vinnikov[1], V. V. Danchuk[1], V. A. Konstantinov[1], Y. Nakazawa[2]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2] Department of Chemistry, Graduate School of Science, Osaka University, 1-1 Machikaneyama-cho, Toyonaka, Osaka 560-0043, Japan*
*e-mail: basnukaeva@ilt.kharkov.ua*

Linear coefficient of thermal expansion α(*T*) of single crystal (BEDT-TTF)$_2$Cu[N(CN)$_2$]C1 was studied along the crystal layers using the method of precise capacitive dilatometry in the temperature range 2-285 K [1,2]. It is positive in this direction over the entire temperature range. Anomalies of thermal expansion were observed at 29-30 K and 74-80 K. The anomaly near 30 K is, apparently, due to the transition between the paramagnetic phase and the antiferromagnetic insulator state. Peak of α(*T*) at 78 K corresponds to a phase transition related to orientational disordering of ethylene groups in dimmers of BEDT-TTF. A broad maximum of α(*T*) in the temperature range 40–70 K, is apparently explained by fluctuations of charge within the dimers, and by spin fluctuations, which first increase with increasing temperature, and then decrease in process of thermal disordering of dimers.

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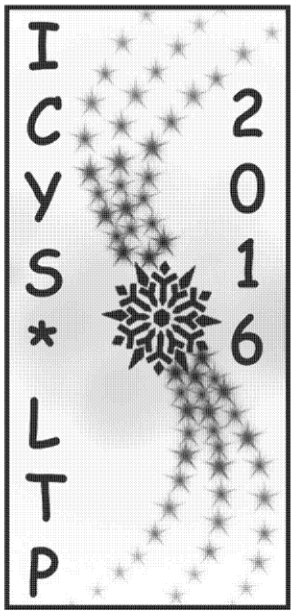
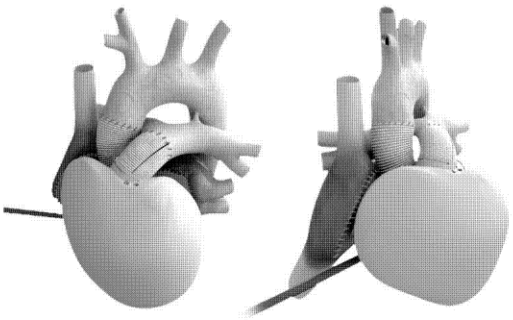
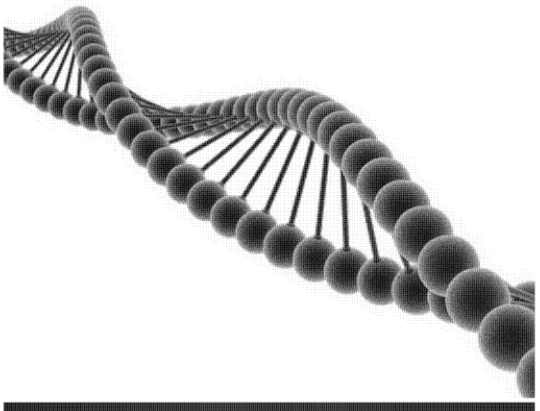
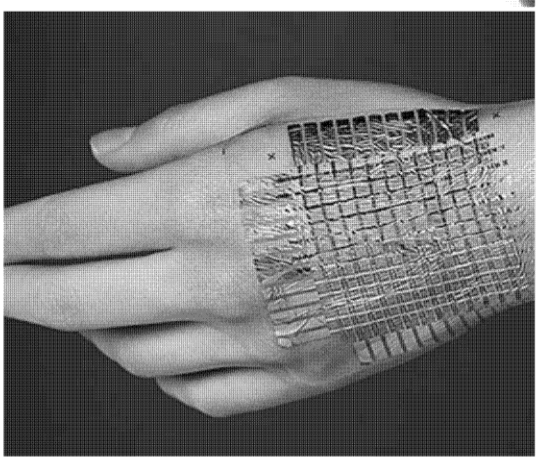
# Biophysics and Physics of Macromolecules







# EFFECT OF DIVALENT CATIONS ON THE PROTON TRANSPORT IN ISOLATED ERYTHROCYTE

**D. F. Astapovich, V. P. Berest**

*V.N.Karazin Kharkiv National University, Svobody Sq., 4, Kharkiv 61022, Ukraine*
*e-mail: astapovich.2012@mail.ru*

Calcium ions among other factors regulate deformability and elasticity of circulating red blood cells (RBC). Cytosol calcium level is critical for conventional RBC physiology aimed at maintaining oxygen delivery. The basal $Ca^{2+}$ influx is mediated by a proton carrier and is under control of intracellular regulatory circuits. To test the assumption that the $Ca^{2+}$ influx is in part driven by the proton-motive force and that the influx and efflux of $Ca^{2+}$ are coupled via the RBC osmotic regulation we performed computer simulations.

We have used an integrated mathematical model of a single RBC homeostasis to study the effect of divalent cations on transient properties of RBC and proton transport in particular. The model does not allow for direct manipulations with intracellular $Ca^{2+}$ and $Mg^{2+}$ concentration, so we did it implicitly by analyzing the behavior of isolated cells in response to the abrupt introduction of a large number of ionophore A23187. The model is given by a system of differential and algebraic equations [1, 2], which are solved numerically to describe the kinetics of erythrocyte relaxation from one equilibrium state to another when an instantaneous change in environmental conditions occur.

The main interest for us was to study the influence of high concentrations of intracellular free calcium on the mechanisms of regulation of the osmotic state of erythrocyte. During a simulation it was found that: a) when we change the nonspecific erythrocyte membrane permeability to $Ca^{2+}$ we observe dehydration, increase of cell volume and intracellular osmotic pressure, i.e. erythrocyte dehydration increases the osmolarity of intracellular medium; b) when the concentration of intracellular calcium reaches $10^{-2}$ M marked hyperpolarization and sudden alkalization/acidification of intra- and extracellular media is observed; c) osmotic relaxation of erythrocyte under conditions of very high concentrations of ionophore A23187 leads to the misbehavior of the model and loss of stability regulation of the osmotic balance of the cells (Fig. 1, Fig. 2). It can be assumed that the erythrocyte hemolysis occurs as a result of the formation of large pores for divalent cations in the erythrocyte cell membrane.

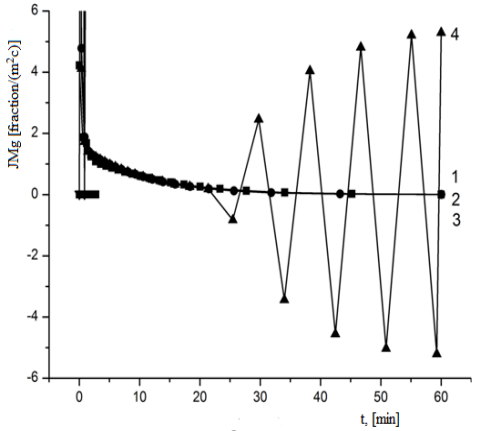



**Fig. 1.** Changes of $Mg^{2+}$ flux density over time with varying amounts of A23187: 1) $10^{10}$ molecules/cell; 2) $10^{18}$ molecules/cell; 3) $5 \cdot 10^{18}$ molecules/cell; 4) $10^{20}$ molecules/cell.

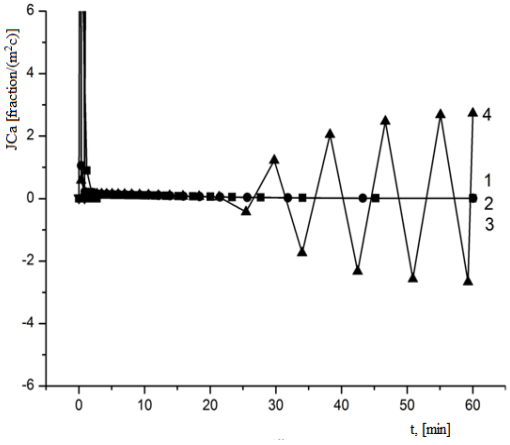



**Fig. 2.** Changes of $Ca^{2+}$ flux density over time with varying amounts of A23187: 1) $10^{10}$ molecules/cell; 2) $10^{18}$ molecules/cell; 3) $5 \cdot 10^{18}$ molecules/cell; 4) $10^{20}$ molecules/cell.

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# PHARMACEUTICAL INTERACTIONS IN MODEL LIPID BILAYERS BY MEANS OF DIFFERENTIAL SCANNING CALORIMETRY

**L. V. Budianskaia, O. V. Vashchenko**

*Institute for Scintillation Materials of NAS of Ukraine,Prospekt Nauky, 60, Kharkiv 61001, Ukraine*
*e-mail: l.budjanskaja92@gmail.com*

Pharmaceutical interactions are important part of drugs action and could be essential for their efficacy [1]. Meanwhile, such investigations are extremely complicated due to multi-compound structure of both drugs and bio-objects. Therefore, model approaches could help to elucidate certain aspects of this problem. Lipid bilayer is known as an obligatory site of drugs effect during their interaction with living organism [2]. So, model lipid bilayers seem to be an adequate model medium to study pharmaceutical interactions.

Pharmaceuticals with diverse properties were chosen for investigation, namely, azithromycin, succinylcholine and povidone. Additionally, cholesterol was examined as a regular component of biomembranes. Model lipid membranes of *L*-α-dipalmitoylphosphatidylcholine (DPPC) containing the substances were examined by differential scanning calorimetry (DSC) using microcalorimeter «Mettler DSC 1». Combined membranotropic effects of pairs of substances were compared with effects of the individual substances by shift of DPPC membrane melting temperature ($\Delta T_m$).

The results obtained are summarized in Table 1. Additivity effect occurs if $\Delta T_m^{12} = = \Delta T_m^{1} + \Delta T_m^{2}$, where $\Delta T_m^{1}$ and $\Delta T_m^{2}$ are effects of individual substances, and $\Delta T_m^{12}$ is an effect of the pair of substances. Antagonism takes place if $\Delta T_m^{12} < \Delta T_m^{1} + \Delta T_m^{2}$.

**Table 1.** Effects of combined membranotropic action of substances in pairs ‘Substance 1 – Substase 2’ on DPPC membranes.

| Substance 2 / Substance 1 | Povidone | Cholesterol |
|---|---|---|
| Azithromycin | antagonism | additivity |
| Succinylcholine | antagonism | additivity |

As one can see, the combined membranotropic effects are the same as for hydrophobic azithromycin as for hydrophilic succinylcholine. So, antagonism took place in the both pairs containing povidone, whereas additivity was observed in both pairs containing cholesterol.

Such experimental results seem to be interesting at least due to the absence of theoretical basis to their prediction.

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# LUMINESCENCE ENHANCEMENT FROM CARBON NANOTUBES INDUCED BY THIOL COMPOUNDS

**N. V. Kurnosov, V. S. Leontiev, V. A. Karachevtsev**

*B.Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: n.kurnosov@ilt.kharkov.ua*

Doping of single-walled carnon nanotubes (SWNTs) aqueous solution with several thiol-containing compounds (dithiothreitol (DTT), cysteine, mercaptoethanol) is accompanied with the intensity increase of photoluminescence (PL) from nanotubes [1, 2]. All these compounds are reducing agents which passivate p-defects on the nanotube surface (that quenched the emission) due to presence of thiol group in the structure.

The results of studies of cysteine and other thiol reducers (dithiothreitol, dithioerythritol, glutathione, mercaptoethanol) influence on the SWNT photoluminescence are presented. PL spectra of semiconducting SWNTs (grown by CoMoCAT method) in aqueous suspensions with adsorbed single-stranded DNA were observed in the range of 1.1-1.6 eV (emission was excited by green laser, $\lambda_{ex}$=532 nm, 5 mW). Such spectra were registered for different concentrations of added reducers (up to $10^{-3}$ M). The integral intensities of nanotube PL bands were determined at each concentration to obtain the dependence of normalized PL intensity on logarithm of concentration (the concentration curve). Concentration curves showed that PL intensity of semiconducting nanotubes was enhanced after doping with each thiol compound, the largest effect was observed for DTT. Also, the emission enhancement was changed for nanotubes of different chiralities containing in the sample.

We have also studied the effect of UV-irradiation and time of sonication (30 or 90 min) of nanotube:DNA aqueous suspension on the enhancement of PL from nanotubes induced by addition of thiol compounds. The UV-irradiation treatment was applied to nanotube suspensions prepared using different sonication methods: tip sonication and bath sonication. In both cases it turned out that UV-irradiation of nanotube aqueous suspension leads to appearance of additional nanotube defects as well as to a change of the DNA coverage of the nanotube surface. This results in a shift of the concentration curve towards lower concentration (titration with cysteine was performed). Longer time of sonication also causes the change of the DNA coverage, which can lead to lower PL intensity from certain nanotube species in pure nanotube suspension, however, it is accompanied with a greater sensitivity of the PL intensity to addition of thiols. The different enhancements of PL from nanotubes of different chiralies were observed as well as from SWNTs exposed to short and long sonication. It was revealed that the discrepancy in the enhancements values obtained after doping with different reducers was smaller for the nanotube suspension with longer sonication treatment. We assume that the effect of the PL enhancement of carbon nanotubes in aqueous suspension due to addition of reducers depends on several factors, concerning both the nanotubes (surface coverage, defects) and the additives (structure and chemical reactivity of added reducing molecules).

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# CORRELATION OF SOME MOLECULAR PARAMETERS OF BIOLOGICALLY RELEVANT SUBSTANCES AND THEIR EFFECT ON MODEL LIPID MEMBRANES

**A. O. Sadchenko, O. V. Vashchenko, N. A. Kasian**

*Institute for Scintillation Materials of the NAS of Ukraine, Prospekt Nauky, 60, Kharkiv 61001, Ukraine*
*e-mail: alina_k@isma.kharkov.ua*

Relationship between lipid membrane properties and molecular parameters of guest molecules is an interesting biophysical problem with important practical applications. It is commonly known that drugs can substantially affect the membrane properties under drug-membrane interactions. Using a wide number of biologically relevant substances (BRS), we made an attempt to establish correlation between molecular parameters of drugs and their effect on model lipid membranes (membranotropic effect).

Various BRS (drugs, cryoprotectants, cell membrane compounds, etc.) were introduced into DPPC model membranes, and the effects were examined by differential scanning calorimetry (DSC) using microcalorimeter «Mettler DSC 1». The most sensitive and informative parameter obtained from DSC-profiles was the temperature of the main phase transition of the lipid membrane ($T_m$). In order to compare the results of different experiments, the membranotropic activity parameter ($a$) was suggested. It corresponds to $T_m$ change resulting from introduction of 1 wt. % of BRS into the membrane.

Analysis of literature and our experimental data allowed us to select and classify the factors important for BRS-membrane interactions, such as chemical structure, geometry, lipophilicity, electrostatic parameters, parametric adequacy, etc. Lipophilicity is generally acknowledged as an important parameter for BRS membranotropic effect. The lipophilicity coefficient *logP* was calculated by 7 techniques using Virtual Computing Chemical Laboratory (http:/www.vcclab.org). Correlations between different *logP* values and $a$ were weak (-0.22 ÷ -0.42) for the whole bulk of the BRS examined. Such result confirms that membranotropic effects are caused by diversity of the molecular parameters marked above.

So, it was necessary to obtain and analyze more molecular parameters of the BRS. Such molecular parameters as total area ($S_{total}$), volume ($V_m$), dipole moment ($\mu$) and geometrical dimensions of the BRS molecules were calculated by semiempirical method AM1 using software MOPAC 2012, version 15.347W. Taking into account the above mentioned classification, we determined parameters of molecular anisotropy and of polar area fraction ($S_{polar}/S_{total}$). Parameter $S_{polar}$ was obtained from free electronic resource http://pubchem.ncbi.nlm.nih.gov.

Correlation between $a$ and $S_{polar}/S_{total}$ was established, which allowed us to select a group of BRS with similar mechanism of membranotropic action (with high linear correlation, -0,83).

Matrices of linear correlation coefficients were obtained for various BRS groups. It was established that parameter $a$ has a high degree of correlation (~ 0.9) with *logP* and $S_{polar}/S_{total}$ for BRS group with different chemical nature, but similar mechanism of membranotropic action. For BRS of similar chemical nature (oxyethylated derivatives of glycerol; quaternary ammonium compounds), parameter $a$ has a high degree of correlation (> 0.9) with *logP*, $S_{total}$, $V_m$ and $\mu$.

The results obtained could be useful for drug-membranes interactions study and development of modern pharmaceutics.

# COMPARISON OF NONCOVALENT INTERACTIONS OF LINEAR HETEROCYCLIC ORGANIC MOLECULES WITH CARBON NANOTUBES OR WITH GRAPHENE

**E. S. Zarudnev, S. G. Stepanian, V. A. Karachevtsev**

*B.Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: zarudnev@ilt.kharkov.ua*

Noncovalent functionalization of novel carbon nanostructures, such as graphene or nanotubes, with conjugated π-systems has opened up great opportunities for various applications including biology and nanomedicine. Noncovalent functionalization is particularly attractive in comparison with covalent functionalization as attaching chemical compounds do not affect the structure and electronic properties of nanostructured carbons and as it is a simple procedure to prepare new nanocomposites.

The linear heterocyclic organic molecules are able to interact noncovalently with single-walled carbon nanotubes SWNTs of various types and chiralities. Such heterocyclic organic molecules like imidazophenazine (F1) and its derivatives ((2-methylimidazo-[4,5-d]-phenazine (F2), 2-trifluoridemethylimidazo-[4,5-d]-phenazine (F3), and 1,2,3-triazole-[4,5-d]-phenazine (F4)) with various side groups in their structure can be perspective in solving the problem of separating or enrichment of the certain species of carbon nanotubes.

In this investigation we compare the optimized structures and interaction energies for complexes of heterocyclic linear molecules with carbon nanotubes of different diameters and chirality and with graphene. As noncovalently attached molecules we select F1-F4 compounds, symmetrical analogue molecule (tetracene) and the molecules of benzene and imidazole, which are building blocs of investigated linear molecules.

As calculation results, the optimized structures of complexes and their interaction energies were obtained for all studied molecules with graphene, zigzag and armchair nanotubes of different diameters. Upon calculations, the molecules studied were located on the graphene along two directions: zigzag and armchair.

Upon studies of interactions of heterocyclic molecules with nanotubes, the increase of interaction energy at the changing nanotubes from armchair (6,6) to zigzag (10,0) ones was observed. In case when investigated molecules interact with graphene the opposite picture (except F3) was observed, namely, the interaction energy was decreased moving from the armchair direction to zigzag one.

Structures and interaction energies of F1 and F4 complexes with nanotubes of various diameters (the diameter changes from 0.77 nm up to 1.54 nm for zigzag type nanotubes and from 0.80 to 1.60 nm for armchair type ones) were determined. For all the structures studied the increase in the energy of interactions between the molecule and the nanotube was observed when the nanotube diameter was enhanced. With increasing of the nanotube diameter the F1 and F4 compounds demonstrate the different enhancements of the binding energy and above 1.4 nm the energy value calculated for armchair nanotubes is predominated over zigzag ones.

In contrast to the TET molecule the electrostatic potentials induced by F1-F4 molecules on the nanotubes and graphene surfaces have an asymmetrical distribution which is explained by the presence of nitrogen atoms in their structures and back side groups in F2 and F3. Note that these molecules induce the stronger electrostatic potentials for graphene in compare with the nanotubes that is caused by the curvature of the nanotube surface.

# INFLUENCE OF FREEZING DOWN TO -196˚C ON STRUCTURE AND ANTIOXIDANT POWER OF SEVERAL PROTEINS

**S. V. Narozhnyi, S. L. Rozanova, O. A. Nardid**

*Institute for Problems of Cryobiology and Cryomedicine of the NAS of Ukraine,*
*Pereyaslavska str., 23, Kharkiv 61015, Ukraine*
*e-mail: stas.narozhnyy@mail.ru*

For a long time proteins were considered as a major target for detrimental action of free radicals. However there are new data supporting proteins antioxidant properties. Herewith their antioxidant capabilities are closely linked to molecule structure [1, 2]. These facts contribute protein and protein compositions application in clinical practice in order to treat oxidation-induced diseases including atherosclerosis, aging, inflammation, and certain nervous system disorders.

One of the most perspective and proper ways of antioxidant properties storing appears to be cryopreservation. However freeze-thawing is known to lead in most cases to protein conformational changes which consist in molecule loosening, increasing accessibility of protein active sites as well as molecule aggregation [3, 4]. Moreover conformational alterations in proteins may change their antioxidant potency.

The purpose of the present work was to investigate influence of different freeze-thawing protocols on structure and antioxidant properties of isolated proteins.

In our experiments we have investigated human serum albumin, human hemoglobin and cytochrome C from horse heart frozen down to -196ºC with 1-2º/min and 300º/min rate with following thawing on a water bath at 20ºC. Native proteins were taken as a control. Influence of freeze-thawing protocols on protein structure was investigated using spectrophotometric and fluorescent assays. Antioxidant activities of isolated proteins were estimated by their ability to reduce ABTS+ radical and by ferrous ions chelating ability. It have been established that unfolding derived from freeze-thawing exposure leads to protein antioxidant activity increasing while decreasing of such an activity may be connected with macromolecule aggregation. Character of freeze-thawing influence on proteins depends on molecule structure particularities and freezing protocols.

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# THE VIBRATIONAL SPECTRA OF 5-FLUOROURACIL MOLECULES ISOLATED IN THE LOW TEMPERATURE Ar MATRICES

**I. I. Shkapo, A. Yu. Ivanov, Yu. V. Rubin, V. A. Karachevtsev**

*B.Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Prospekt Nauky, 47, 61103 Kharkov, Ukraine*
*e-mail: shkapoiliya@gmail.com*

The halogen-substituted DNA bases and nucleosides are already known for an array of biological properties [1]. In particular, 5-fluorouracil is in many cases the first-line chemotherapeutic agent and used for anticancer therapy. Because of this 5-halouracils are the objects of scientific studies with the most modern techniques [2]. The low temperature spectral methods play a significant role in the modern studies on structures of isolated biomolecules. For this work the FT-IR spectra of 5-fluorouracil molecules isolated in low temperature Ar matrices were obtained in the range of 3800-200 $cm^{-1}$ with resolution 0.3 $cm^{-1}$. The populations of main structural isomers of 5-fluorouracil at the different temperatures of evaporation were estimated by means of the quantum-mechanical calculations at the DFT/B3LYP and MP2 levels. It was established that the population of the minor isomers of 5-fluorouracil does not exceed the threshold of detection of 0.1-0.2% at the temperature of evaporation 380 K. In the spectral range of 1900-500 $cm^{-1}$, the splitting of a number of the absorption bands is caused by Fermi resonance. New software was developed for the synthesis and analysis of the calculated spectra with anahrmonic bands. By using the DFT/B3LYP/ 6311++G(df,pd) method of calculations (harmonic and anharmonic) and polynomial correction [3] of frequencies of the vibrational spectra the combination bands enhanced by Fermi resonance were established, in particular in the νCO region (Fig. 1): FR1 (1705.1 $см^{-1}$ ), FR2 (1767.8 $см^{-1}$), FR3 (1755.1 $см^{-1}$ ), FR4 (1780.2 $см^{-1}$).

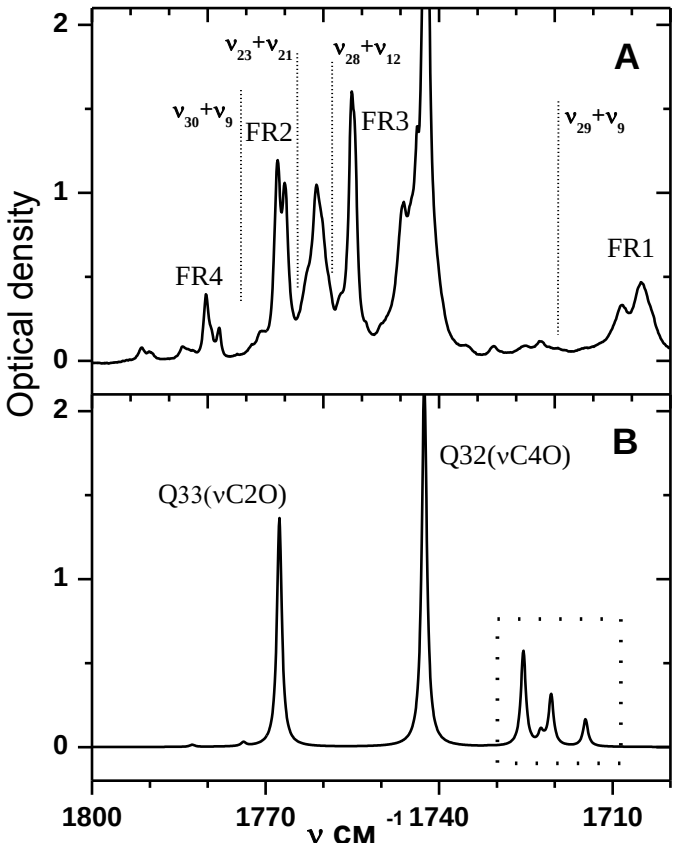


**Fig. 1.** FTIR spectra of 5-fluorouracil molecules in the νCO stretching region (1800-1700$cm^{-1}$): A – experiment in Ar matrix (T= 6 K, matrix to sample ratio = 700:1). B - calculation by the DFT/B3LYP/6311++G(df,pd) method.

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# MASS SPECTROMETRIC INVESTIGATION OF INTERACTION OF PUTRESCINE WITH OLYGOMERS OF POLYETHYLENE GLYCOL

**V. G. Zobnina[1], O. A. Boryak[1], M. V. Kosevich[1], K. Vekey[2], A. Gomory[2]**

*[1] B.Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2] Core Technologies Centre of Research Centre for Natural Sciences of the Hungarian Academy of Sciences, Magyar tudosok korutja, 2, Budapest, H-1117, Hungary*
*e-mail: zobnina@ilt.kharkov.ua*

The natural polyamines are ubiquitous constituents of human cells; they attract attention of molecular biophysics and medicine because of the well known increase of polyamines content in malignant and proliferating cells. A new strategy to inhibit «bad» cell growth is the addressing polyamines depletion. In the framework of systematic investigation of nanoparticles based on pegylated active compounds for targeted drug delivery, the extreme need for molecular information concerning the possibility of complex formation between the representatives of polyamines and polyethylene glycol (PEG) comes to the fore.

In the present work we report the data on noncovalent intermolecular interactions of polyamine putrescine (Put) with PEG-400, obtained by electrospray mass spectrometry.

In the electrospray positive ion mass spectra (Fig. 1) of putrescine-polyethylene glycol mixture in methanol sets of cationized and protonated oligomers $PEG_n \cdot Na^+$, $PEG_n \cdot H^+$, and the Put in protonated form $Put \cdot H^+$ were recorded. The important result is the observation of the abundant signals of solvated complexes $PEG_n \cdot Put \cdot H^+$. In the positive ion mode along with the above signals we recorded an unexpected set of doubly charged clusters of putrescine with $PEG_n$. Dependence of cluster sets abundances on cone voltage variation has shown that doubly charged $PEG_n \cdot Put \cdot 2H^{2+}$ clusters which start to decrease in abundance from the cone voltage value as low as 10 V, are significantly less stable than those of the oligomers with Put in the protonated form - $PEG_n \cdot Put \cdot H^+$.

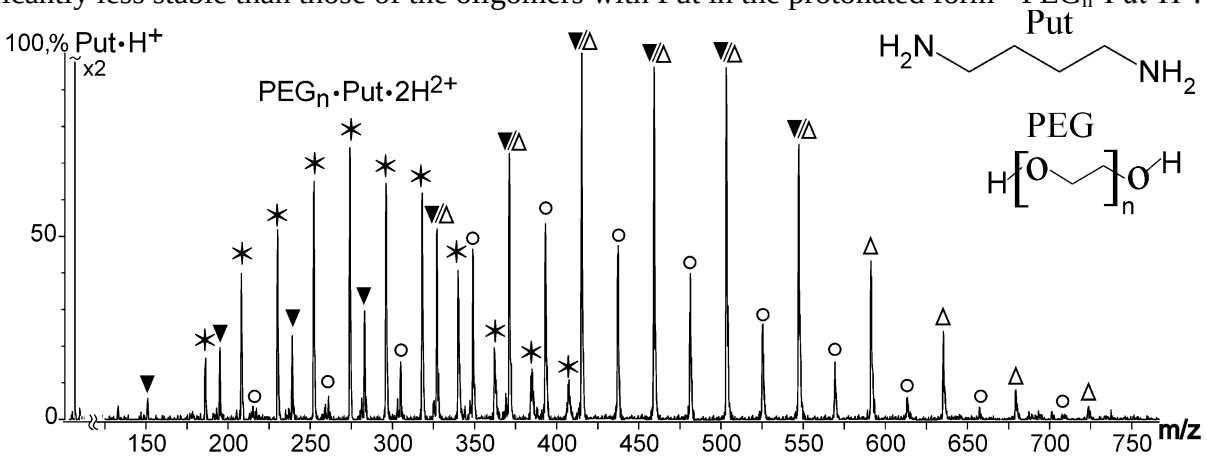


**Fig. 1.** Electrospray mass spectrum of positive ions of "putrescine – PEG" system and structures of Put and PEG–400 ($PEG_n$) oligomers. Designations of peaks series: ○ – cationized oligomers of $PEG_n$ – $PEG_n \cdot Na^+$ ; ▼ – protonated oligomers of $PEG_n$ – $PEG_n \cdot H^+$ ; Δ – protonated complexes of $PEG_n$ oligomers with Put – $PEG_n \cdot Put \cdot H^+$ ; * – doubly charged protonated complexes of $PEG_n$ oligomers with Put – $PEG_n \cdot Put \cdot 2H^{2+}$.

Of course, to get answers to the questions concerning the structural parameters and features of complex formation and charge location in doubly charged nanoparticles, the computer modeling involving molecular dynamic simulation are required.

At the moment, however we can confidently say that the observations of discussed noncovalent complexes are of interest both for fundamental molecular biophysics and for applications in the production of pharmaceutical organic nanoparticles.

# THE INFLUENCE OF THE PROTONATION ON THE STABILITY OF THE SPIROPYRAN AND MEROCYANINE MOLECULES

**O. A. Kovalenko[1], Yu. M. Lopatkin[1], P. O.Kondratenko[2]**

*[1] Sumy State University, Rymsky-Korsakov str., 2, Sumy 40007, Ukraine*
*[2] Aerospace Institute, National Aviation University, Kosmonavt Komarov Prospekt, 1, Kiev 03680, Ukraine*
*e-mail: olya.sumy.ua@gmail.com*

The investigation of the molecular photochromic switches is very actual to date because of the possibility of their use in new technologies, such as optical data storage, molecular logic gates and optical switches. The main advantage of these compounds is that they permit to manage a plenty of properties by radiation [1]. Photochromic molecules of the spiropyran(SP) class can reversibly switch between a spiro form, that absorbs only in UV region, and merocyanine(MC) form that absorbs in the visible region of the spectrum [2].

As it is known, the closed neutral form of the SP molecule is more stable than the corresponding MC form. Protonation of the molecules leads to the considerable decrease of their excitation energy [3]. MC can be done stable due to its protonation.

The aim of this study was to elucidate the protonation influence on the stability of the SP molecule and to determine the protonation center of model molecules. Also the aim was to identify the protonation features of the model molecules. Different ways of SP (Fig.1) and MC protonation were considered, namely O(30)-protonation, N(11), and also N(37)-protonation.

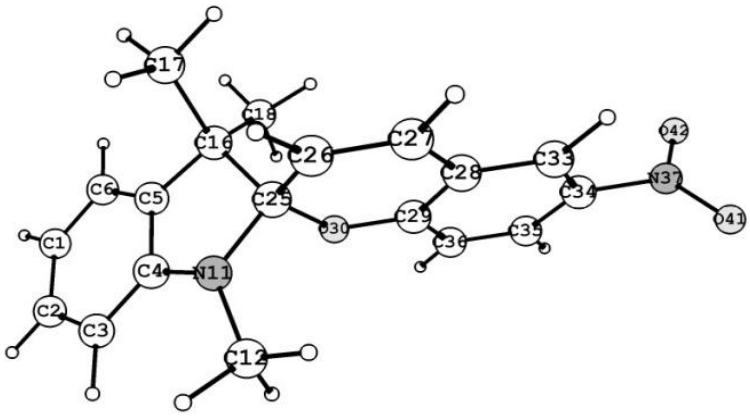


**Fig. 1.** General structure of the spiropyran

Energies of the protonated forms of the SP and MC molecules have been obtained (Table 1). It has been done for fully optimized molecules using the semi-emperical method AM1.

| | MC | SP |
|---|---|---|
| $11H^+$ | -191.3 | -192.1 |
| $37H^+$ | -189.6 | -189.4 |
| $OH^+$ | -192.6 | -192.4 |
| Cationn | -189.2 | -189.0 |

**Table 1.** The binding energies (eV) of the spiropyran and merocyanine molecules before and after protonation.

Thus, it is possible to make a conclusion that in the cation form energetically preferential is MC. On the contrary, attaching a hydrogen atom to cations of both forms in the N(37) position is energetically less favorable. Attaching a hydrogen atom to N(11) and to O(30) in the cation of the SP is practically equiprobable. For the cation of the MC a hydrogen atom attached to O(30) gives considerable energetic advantage.

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# STRUCTURE AND FUNCTIONAL STATE OF HUMAN HEMOGLOBIN IN ALGINATE MICROSPHERES AFTER FREEZING DOWN TO -196 °C

**V. N. Kuchkov, S. L. Rozanova**

*Institute for Problems of Cryobiology and Cryomedicine of the NAS of Ukraine,*
*Pereyaslavska str., 23, Kharkiv 61015, Ukraine*
*e-mail: vkuchkov@yahoo.com*

Treatment of some diseases requires the transportation of some drugs or proteins directly to a place of their action in an organism. As the transporters allowing to keep structure and functions of transferable proteins there are used the alginate hydrogels. Hemoglobin is one of the proteins, widely applied in transfusion medicine. Unfortunately, in alginate microspheres the heme of this protein is exposed to oxidation that lowers its functional efficiency and reduces storage duration. The optimal solution of this problem is storage at –196 C. At the same time it is known that freeze-thawing leads to protein conformational changes which consist in molecule loosening, increasing an accessibility of protein active sites and severe loss of their activity.

The study of various freezing rates impact on the hemoglobin structure and functionality in alginate microspheres was the aim of this work.

Hemoglobin-loaded alginate microspheres were obtained by ionotropic gelation. Their freezing down to –196 °C was carried out with 1-2 °C/min and 300 °C/min cooling rates. The thawing temperature was fixed at 22 °C. Functional activity of hemoglobin was analyzed by ability to release oxygen in anaerobic conditions with sodium dithionite use. Percentage of various forms of hemoglobin in microspheres was estimated by absorption spectroscopy. Structural changes of hemoglobin are detected through decolorization of protein $ABTS^+$ radical assay.

It has been shown that freeze-thawing of encapsulated hemoglobin leads to its partial release from the microspheres. Here with the decreasing of hemoglobin $ABTS^+$ radical reducing ability was observed. This may be a result either of hemoglobin leaking from microspheres or protein conformational changes. Frozen with the rate of 1-2 °C/min hemoglobin as a component of alginate microspheres has more manifested differences in structural-functional state if compared with rapidly frozen. Slow cooling rate results to greater loss of hemoglobin alginate microspheres after thawing. The ability to release oxygen under anaerobic conditions does not depend on the mode selected for cryopreservation.

# THE CONFORMATIONAL FEATURES OF PROTEINS AND LIPOPROTEINS FROM *TENEBRIO MOLITOR* LARVAE DURING COLD ACCLIMATION

**D. V. Tretyak[1], O. K. Gulevsky[1], A. L. Tatarets[2], L. D. Patsenker[2]**

*[1]Institute for Problems of Cryobiology and Cryomedicine of the NAS of Ukraine, Pereyaslavska str., 23, Kharkiv 61016, Ukraine*
*[2]State Scientific Institution "Institute for Single Crystals" of the NAS of Ukraine, Prospekt Nauky, 60, Kharkiv 61001, Ukraine*
*e-mail: tretyak_diana@mail.ua*

One of the most effective, informative and highly-sensitive methods for studying structural features of proteins is fluorescence spectroscopy using fluorescent probes (dyes) based on the detection of changes in fluorescence parameters of specific fluorescent dyes depending on physico-chemical properties of their microenvironment. It is extremely important that today SSI "Institute for Single Crystals" of NASU (Kharkiv, Ukraine) has already synthesized a number of fluorescent probes, which enable studying conformation not only of isolated proteins but also of protein mixtures with other molecules. It is known that some proteins of cold-tolerant organisms, including enzymes, are able to change their spatial configuration under the low temperatures influence, which leads to changes in their hydrophobicity [1, 2] and enhancement in their flexibility [3-5], being a molecular adaptation strategy of such organisms in unfavorable environmental conditions. It is still remained unclear whether the overall hydrophobicity of all proteins in cold-tolerant organisms changes or such alterations only affect certain groups of proteins during cold adaptation.

The aim of this study was to investigate conformational features of proteins and lipoproteins from Tenebrio molitor larvae during cold acclimation by fluorescence spectroscopy.

The studies were carried out in T. molitor last instar larvae, which were acclimated at 5–7°C for 3 weeks. To isolate proteins and lipoproteins, larvae were homogenized in 0.6% NaCl in 0.1 M Na-phosphate buffer (pH 7.4). Homogenates were centrifuged at 1,800 g for 15 min. Then supernatants were filtered using a membrane module "Vivaflow-50" (Sartorius, Germany), which cuts off molecules with the molecular weight of ≥1,000 kDa. Aliquots were taken from ultrafiltrates for fluorescence spectroscopy. The protein concentration was determined by the Bradford method [6].

The study used fluorescent probe DSP-13-2 (SSI "Institute for Single Crystals" of NASU, Ukraine), which binds to hydrophobic parts of proteins, and lipoprotein-binding probe K-37 (SSI "Institute for Single Crystals "of NASU, Ukraine). The concentrations of DSP-13-2 and K-37 were $4.05\times10^{-12}$ M and $4.70\times10^{-12}$ M, respectively. All fluorescence emission spectra were recorded on a Cary Eclipse spectrophotometer (Varian, Australia) in the wavelength range from 400 to 650 nm upon excitation at 410 and 420 nm for K-37 and DSP-13-2, respectively.

Using fluorescence spectroscopy with fluorescent dye DSP-13-2, we found that total proteins from non-acclimated T. molitor larvae were more hydrophobic than those from cold-acclimated insects. The studies with fluorescent probe K-37 revealed that lipoproteins in non-acclimated T. molitor larvae were significantly more abundant than in acclimated T. molitor larvae or lipoproteins of the latter had more sites capable of binding probe K-37.

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# METHODS AND MEANS OF FOURIER-STOKES POLARIMETRY AND THE SPATIAL FREQUENCY FILTERING OF PHASE ANISOTROPY MANIFESTATIONS IN DIAGNOSIS OF KIDNEY PATHOLOGY

**A. V. Dubolazov, V. O. Ushenko, I. V. Soltys, R. M. Besaga**

*Chernivtsi National University, Kotsyubinskogo str., 2, Chernivtsi, Ukraine*
*e-mail: yuriyu@gmail.com*

The optical model of polycrystalline networks of histological sections of rectum wall is suggested. The results of investigating the interrelation between the values of statistical (statistical moments of the 1st-4th order) parameters are presented. They characterize the coordinate distributions of the fourth parameter of Stokes vector of Fourier transforms of laser images of rectum wall histological sections and oncological changes. The diagnostic criteria of rectum cancer are determined [1].

Histological sections of rectum wall biopsy with benign (group of samples 1-9) and malignant (group of samples 2-10) were used as objects of investigation. This research is confined to the analysis of distributions structure of the 4th Stokes vector parameter most vividly characterizing the changes in optical anisotropy of polycrystalline biological networks (Fig. 1 and Fig. 2) [2].

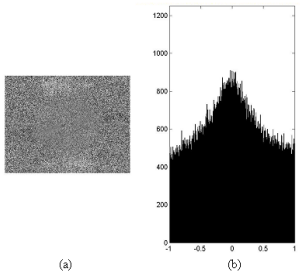

**Fig. 1.** Coordinate structure and histogram of values distribution of the 4th parameter of Stokes vector scattered by histological section of group 1 in Fourier plane

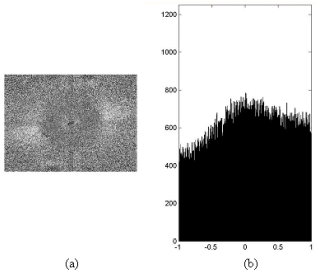

**Fig. 2.** Coordinate structure and histogram of values distribution of the 4th parameter of Stokes vector scattered by histological section of group 2 in Fourier plane

The results of the 1st-4th order moments calculation characterizing the coordinate distributions in Fourier plane of the field of laser radiation transformed by histological sections of rectum wall with benign (group 1) and malignant (group 2) tumors are presented in Table 1.

**Table 1.** Statistical moments of the 1st-4th orders of Fourier spectrum $S_4$

| Parameters | Benign changes | Malignant changes |
|---|---|---|
| $R_1$ | $0{,}28 \pm 0{,}0012$ | $0{,}07 \pm 0{,}021$ |
| $R_2$ | $0{,}11 \pm 0{,}008$ | $0{,}39 \pm 0{,}014$ |
| $R_3$ | $1{,}14 \pm 0{,}009$ | $0{,}59 \pm 0{,}016$ |
| $R_4$ | $2{,}47 \pm 0{,}017$ | $0{,}79 \pm 0{,}027$ |

A model of generalized optic anisotropy of the fibrillar protein matrices has been suggested and the method of Fourier's polarimetry for the parameters of linear and circular birefringence has been substantiated.

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# RELATIONSHIP OF THE PHASE AND AMPLITUDE PARAMETERS WITH ANISOTROPY OF MULLER-MATRIX INVARIANTS

**Yu. O. Ushenko, A. V. Dubolazov, V. O. Ushenko, L. Pidkamin**

*Chernivtsi National University, Kotsyubinskogo str., 2, Chernivtsi, Ukraine*
*e-mail: yuriyu@gmail.com*

The principles of optical model of human blood plasma polycrystalline structure are described. The results of investigating the interrelation between the values of statistical, correlation and fractal parameters are presented. They characterize the coordinate distributions of mutual polarization degree of the points of laser images of blood plasma smears of patients with malignancy of the breast in combination with other pathologies. The diagnostic criteria of the malignancy of the breast and its severity degree differentiation are determined [1-3].

Laser images of three groups of blood plasma samples of the patients of different pathological state are analyzed:

- healthy patients – group 1 (11 patients);
- patients with benign breast changes – group 2 (10 patients);
- patients with malignancy of the breast – group 3 (12 patients).

The ensemble of data about the values of diagnostic parameters $M_{k=1;2;3;4}(V=0,5)$ is presented in Table 1.

**Table 1.** Statistical moments of the 1st-4th orders of distributions $V(x,y)=0,5$ of blood plasma layers of all groups of patients

| Parameters | Group 1 | Group 2 | Group 3 |
|---|---|---|---|
| $M_1(V=0,5)$ | $0,09\pm0,008$ | $0,21\pm0,027$ | $0,32\pm0,019$ |
| $M_2(W=0,5$ | $0,26\pm0,031$ | $0,13\pm0,023$ | $0,12\pm0,019$ |
| $M_3(W=0,5$ | $0,11\pm0,021$ | $1,28\pm0,41$ | $4,26\pm0,58$ |
| $M_4(W=0,5$ | $0,09\pm0,009$ | $2,12\pm0,52$ | $5,29\pm0,0096$ |

The difference between statistical moments $M_k(W)$ of laser images of test group blood plasma (group 1) and the patients with various pathologies (groups 2 and 3) – mean (increasing by 2.7 – 3.5 times); dispersion (decreasing by 2.5 – 3.3 times); skewness (increasing by 3.3 – 5.4 times) and kurtosis (increasing by 4.5 – 6.1 times) – are determined [3].

Thus, diagnostic effectiveness of the phase and amplitude parameters with anisotropy of Muller-matrix invariants of myocardium tissue histological sections was demonstrated for diagnosing different types of pathologies.

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# MUELLER-MATRIX DIFFERENTIATION OF FIBRILLAR NETWORKS OF BIOLOGICAL TISSUES WITH DIFFERENT PHASE AND AMPLITUDE ANISOTROPY

**Yu. O. Ushenko, A. V. Dubolazov, V. O. Ushenko**

*Chernivtsi National University, Kotsyubinskogo str., 2, Chernivtsi, Ukraine*
*e-mail: yuriyu@gmail.com*

The optical model of polycrystalline networks of myometrium is suggested. The results of investigating the interrelation between the values correlation (correlation area, asymmetry coefficient and autocorrelation function excess) and fractal (dispersion of logarithmic dependencies of power spectra) parameters are presented [1]. They characterize the distributions of Mueller matrix elements in the points of laser images of myometrium histological sections. The criteria of differentiation of death coming reasons are determined [2].

The results of experimental investigations of coordinate $Z_{44}(m\times n)$ – fragments (a), (b); statistical $h(Z_{44})$, – fragments (c), (d); correlation $K(Z_{44})$, – fragments (e), (f) and fractal $\log J(Z_{44})-\log d^{-1}$, – fragments (g), (h) structure of Mueller matrix phase elements $Z_{44}$ of myometrium of the heaths patients – group 1 (left column) and sick patients - group 2 are illustrated by Fig. 1 and Table 1.

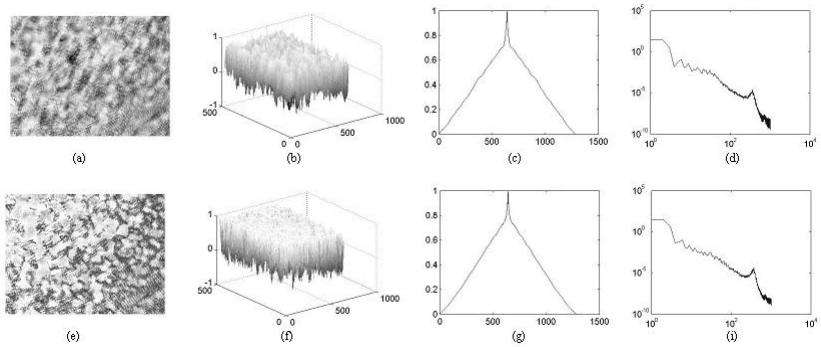

**Fig. 1.** Statistical, correlation and fractal parameters of myometrium phase element $Z_{44}$ distributions

**Table 1.** Statistical moments $M_{j=1;2;3;4}(Z_{44})$ of coordinate distributions $Z_{44}(m\times n)$ of myometrium tissue for group 1 and group 2 cases

| Parameters | Group 1 | Group 2 |
|---|---|---|
| $S(Z_{44})$ | $0{,}21\pm0{,}026$ | $0{,}26\pm0{,}037$ |
| $Q_2(Z_{44})$ | $0{,}35\pm0{,}044$ | $0{,}31\pm0{,}039$ |
| $Q_4(Z_{44})$ | $0{,}43\pm0{,}051$ | $0{,}53\pm0{,}062$ |
| $M_1(Z_{44})$ | $0{,}21\pm0{,}026$ | $0{,}26\pm0{,}037$ |
| $M_2(Z_{44})$ | $0{,}35\pm0{,}044$ | $0{,}31\pm0{,}039$ |
| $M_3(Z_{44})$ | $0{,}43\pm0{,}051$ | $0{,}53\pm0{,}062$ |
| $M_4(Z_{44})$ | $1{,}16\pm0{,}14$ | $1{,}37\pm0{,}16$ |

The efficiency of the method of azimuthally invariant Mueller-matrix mapping of laser polarization polarimetry of biological tissues in the task of differentiation was demonstrated.

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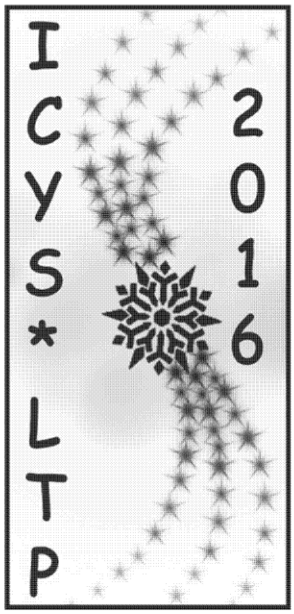
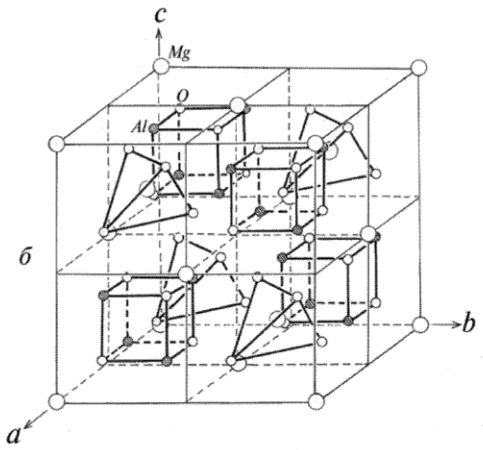
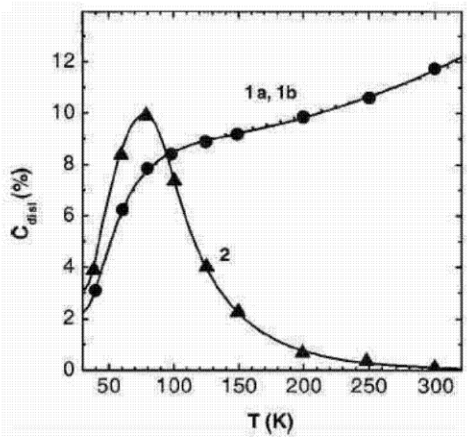
# Materials Science




# CHANGE OF STRUCTURE OF POLYIMIDE PM-A AFTER EXPOSURE TO LOW TEMPERATURE AND DEFORMATION

**V. G. Geidarov, Y. M. Plotnikova**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: geydarov@ilt.kharkov.ua*

Polyimide polymers are widely used in various fields of modern technology due to its unique physical properties. [1,2]. However, because of the complex molecular structure of some of the questions still no clear answer. So, there is no information about what happens to the objects under the influence of low temperatures. In this work, we suggest one explanation for the reaction of the sample processing method. For X-ray study of these substances give typical for amorphous solids X-ray scattering pattern, characterized by short-range order.

The work presents results of a study by X-ray diffraction, the polymer subjected to linear deformation and low temperature cooling. Samples for the experiments took the form of strips dimensions 70x5x0,08 $мм^3$, X-ray diffraction studies were performed on a DRON-2.0. Measurements were carried out over a wide range of angles.

All radiographs observed halo typical of amorphous solids. Halo symmetrical to the initial film. External influence (low temperature and deformation) leads to redistribution of intensities and to the asymmetric form of halo consisting of two maxima: the main and "satellite". Emergence of an additional maximum demonstrates formation of area of a near order with density of distribution of atoms other than an initial sample. As part of our reasoning this behavior can be explained by the ordering of polyimide molecules under the influence of uniaxial tension and loss of intramolecular degrees of freedom when cooled.

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# X-RAY DETERMINATION OF STRUCTURAL PARAMETERS IN CP-TITANIUM UNDER CRYOROLLING

**Y. M. Plotnikova**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: Plotnikova@ilt.kharkov.ua*

The investigation nanocrystallinel structure causes a great interest. It is associated with unique physical and mechanical properties of these materials. An effective way of producing such materials is the method of cryomechanical fragmentation of grain [1].

The samples were repeatedly rolled at a temperature of liquid nitrogen with achievement of deformation $|e| = 0{,}06 - 3$ to obtain a nanostructural state.

The structure of the samples has been studied on the diffractometer DRON-2.0 (method $\theta$-$2\theta$), using X-ray diffraction with filtered Cu-Kα radiation, collimation slits and subsequent computer data processing. Intensity of scattering was registered in the range of angles $20^\circ < 2\theta < 140^\circ$. Samples removed in the rolling plane. Parameters structures such as: the values of regions coherent scattering $L$ (RCS), the level of average micro deformations $\Delta\varepsilon$ and macro stresses $\sigma$ were assessed by the analysis of the intensities, the shape of the line profiles and width of diffraction reflections [2].

The sizes of RCS decreases approximately by 50% compared to the initial sample with increasing in extent of deformation to $|e| \approx 0{,}6$. Observed decreasing in the sizes of RCS may indicate on raising a contribution of twinning in the formation of a nanostructural state. At further deformation the sizes of RCS virtually unchanged.

It was found that the value of the average micro deformations is characterized by sudden growth when $|e| = 0 \div 0{,}3$. That is why associated with intense fragmentation of the grain structure at this stage. The value of micro deformations at high achievement of deformation gradually increases from $\Delta\varepsilon = 1{,}5 * 10^{-3}$ to $\Delta\varepsilon \approx 2{,}5 * 10^{-3}$.

In the initial sample according to the received results the tensile stresses $\sigma$ is equal 1,5 GPa. On the other hand, all samples after cryodeformation are characterized by compressive residual stresses. The average value is about 2 GPa.

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# INDENTATION SIZE EFFECT IN TITANIUM VT1-0

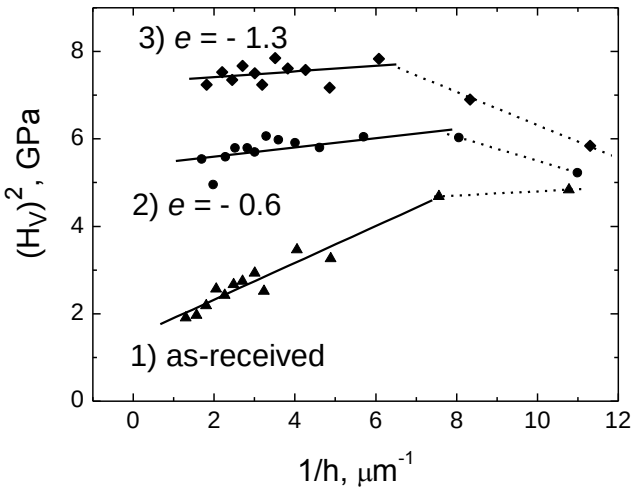
**A. V. Rusakova**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: rusakova@ilt.kharkov.ua*

The dependence of microhardness on the load $H(P)$ or on the depth $H(h)$ is often observed at the indentation of solids. It is so-called indentation size effect (ISE). To obtain the correct values of microhardness it is necessary to carry out the measurements provided that $H(P)$ = Const.

To study ISE in titanium VT1-0 the detailed dependences $H_V(P)$ for the as-receive sample and the samples rolled to the true strain $e$ = - 0.6 and $e$ = - 1.3 at the temperature $T \approx 77$ K [1] were obtained. These measurements also provide data about the structure states of the surface layer and the bulk of the sample.

The concept of geometrically necessary dislocations (GNDs) [2] is the most frequently used to interpret ISE. In the model of GNDs the indenter penetration resistance was calculated with regard to the contribution of statistically stored dislocations (SSDs) with density $\rho_s$ and GNDs with density $\rho_G \propto \frac{1}{h}$. The model leads to the following form for the depth dependence of the microhardness:




$$\frac{H}{H_0} = \sqrt{1 + \frac{h^*}{h}}, \qquad (1)$$

where $H_0 = 3\sqrt{3}\alpha\mu b\sqrt{\rho_s}$ is the hardness of material in the absence of any GNDs ($H_0 = H_{h\to\infty}$), $h^*$ is a characteristic length that depends on the SSDs density. The model of GNDs gives the expression

$$h^* = \frac{81}{2} b\alpha^2 \mathrm{tg}^2\theta \left(\frac{\mu}{H_0}\right)^2, \qquad (2)$$

where $b$ is the modulus of dislocation Burgers vector, $\alpha \approx 0.5$, $\theta$ is the angle between the surface of the sample and the pyramid face of indenter, $\mu$ is the shear modulus. It can be seen from (2) that $h^* \propto \frac{1}{\rho_s}$.

In the Figure the data of measurements $H_V(P)$ are presented in the coordinates corresponding to the expression (1). The experimental data are satisfactorily described by this model with the exception of the points at $h \leq 0.2$ μm. The cryorolled samples (the curves *2* and *3*) are characterized by the larger values $H_0$ and significantly smaller values of characteristic length $h^*$ as compared with the as-received sample (the curve *1*) [3].

Thus, the dependences of microhardness on the load (or on the depth of indenter penetration) can be caused by two reasons. The first reason is the presence of gradient of micromechanical properties in the surface layer of the samples (the region of small values of $h$). The second one is the generation of geometrically necessary dislocations under the impression.

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# STRAIN HARDENING, STRAIN RATE SENSIITIVITY AND DUCTILITY OF THE NANOCRYSTALLINE TITANIUM

**R. V. Smolianets**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: smoljanets@ilt.kharkov.ua*

The general tendency of the nanocrystalline (NC) and ultrafine-grained (UFG) metals is a strong increase of strength with a significant loss of ductility. The tendency to stability for NC and UFG metals during tensile deformation associated primarily with a decreasing ability to the strain hardening $\theta$. According to the criterion Considére, the inhomogeneous deformation (necking) begins when

$$(\partial\sigma/\partial\varepsilon)_{\dot{\varepsilon}} = \theta \lesssim \sigma, \qquad (1)$$

where $\sigma$ and $\varepsilon$ is the true strain and true strain, respectively. For materials sensitive to the strain rate of flow strain in addition to a sufficient level of strain hardening to the maintenance of the uniform deformation also contributes the availability of the strain rate sensitivity $m = (\partial\ln\sigma/\partial\ln\dot{\varepsilon})_{\varepsilon}$. In this case, the instability criterion (Hart) has the following form:

$$(1/\sigma)\,(\partial\sigma/\partial\varepsilon)_{\dot{\varepsilon}} - 1 + m \lesssim 0, \qquad (2)$$

i.e. a material with a high value of m is more stable.

In this paper, the effect grain size (d) and the grain size distribution on the parameters $\theta$ and $m$ of the equations (1) and (2) has been studied for NC unimodal ($d$ = 45 nm), NC bimodal (~ 18% of the submicron grains in NC matrix) and CG ($d$ = 3 μm) of commercial purity titanium VT1-0 during tensile deformation at the temperature range 77 - 400 K. NC titanium was produced by using the method of cryomechanical fragmentation grains (in this case, cryorolling at 77 K) [1]. This structural state was obtained by annealing of the samples with an average grain size of 35 nm at temperatures of 523 K, 723 K and 943 K for 45 min.

It is found the sharp decrease of the strain rate hardening $\theta$ with decreasing grain size to nanometer values at lower levels of plastic deformation. The reason for this considered to the impossibility of effective accumulation dislocations inside tiny NC grains due to image forces and interaction with grain boundaries.

Concurrently, the two-fold decreasing strain rate sensitivity $m$ at reducing the grain size from 3 microns to 45 nm is observed. In particular, the value of $m$ at $T$ = 293 K is changed from 0.022 for CG to 0.01 for NC titanium. It should be noted that such tendency of change $m$ for BCC metals is observed, while the creating of NC / UFG state in FCC metals give rise to an increase of the strain rate sensitivity.

For stable plastic flow of the assistance m, as follows from eq. 2, is insufficient. This can be explained by progressive necking, when decreasing $\theta$ can`t compete with the decreasing cross-sectional area. Thus, the lack of a sufficient strain hardening $\theta$ and strain rate sensitivity $m$ result to the work softening mechanism (adiabatic or geometric), which leads to the formation of shear banding during tensile deformation of the flat specimens, as a fundamental mode of plastic deformation NC / titanium UFG.

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# PEIERLS BARRIERS FOR <A>-TYPE SCREW DISLOCATIONS IN MAGNESIUM

**O. M. Vatazhuk[1], A. Ostapovets[2], R. Gröger[2]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2]CEITEC-IPM, Institute of Physics of Materials ASCR, Žižkova 22, Brno, Czech Republic*
*e-mail: vatazhuk@ilt.kharkov.ua*

Magnesium and its alloys are actively studied as perspective low weight construction materials that have relatively high specific strength and excellent corrosion resistance for which they are favored in automotive and aerospace applications [1]. However, their practical applications are limited due to lack of deformability. Magnesium has hexagonal crystal structure which results in significant anisotropy of plastic deformation in this material. Critical resolved shear stress (CRSS) is about one order of magnitude higher for non-basal slip than CRSS for basal slip. Deeper understanding of plasticity mechanisms is necessary in order to improve mechanical properties of magnesium alloys.

Computer modeling of dislocation motion is a perspective way to investigate slip mechanisms in atomistic level. However, modeling of thermal activation of slip by atomistic methods is limited by timescale of molecular dynamics. In practice, the molecular dynamics allow the calculations at stresses and strain rates much higher than those at real deformation experiments. Hence, analytical models of thermally activated formation of kink pairs can provide appropriate solution of the problem. Such models can use the results of atomistic simulations as input. However, the models based on reaction rate theory depends sensitively on the form of Peierls barrier that the dislocation overcome when moving in the crystal [2]. The reason is that activation enthalpy, which determines the dislocation motions, is obtained by integrating over the Peierls barrier.

The calculations of the core structures and Peierls stresses for dislocations in magnesium are widely presented in literature [3-5]. However, the calculations of complete Peierls barriers are more rare [6]. The aim of present work is calculation of exact shape of Peierls barriers for <a> screw dislocation gliding on basal and prismatic planes in magnesium by using of several popular interatomic potentials for magnesium. We would like to compare predictions of models based on these potentials and to describe their abilities and limitations. We first investigate stability of different typs of dislocation core. Then, employing the Nudged Elastic Band method, we calculate the Peierls barriers between equivalent minimum-energy configurations on basal and prismatic slip systems and determine the transition paths of the dislocation. Three EAM potentials are used in the present work. The results are compared with available first-principles calculations and experiments.

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# PECULIARITIES OF PLASTIC DEFORMATION OF UFG AZ31 AT LOW TEMPERATURE

**P. A. Zabrodin**

*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: pavel.a.zabrodin@gmail.com*

The increasing shortage of natural resources, together with the world-wide implementation of stricter environmental regulations, is making it necessary to produce and utilize a range of light-weight metallic alloys for the transportation industry. Magnesium is currently the lightest metal in use for structural applications [1, 2].

In addition, magnesium alloys are attractive for use in a future hydrogen economy since magnesium is the only metallic element capable of reversibly storing a high volume of hydrogen in the form of metal hydrides [1].

The only drawback of magnesium alloys is poor plasticity, which complicates the forming. One effective way of improving the properties of the cast magnesium alloy AZ31 (Mg–Al–Zn) is to combine hot rolling and equal-channel angular pressing (ECAP) at high temperatures [2, 3].

Because of reduced grain sizes, changes in the nature of the grain boundaries, and enhancement of a texture that favors basal dislocation glide, after this kind of processing, increase yield stress and ductility.

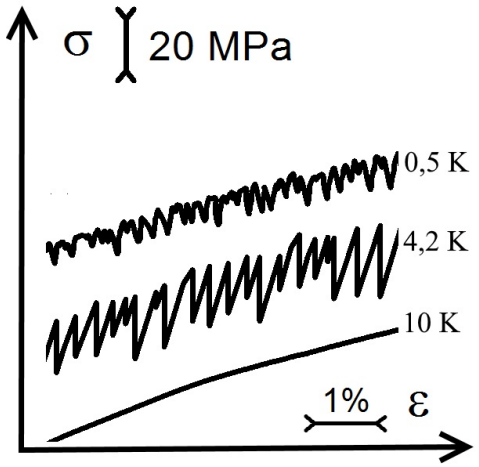


*Fig.1. The influence of temperature on the features of low-temperature jump-like deformation.*

For further study of the effect of microstructure, after annealing, on the mechanisms for plastic deformation, there is some interest in investigating the mechanical properties of the ultrafinegrained (UFG) Mg alloy at low temperatures.

It found that the amplitude and statistics at the low-temperature jump-like deformation Mg–Al–Zn dependent on microstructure. Reduction of the average density of dislocations and grain growth during annealing causing a reduction in the amplitude of the jump-like deformation and changes in the distribution of surges in amplitude.

It found that the amplitude and statistics at the low-temperature jump-like deformation UFG alloy dependent on temperature of deformation (Fig.1). Plastic deformation of UFG alloy at a temperature of 10 K occurs uniformly - peculiarities is not observed. Increasing of the temperature of deformation from 4,2 to 0,5 K causing a reduction in the amplitude and increasing the frequency of the jump-like deformation.

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# EFFECT OF DOPING AMINO ACIDS L-ARGININE ON THE STRENGTH AND NONLINEAR OPTICAL PROPERTIES OF KDP CRYSTALS

**E. I. Kosteniukova, O. N. Bezkrovnaya**

*STC ''Institute for Single Crystals'' of NAS of Ukraine,*
*Prospekt Nauky, 60, Kharkiv 61001, Ukraine*
*e-mail: e.kostenyukova@gmail.com*

The KDP ($KH_2PO_4$) sigle crystals are of great interest because of the large number of devices that use solid-state laser light sources. KDP crystals have become popular due to their transparency in the UV spectral region, high structure perfection, relatively high laser damage threshold and low cost of the fabrication of optical elements and widely used in nonlinear optics as harmonic generators for high-powerful lasers. However, one of the main functional restrictions for KDP crystals is relatively low value of quadratic susceptibility. One method of increasing of the efficiency SHG is doping of the KDP crystals by organic molecules, such as amino acids, which possess high polarizability and contain the groups which can effectively form hydrogen bonds with the growing crystal face. The amino acid molecules have high polarizability due to the processes of internal charge transfer between the donor ($COO^-$ and acceptor ($NH_2^+$) groups and have nonlinear optical properties. Thus, the addition of L-arginine (L-arg) amino acids to KDP crystal matrix led an increase in the efficiency of SHG in 1.33-1.74 times [1].

The aim of our work was the obtaining of a composite KDP:L-arg crystal, investigation of its mechanical strength and the efficiency of SHG. KDP and KDP:L-arg crystals (with 0.3-1.4 wt. % concentrations of L-arg in the mother liquor) were grown by the method of temperature reduction. Samples for studies were cut from growth sectors {100} and {101}. For the study of the Vickers microhardness were used a z-slices (the indentation load was in the range 0.2 - 2 N), and for the study the efficiency of SHG – carved out at an angle 59°. The efficiency of SHG in KDP and KDP:L-arg crystals was studied on a special laboratory setup with using of a solid-state laser with Nd:YAG active element. The investigated samples were preliminarily treated by mechanical grinding and polishing.

For pure KDP crystal the value of microhardness at loads of 0.5 to 2N does not depend on the load and makes 1.85-1.9 GPa for the planes (100) and (001) for the sector {101} and 2.0-2.15 GPa for the sector {100}. All the samples show "reverse indentation size effect" connected with the influence of the surface crystal layer which is most essential at low indenter loads [2]. It has been found that at 0.3-1.0 wt. % concentration of L-arg the microhardness value $H_V$ in the sector {101} increases in comparison with the one of pure KDP. The rise of the mechanical strength of the crystals result in from their doping may be bound up either with changes in the crystal structure or with a decrease of the mobility of point and linear defects [3]. With the increase of the concentration of L-arg to 1.4 wt. % the microhardness of both crystal faces diminishes by ~5-9 % and ~14-18 % for the sectors {101} and {100}, respectively. This is caused by disturbance of the crystal structure due to the entering of much larger quantity of L-arg molecules into the crystal.

Investigation of the NLO properties of KDP and KDP:L-arg shows that in the samples of the doped crystals the efficiency of SHG is higher in comparison with that in the pure KDP. With the rise of the concentration of L-arg molecules the radiation conversion intensity increases. Thereat, the efficiency of SHG grows proportionally to the rise of the concentration of L-arg in the crystal and for KDP:L-arg crystals (1.4 wt. % L-arg in the solution) was in 2.5 times higher than the pure KDP.

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# PLASTIC PROPERTIES OF TUNGSTEN-POTASSIUM IN A WIDE TEMPERATURE RANGE

**S. V. Lebediev[1], T. V. Khvan[1], V. I. Dubinko[2], D. Terentyev[3]**

*[1]V. N. Karazin Kharkiv National University,*
*Svobody Sq. 4, Kharkiv 61022, Ukraine*
*[2]National Scientific Centre Kharkiv Institute of Physics and Technology,*
*Academicheskaya 1, Kharkiv 61108, Ukraine*
*[3]Belgian Nuclear Research Centre SCK·CEN*
*e-mail: timofii.khvan@gmail.com*

Tungsten is a promising material for building a first wall or divertor of nuclear reactors, because it has such a good properties like high melting temperature and good thermal conductivity. That is why this metal toughness properties research, pure, with different impurities and with different grains size, are interesting, as a physical point of view and as a safety question.

The using of tungsten gave us a possibility to suppress erosion and to work with high heat loads [1]. However, tungsten suffers from transit to brittle condition below a certain temperature [2], which is called ductile-to-brittle transition temperature. Depending on mechanical, chemical and (micro-)structural parameters, this temperature is between 500 and 900 K. In addition, tungsten can be embrittled by overheating or neutron irradiation [3].

In this work we researched the temperature influence on tungsten doped by potassium plastic properties in a 77 – 873 K interval. Specimens used was a wires with a 0.15 mm cross section diameter and a 30 mm working part length. Using the wire like this in fiber-reinforcing of building materials adds some strengthening properties. The specimens heating was implemented by an external heating element.

It was found, that increasing of temperature decreased the ultimate stress in a ~2300 - ~1600 MPa range. In an electron microscope has been seen the change of specimens' destruction places. The destruction works by cracks appearance, predominantly on the surface. The temperature influence increases the geometric sizes of these cracks. In spite of toughness decreasing, the relative elongation of the specimen was ~1% in all experiments.

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# EVIDENCE FOR THE GAS ACTION ON THE PROCESS OF DENDRITIC NANOSCALE POINT CONTACTS CREATION

**A. O. Gerus[1], A. V. Savitsky[1], A. P. Pospelov[2], G. V. Kamarchuk[1]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2] National Technical University "Kharkov Polytechnic Institute" 21 Bagalia Str., Kharkiv, 61002, Ukraine*
*e-mail: gerus@ilt.kharkov.ua*

Point contact is a well-known nano-object which displays original physical properties and can serve as a modern tool of research and technology. Yanson point contact spectroscopy is a good example of where point contacts can be used [1]. At the temperature of liquid helium, the current-voltage characteristic of a point contact has a non-linear contribution, in addition to the linear one of Ohm's law, which is due to nonequilibrium processes of electron relaxation. Information about these processes can be obtained by using Yanson point contact spectroscopy thanks to the specific distribution function of electrons in the contact formed in the current mode.

Another characteristic property of point contacts is the original potential distribution. As current flows in the electrode – point contact – electrode system all the potential drops in the narrow area of the contact. This makes it possible for a new type of electrochemical electrode system called nanostructured elongated element to arise at the ends of the point contact channel at room temperature upon placing point contact in a liquid medium [2]. The main condition for its operation is a nonzero potential difference at the opposite ends of the point contact conduction channel which gives rise to electrochemical processes. This condition can easily be met for the point contact system. As a result, the point contact nanostructured elongated element can be used as a tuneable instrument to detect new physical effects and electrochemically synthesize a broad range of low-dimensional structures and functional materials. This can be illustrated, for example, by the cyclic electrochemical switchover effect discovered in the process of creation of dendritic point contacts [2].

Here we study the action of external gas agent on the process of creation of dendritic point contacts in a liquid medium. We found a change in the process of formation of point contact channel structure caused by gas molecules diffusing into the electrocrystallization area. It affects the form and behaviour of the conduction histograms obtained from the stepped conduction dependences of the dendritic point contact system formed cyclically in a controlled gas medium. The high sensitivity of quantized electrical conduction to the condition of the interphase boundary makes it possible for the arising dendritic point contacts to detect gases diffusing into electrolyte and become a prototype of quantum differential detectors of gas media.

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# INFLUENCE OF GROWTH CONDITIONS ON THE PROPERTIES OF $PbMoO_4$:Nd SINGLE CRYSTALS

**Yu. N. Gorobets, A. N. Shekhovtsov**

*Institute for Single Crystals, NAS of Ukraine,*
*Nauki Ave., 60, Kharkov 61001, Ukraine*
*e-mail: ygorobets@yuandex.ru*

$PbMoO_4$:Nd single crystals are considered to be promising active media for Raman lasers, which combine lasing and conversion functions due to stimulated Raman scattering (SRS). Efficient SRS conversion calls for high pump densities. This circumstance imposes stringent requirements on the radiation resistance of SRS materials. The dependence of the optical breakdown of $PbMoO_4$:Nd crystals on the neodymium concentration and the phase composition of dopant (the use of simple and multicomponent neodymium oxides) was studied in [1]. The high optical breakdown value demonstrated the $PbMoO_4$:Nd crystal grown at the use of simple neodymium oxide $Nd_2O_3$.

For this reason the $PbMoO_4$:$Nd^{3+}$ single crystals were grown by the Czochralski method by the use of simple neodymium oxide $Nd_2O_3$. Dielectric properties have been studied in the temperature range of 20–550°C at frequencies from 25 to $10^6$ Hz. The frequency dependence of tan δ was analyzed in the frame of computer model for the substitution of the insulator under study using the equivalent electric scheme. The parameters of the substitution electric scheme for different temperatures were defined and analyzed. The absorption and luminescence spectra of $PbMoO_4$:Nd single crystals were studied at the room and liquid nitrogen temperatures and discussed.

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# FIRST PRINCIPLES STUDY OF VIBRATIONAL PROPERTIES OF $In_XTl_{1-X}I$ SUBSTITUTIONAL SOLID SOLUTIONS

**A. V. Franiv, A. I. Kashuba**

*Ivan Franko National University of Lviv, Department of Physics,*
*8a, Kyryla i Mefodiya St., 79005, Lviv, Ukraine*
*e-mail: AndriyKashuba07@gmail.com*

Searching for new functional materials and ways to control their properties belongs to the primary tasks of physics of semiconductors and insulators. For a rather long time, the attention of scientists has been attracted to studying the properties of semiconductors and insulators with a layered crystalline structure [1-2].

First-principles methods based on density-functional theory are common and well established tools for studying structural and vibrational properties of semiconductors and insulators with various structural ordering. This method gives the ability to determine the basic properties of many materials without experimentally determined parameters. For example, the equilibrium structure, elastic constants, and high-symmetry phonon frequencies can be determined very accurately.

One of the most popular methods of first-principles calculation of lattice dynamics is the linear response method [3].

We present lattice dynamics calculations of $In_xTl_{1-x}I$ substitutional solid solutions (SSSs) layered crystals based on first-principles pseudopotentials which allow obtain the dynamical matrix directly from set of wave vectors. The modeling of these structures is rather difficult because they have strong interlayer ion-covalent binding and weak electrostatic interlayer interaction.

The $In_xTl_{1-x}I$ SSS crystallizes in a layered orthorhombic structure with the space group of symmetry $D_{2h}^{17}$ (*Cmcm*).

The group theory analysis results in the following classification of the $In_xTl_{1-x}I$ lattice vibration modes in the $\Gamma$ point of the Brillouin zone:

$$\Gamma_v = 4A_g + 4B_{1g} + 4B_{3g} + 4B_{1u} + 4B_{2u} + 4B_{3u}.$$

The $B_{1u}$, $B_{2u}$ and $B_{3u}$ modes corresponding to the $T_Z$, $T_Y$, $T_X$ translations are acoustic. The twenty one optical modes correspond to normal vibrations, namely, the fully symmetrical ($4A_g$), external translation ($3B_{1u}$, $3B_{2u}$ and $3B_{3u}$), and close to libration ($4B_{1g}$ and $4B_{3g}$) ones.

The lowest-energy $B_{1g}$ mode is a bending mode, where the atoms move in the vertical and horizontal plane around the 90 degrees equilibrium position and thus it is expected have the lowest frequency. The next mode, $B_{3g}$, is a combination of stretching and bending. The first $A_g$ mode is a kind of torsional mode, where the distorted rhombus is twisted by the atomic movement. The other $A_{1g}$ mode is the only pure stretching mode. The other even-numbered modes as well as the infrared-active odd ones involve combinations of stretching and bending.

The phonons were calculated from optimized geometries of $In_xTl_{1-x}I$ by employing the linear response method. The exact phonon frequencies were obtained at all high-symmetry points of the Brillouin zone. The calculated frequencies are compared to Raman and infrared experimental data.

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# THE INFLUENCE OF COMBINATION OF DIFFERENT TYPES OF LOW-TEMPERATURE DEFORMATION ON STRUCTURE AND MECHANICAL PROPERTIES OF TITANIUM GRADE VT1-0

**Y. S. Osadchuk[1], N. A. Shulgin[2], A. A. Chupikov[2]**

*[1]V. N. Karazin Kharkiv National University,*
*Svobody Sq. 4, Kharkiv 61022, Ukraine*
*[2]National Scientific Centre Kharkiv Institute of Physics and Technology,*
*Academicheskaya 1, Kharkiv 61108, Ukraine*
*e-mail: osadchukevgeny@gmail.com*

It is known, that the physical and mechanical characteristics of metals and alloys, particularly strength, plasticity, degree of thermal stability are determined by the spectrum of defects of crystal lattice and their changes at different types of external actions. One of the methods of improvement of exploitative properties of metals and alloys is a method of thermomechanical processing. The main task of this processing is creating structures with high defect concentration of crystalline structure and receiving nanostructured states. Nowadays, the methods of severe plastic deformation (SPD) by torsion, rolling and drawing are used. The processing of metals by high hydrostatic pressure at cryogenic temperatures under hydrostatic compression method of quasi-hydroextrusion (QHE) is a perspective methods of receiving functional nanomaterials that have unique physical and mechanical properties.

Titanium and its alloys have a unique combination of physical and mechanical properties such as low density, high strength and plasticity, corrosion resistance in many hostile environments. An important feature of titanium is the ability to plastic deformation without disturbing the continuity of material in a wide temperature range including low temperatures.

In the article the physical and mechanical properties of commercially pure titanium grade VT1-0 after deformation by method of quasi-hydroextrusion and subsequent rolling at 77 K and 300 K were studied.

The structural research have shown that the deformation by hydrostatic compression method of quasi-hydroextrusion at 77 K depresses the process of twinning which is typical for deformation of titanium at low temperature (77 K) in case of uniaxial load. The influence of temperature on deformation by the method of quasi-hydroextrusion at 77 K is evident in formation of more powerful dislocation charges and higher concentration of these dislocation charges after deformation at 77 K.

It is shown that the microhardness is increases on 40% in comparison with the initial state after the deformation by the method of quasi-hydroextrusion at 77 K on 30%. The subsequent deformation by rolling at 77 K and 300 K further increases microhardness on 17% and 12% respectively. Electrical resistivity increases on 109% and 98% in comparison with the initial state after the deformation by the method of quasi-hydroextrusion at 77 K and subsequent rolling at 77 K and 300 K respectively.

# LOW TEMPERATURE MECHANICAL PROPERTIES OF THE $Ti_{30}Zr_{25}Hf_5Nb_{20}Ta_{10}$ HIGH ENTROPY ALLOY

**V. V. Voloschuk[1], E. D. Tabachnikova[1], A. V. Podolskiy[1], V. F. Gorban[2]**

*[1]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*[2]Frantsevich Institute for Problems of Materials Science NASU, 3, Krzhizhanovsky str., Kyiv, 03680, Ukraine*
*e-mail: valya93voloschuk@mail.ru*

The traditional technology for producing high-strength multi-component metal alloys is based on the use of one or two "basic" elements, to which a large number of alloying elements is added. Recently, a new class of multi-component metal alloys, called high-entropy alloys (HEA), due to higher values of the mixing entropy S mix, the value of which is within a 13- 19 J / mol K., attracted attention due to the unique combination of different physical properties, including mechanical.

The mechanical behavior of the $Ti_{30}Zr_{25}Hf_5Nb_{20}Ta_{10}$ high entropy alloy, which has the only solid solution bcc crystal phase, was examined in the temperature range of 4.2 – 300 K by uniaxial compression. Samples (3.7x2.2x1.8 mm) were deformed along the longest size with a strain rate of $2.7 \cdot 10^{-4}$ $s^{-1}$. From the experimental stress – plastic strain curves $\sigma(\varepsilon)$ the yield strength $\sigma_{0.2}$ and the maximal achieved strength $\sigma_{max}$ were determined. During the tests, the strain-rate sensitivity was measured by increasing the strain rate. Temperature dependences of the strain hardening, yield strength, ultimate strength, strain rate sensitivity and plasticity was measured and analyzed.

High yield strength of 1.1 GPa was registered at ambient temperature 300 K, which is probably associated with severe distortions of the crystal lattice due to presence of elements with different atomic radius in this multi-component alloy. Significant increase of strength was registered with decrease of compression temperature down to 4.2 K (1.9 times) indicating thermally activated type of plastic deformation. High plasticity (more than 30 % of plastic strain) is observed in temperature range of 77-300 K, at lower temperatures plasticity decreases down to 1 % at 4.2 K.

Peculiarities of microstructure, its impact on the low temperature mechanical characteristics and low temperature mechanisms of plastic deformation of the $Ti_{30}Zr_{25}Hf_5Nb_{20}Ta_{10}$ high entropy alloy are discussed.

# INFLUENCE OF PHYSICAL AND CHEMICAL PARAMETERS OF SOLIDS ON THE YIELD OF PARTICLES IN THE EXCITED

**I. S. Zelenina, V. V. Bobkov**

*Karazin Kharkiv National University, Svobody sq. 4, Kharkiv, 61022, Ukraine*
*e-mail: irs3359@mail.ru*

Ion bombardment of the solid surface of the particles is accompanied by the departure of the excited state, followed by the emission of electromagnetic radiation. This phenomenon is called the ion-photon emission (IFE) and is widely used as a base for the expansion of representations about the basic mechanisms of IFE, and for the development of analytical methods for the study of solids.

In this study we investigated the basic parameters of IFE (spectral composition, the quantum yield, the spatial distribution of the radiation) arising in the bombardment of $Ar^+$ ions and the surface of the yttrium and aluminum-yttrium garnets (YAG). The studies were conducted in a pilot plant that produces highlighted by mass $Ar^+$ ion beam with an energy of 20 keV and a current density of 15 mA* $cm^{-2}$. The emission spectra were studied in the wavelength range 250.0-800.0 nm.

In the spectrum of the radiation particles ejected from AIG, we observed lines emitted by excited atoms of aluminum, yttrium atoms and ions. In the spectrum of particles ejected from the metal yttrium, present atomic and ionic lines of yttrium. It is noted that the atomic line intensity distribution for the case of various yttrium YAG and Y. For spectral lines YI, emitted yttrium atoms excited in the low-lying excited states, there was a significant (2-3 fold) increase in the quantum yield values for comparison with a YAG and Y. For the spectral lines of the YI, due to transitions from the high-lying states of yttrium atoms practically not observed differences in the value of the quantum yield for the AIG case, and Y. in addition, in the spectra of YAG and Y attended a number of edges orange band system YO molecule.

The paper also evaluated the rate of knocked-out excited yttrium atoms. It was found that for the majority of the lines due to transitions from highly excited states, there was a two-speed part of reflected excited atoms of yttrium, "slow" particle energy from 100 - 300 eV and the "fast" - with the energy of more than 4 keV. At the same time, the lines due to the transitions of the low-lying states, the value of the kinetic energy of atoms of yttrium was a fraction eV for YAG and yttrium.

In summary, one can imagine the following action mechanisms of the excited states of atoms of yttrium under ion bombardment Y and AIG. The particles whose radiation caused transitions from highly excited states, embossing processes in multiple collisions with the incident ion and solid-state atoms of the cascade of collisions in solids. The radiation is very slow atoms in the low-lying states can be attributed to the collapse of the YO molecule excited by ion bombardment AIG and Y.

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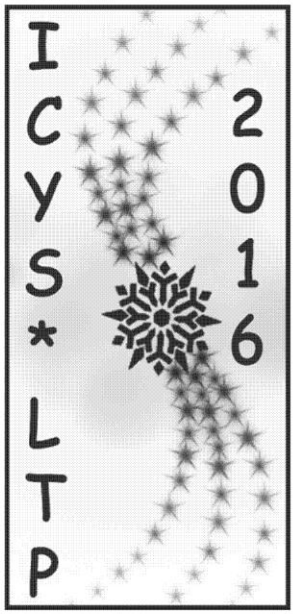
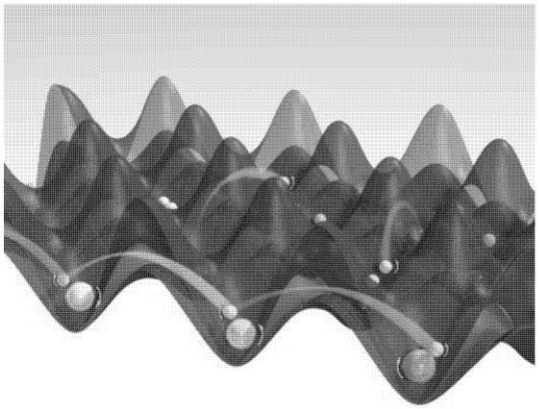
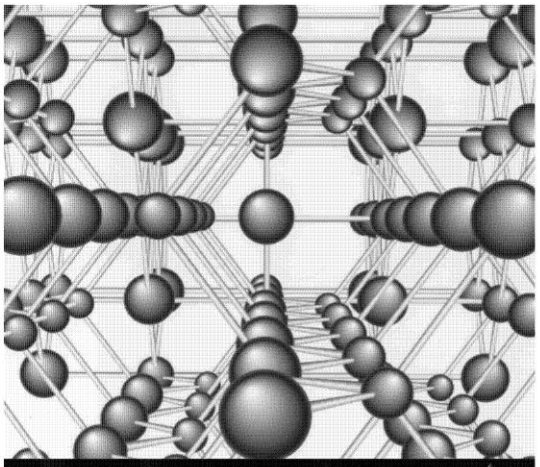
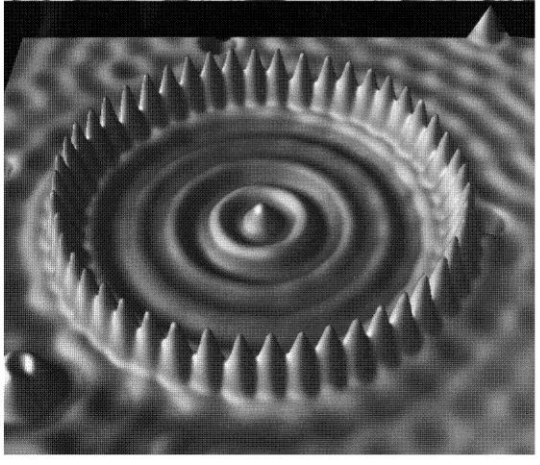
# Theory of Condensed Matter Physic







# ELECTROMAGNETIC WAVE ABSORPTION AND SURFACE PLASMON PROPAGATION IN A DOUBLE LAYER GRAPHENE SYSTEM WITH ELECTRON-HOLE PAIRING

**K. V. Germash, D. V. Fil**

*Institute for Single Crystals of NAS of Ukraine, Prospekt Nauky, 60, 61001 Kharkiv, Ukraine*
*e-mail: germash@isc.kharkov.ua*

In a double layer graphene system (DLGS), in which the graphene sheets are parallel and spatially separated, the electrons from one layer and the holes from the other layer may form electron-hole pairs [1,2]. We develop the approach based on the generalized Nambu formalism and calculate the gauge-invariant linear response functions. Basing on this approach we consider the influence of the electron-hole pairing on the absorption, reflection, and transmission of normally incident electromagnetic waves, and on the propagation of TM and TE surface plasmons.

It is shown that the pairing significantly changes spectral properties of a DLGS in the terahertz range. A sharp peak appears in the coefficients of reflection and absorption at the frequency equal to the gap in the energy spectrum. The coefficient of transmission has a deep minimum at the same frequency.

It was found that the pairing influences essentially the surface symmetric TM mode. This mode splits into the lower and the upper branches. The frequency of the lower branch lies inside the gap $2\Delta$ in the energy spectrum, and the frequency of the upper branch lies outside the gap. The lower branch is weakly damped, and the upper is strongly damped. The lower branch is thermally activated one: it exists only at nonzero temperature. Under increase in temperature the frequency of the lower branch grows up, and the range of wave vectors, in which the lower branch is weakly damped, expands.

It is shown that the pairing has a minor effect on the antisymmetric TM mode.

It is established that in the paired state the low frequency symmetric TE mode can propagate. In the normal state the frequency range of this mode is restricted from below by the inequality $\omega > 1.67\mu$, where $\mu$ is the chemical potential. In the paired state an additional frequency range $\omega_{min} < \omega < 2\Delta$ emerges. The lower edge frequency $\omega_{min}$ goes to zero at $T \to 0$.

In a DLGS with the electron-hole pairing the diamagnetic response is extremely small [3] and it cannot be used for registering the pairing. Another recently proposed method of registration of the electron-hole pairing [3] is based on the measuring the potential of the point charge located near the DLGS, but this method requires sensitive sensors of the electric field. The results presented in this report allows us to make the suggestion that a strong absorption and reflection of an incident electromagnetic wave at the frequency equal to the gap in the energy spectrum could be an indicator of the electron-hole pairing in a double layer graphene.

The strong temperature dependence of the spectrum of the symmetric TM mode could be used in graphene plasmonics for creating the transformation optic devices with a thermal control.

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# SHUTTLE INSTABILITY INDUCED BY TEMPERATURE GRADIENT

**O. A. Ilinskaya**

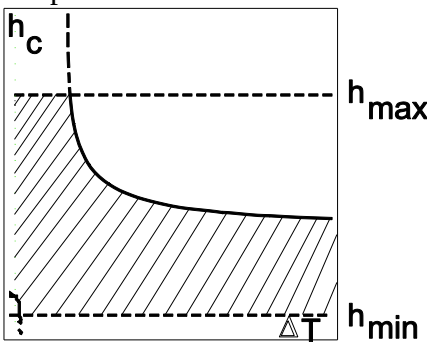
*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
*Prospekt Nauky, 47, 61103 Kharkiv, Ukraine*
*e-mail: ilinskaya@ilt.kharkov.ua*

We formulate a model of thermo-induced single-electron magnetic shuttling where thermoelectric and thermomechanic effects are crucial in magnetic shuttle instability. Thermoelectric effects are known to be important in solid state physics because they allow one to convert thermal energy into electric energy. For example, the temperature difference between two ends of a conductor induces an electric current in the closed circuit without voltage source [1].

Electron shuttling [2] appears due to inter-relation between electron tunneling and mechanical vibrations of a grain (quantum dot) in the gap between two electrodes. At certain conditions, electron tunneling in such a system leads to exponential increase of the dot oscillation amplitude. In the presence of dissipation, the system reaches a steady state, and electrons are mechanically ”shuttled” from source to drain electrodes by moving quantum dot. Such an oscillation regime is called shuttle instability and it is characterized by the current that is larger than ordinary tunnel current by several orders.

The motion of “electric” shuttle [3, 4] is impossible without voltage bias because instability is caused by electric forces. In “magnetic” shuttle [5] which has ferromagnetic leads the instability is caused by magnetic (exchange) forces between the electron spin and magnetic leads in the system. The voltage bias plays the role of an energy source. When electrons in the leads are fully [5] or partially [6] spin-polarized, the shuttle instability occurs only in the presence of an external magnetic field $H$. In these papers, the conditions of shuttle instability were obtained: $H<H_c$ ($H_c$ is critical magnetic field) for 100%-polarization and $H_{c1}<H<H_{c2}$ for partial polarization.

We put a question: is thermally driven magnetic shuttle possible? In our model the voltage bias equals zero, and temperature gradient is applied to the electrodes. We obtain dependence of critical magnetic field on temperature difference, $H_c$ ($\Delta T$), and the increment $r$ $(H, \Delta T)$ of the exponential growth of amplitude of shuttle oscillations as a function of magnetic field and temperature difference.




The dependence $h_c$ $(\Delta T)$ (for dimensionless parameters) is shown in the Figure. The shuttle domain (shaded) is restricted by two curves and two straight lines parallel to $\Delta T$-axis. The upper magnetic field $h_{max}$ $(\varepsilon_0)$ depends on the energy of electron level in the dot and the condition $h<h_{max}$ shows the validity of our approximation (non-resonant electron tunneling). The lower magnetic field $h_{min}$ is determined by the rate of dissipation $\gamma_f$ for quantum dot motion ($h_{min}$ $(\gamma_f \to 0) \to 0$).

Our work predicts a novel effect of thermomechanic shuttle instability which can occur in molecular transistors with spin-polarized electrons in external magnetic field.

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# OPTIMAL EFFICIENCY OF THERMOELECTRICS BASED ON THERMOMAGNETIC EFFECT IN TUNNELING OF SPIN-POLARIZED ELECTRONS THROUGH A QUANTUM DOT IN EXTERNAL MAGNETIC FIELD

**Yu. D. Zubov[1], O. A. Ilinskaya[2]**

*[1] V. N. Karazin Kharkiv National University, Svobody sq., 4, 61022 Kharkiv ,Ukraine*
*[2]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine, Prospekt Nauky, 47, Kharkiv 61103, Ukraine*
*e-mail: ilinskaya@ilt.kharkov.ua*

At present, solid state physics occupies an important place to explore the possibility to improve transistors. In this connection the question arises about the fabrication and application of molecular transistors. This problem is studied both theoretically (in different systems, see, e.g., [1]) and experimentally [2]. In single molecule transistors, the electron transport occurs through a molecule (quantum dot) which is tunnel coupled to the source and drain electrodes.

In our model, the quantum dot is coupled to two magnetic leads where electrons are partially spin-polarized. The source and drain electrodes have different chemical potentials (due to bias voltage) and are kept at different temperatures. An external magnetic field perpendicular to the magnetization of the leads is applied. When electrons in the electrodes are fully spin-polarized (what is the case of half-metals), the electron transport in this system is possible only in the presence of external magnetic field that induces spin precession. If spin polarization is partial, there are two electron transport channels, (i) "direct" (without spin-flip) and (ii) arising due to spin-flips caused by magnetic field.

We analytically calculated dependences of thermoelectric coefficients $G$, $S$, $K$ ($G$ is the electric conductance, $S$ is the thermopower, $K$ is the heat conductance) on the parameters of the system (external magnetic field, degree of spin polarization, molecule/electrode coupling energies $\Gamma_{S/D}$, and gate voltage). We found optimal conditions on model parameters under which the system attains the high thermoelectric efficiency.

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# INVESTIGATION OF STRUCTURAL AND ELECTRONIC PROPERTIES OF BN COMPOUND UNDER HIGH PRESSURE: AN AB-INITIO MOLECULAR DYNAMICS STUDY

**C. Kurkcu, H. Ozturk**

*Ahi Evran University, Faculty of Arts and Sciences, Department of Physics, 40200 Kirsehir, Turkey*
*e-mail: ckurkcu@ahievran.edu.tr*

The structural and electronic properties of the boron nitride (BN) are investigated in the generalized gradient approximation (GGA) of density functional theory (DFT) with the Perdew–Burke–Ernzerhof (PBE) functional. BN crystallizes in a hexagonal structure under ambient conditions. BN undergoes a structural phase transition from the hexagonal structure with space group $P6_3/mmc$ (No:194) to the wurtzite structure with space group $P6_3mc$ (No:186) [1,2]. This phase transition is also studied by total energy and enthalpy calculations. According to these calculations, we obtained this phase transition at about 31 GPa.

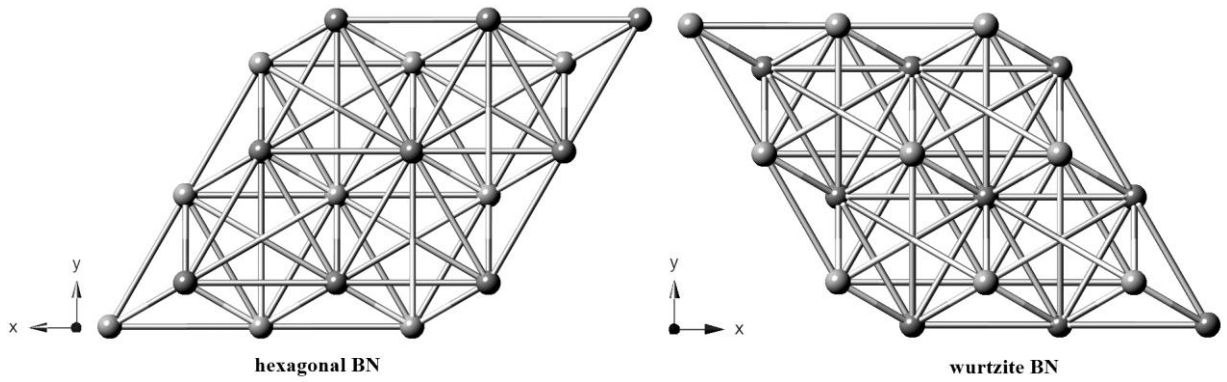


Figure 1. Crystal structures of BN.

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# JOSEPHSON EFFECTS IN ATOMTRONIC CIRCUITS

**O. Y. Matsyshyn[1], Y. M. Bidasyuk[2], M. Weyrauch[2], A. I. Yakimenko[1]**

*[1]Department of Physics, Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Str., 01601 Kyiv, Ukraine*
*[2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany*
*e-mail: oles.matshyshyn@gmail.com*

The dramatic progress of the field of Bose--Einstein condensates (BEC) of atomic gases continuing last two decades is driven by the combination of new experimental techniques and theoretical advances. BECs have become an ultralow-temperature laboratory for nonlinear physics, many-body physics and condensed matter physics, exhibiting superfluidity, quantized vortices, solitons, Josephson junctions and quantum phase transitions.

Electronics deals with the transport and interaction of electrical charges whereas atomtronic devices utilize neutral atoms, whose characteristics include an internal structure, tunable interactions and long coherence times. In the future it may be possible to fabricate atomtronic devices analogous to batteries, diodes and transistors, as well as fundamental logic gates. Nowadays, the effects, which are conventional in electronic devices, find their counterparts in BEC.

One of the most remarkable properties of superconducting devices is the existence of Shapiro resonances. If the external current consists of a dc contribution and a weak ac perturbation of frequency $\Omega$, the Josephson link displays a dc volt-ampere characteristic with voltage plateaus at the values satisfying the resonance condition $2eV = m\hbar\Omega$, where $V$ is voltage of the dc component, $2e$ is the Cooper pair charge, and m is an integer. The Shapiro steps in supecronducting Josephson link are used now to define a standard unit of voltage. In context of BEC, the ac-driven atomic Josephson devices could be used to define a standard of chemical potential [1]. However, due to inevitable technical problems, an experimental demonstration of the Shapiro steps in atomic BEC still is a challenging issue. The impressive achievements in atom circuit technology [2] have opened radically new directions for the quest of this fascinating effect in BEC.

Therefore, a tunable chemical potential difference between two weakly coupled condensates is the key feature required for observation of the Josephson effects. We perform a numerical simulation of the ring-shaped condensate with two moving barriers [3]. We analyze the mechanism of the transition of the condensate from the superfluid to the resistive regime. It turns out that the vortex excitations appear simultaneously with chemical potential difference for a squeezed in vertical direction potential trap. As the result, substantial fluctuations of the phase difference destroy coherence between subsystems of the atomic cloud. It is shown that the vortex excitations do not appear in elongated in vertical direction condensate, which implies the Josephson mechanism for formation of the chemical potential difference. Our theoretical results not only clarify the physical background for the experiments with Josephson effects in atomic BEC, but also suggest the parameters which can be used for observation of the Shapiro resonance in accessible atomtroinic circuits.

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# REALIZATION OF COMPOSITE FERMION TYPE (QUASI)PARTICLES BY DEFORMED FERMIONS. ENTANGLEMENT MEASURES

**Yu. A. Mishchenko, A. M. Gavrilik**

*Bogolyubov Institute for Theoretical Physics of NAS of Ukraine,*
*14b Metrolohichna Str., 03680 Kyiv, Ukraine*
*e-mail: mishchenko@bitp.kiev.ua*

The realization of composite (quasi)particles, particularly of composite fermions analogously to composite bosons [1], by deformed oscillators presents interest from the viewpoint of the effective description in more simple terms abstracting away from the internal structure details. In this work we construct [2] the operator realization of two-component composite fermions built of fermion and of either usual or deformed boson by deformed fermions. Thus, the composite fermion creation and annihilation operators ($a_\mu$, $b_\nu$ – constituent boson resp. fermion operators)

$$A_\alpha^\dagger = \sum\nolimits_{\mu\nu} \Phi_\alpha^{\mu\nu} a_\mu^\dagger b_\nu^\dagger, \qquad A_\alpha = \sum\nolimits_{\mu\nu} \overline{\Phi_\alpha^{\mu\nu}} b_\nu a_\mu$$

are modeled on the states by the fermionic ones for certain wavefunctions $\Phi_\alpha^{\mu\nu}$. The general solution for $\Phi_\alpha^{\mu\nu}$ was found in the case of non-deformed constituent boson, whilst for a deformed one only particular $\alpha = 1,2$ and $\mu,\nu = 1,..,3$ cases were treated. Like in the case of composite bosons [3], such entanglement measures as entanglement entropy and purity for the realized composite fermions were expressed through the parameters involved in matrices $\Phi_\alpha^{\mu\nu}$ and illustrated graphically [2].

The mentioned realization of composite fermion type (quasi)particles can be applied to an effective description of trions or baryons when two constituents form a bound state modeled by deformed boson.

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# MODELING OF KINETICS OF THE MATERIALS FRAGMENTATION MODES AT SEVERE PLASTIC DEFORMATION

**A. V. Khomenko, D. S. Troshchenko, I. O. Solonar**

*Sumy State University, 2, Rimsky Korsakov Str., 40007 Sumy, Ukraine*
*e-mail: o.khomenko@mss.sumdu.edu.ua*

Current technological process requires the production of metal goods, which have high physical and mechanical properties. The application of the methods of severe plastic deformation (SPD) allows to obtain the bulk metallic samples with almost pore-free submicrocrystal (SMC) or nanocrystal (NC) structure, which cannot be obtained by ordinary thermomechanical processing. The application of repeated plastic deformation of shear at the expense of heavy-loaded application in rather low temperatures conditions [1] is the base of SPD methods. As a result of such processing the crystalline grains are being fragmented and the SMC or NC structure with the large-angle of grain boundaries (up to 20°) is being formed.

Recently, the construction of the theoretical models allowing to describe the processes of microstructure grinding of metal at SPD acquires significant importance. As a result, the special approach within nonequilibrium evolutional thermodynamics is developed [2-4]. It helps to establish unambiguously the course of nonequilibrium processes (heating and defect generation) and transformation nature of internal energy during material processing. The introduced variables allow to reflect the specifics of structural defects formation and the accompanying processes of formation of limiting structure under the influence of SPD.

The phase diagram in approximation of a two-defect model is obtained. It sets the conditions of formation of various types of limiting structures under the SPD. The kinetics of the evolution of density of grain boundaries and dislocations at SPD is investigated in details. As the initial conditions, two basic cases are considered corresponding to the nonhardened metals or alloys and to the defectsfull materials, which have the high strengthening properties. It is shown that various types of stationary structures are formed depending on the values of shear strain and the initial states of the material. The defects density of these steady-states correspond to experimentally observed regularities (with the linear size of grains 100 nm and dislocations density within range of $10^{15} – 10^{16}$ $m^{-2}$). Moreover, the close interaction of the defects of different structure levels in the course of steady-states establishment is observed. It is revealed that nonequilibrium variables undergo structural and phase transition. As the result, the evolution of defects density performs sharp transition. It is established that formation of limiting structures is followed by both processes of dislocations accumulation and grains grinding on the one hand and annihilation of dislocations and grains growth on the other. Comparison of exact evolution of a defects' substructure to evolution of grain boundaries within the adiabatic approach is carried out. It shows a high convergence of the obtained results and confirms the rightfulness of its use in the previous calculations.

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# MODELING THE NOISE EFFECT ON ICE SURFACE PREMELTING DURING FRICTION

**A. V. Khomenko[1,2], B. N. J. Persson[2], M. A. Khomenko[1], S. V. Rudenko[1]**

*[1]Sumy State University, 2, Rimsky Korsakov Str., 40007 Sumy, Ukraine*
*[2]Peter Grünberg Institut-1, Forschungszentrum-Jülich, 52425 Jülich, Germany*
*e-mail: o.khomenko@mss.sumdu.edu.ua*

The studies [1-5] reveal that the stick-slip friction, i.e. inhomogeneous dependences of friction force on time and displacement, is inherent for ice dynamics. For example, interrupted rubbing is observed at friction of freshwater, granular ice and columnar, saline ice over themselves [1,2] and polymer (poly(methyl methacrylate) PMMA) on ice [3] for sliding velocities and temperatures in the ranges of $V = 10^{-6} – 10^{-1}$ m/s and $T = 173 – 270$ K. It is widely accepted that surface roughness ascents the real contact area due to interlocking of asperities and, consequently, increases friction. Besides, for our study it is significant that thickness of premelted ice layer decreases between asperities tips and it grows in places of cavities randomly [4]. Therefore the non-homogeneous distribution of thermal and elastic fields is realized. Research [5] demonstrates that due to the small system dimension the fluctuations widen the softened ice surface layer. In this study we found on the line that interrupted friction can occur at the expanse of shear strain, stress and temperature fluctuations in the ice surface layer.

The basic goal of the work is the research of the influence peculiarities of additive non-correlated fluctuations of thermal and deformational fields on the premelting of ice surface film. According to our approach the ice - softened ice transition is presented by shear strain appearance induced by heating of ice surface above critical value [6]. We assume that ice rubbing does not depend on the manner of loading, i.e., stiffness and mass of the contacting blocks [2], although the named dependence can change behavior of such systems. But, it is noteworthy that in our method the background ice temperature plays the role of the parameter of external influence. The phase diagrams are calculated where noises intensities of shear strain, stress and temperature and thermostat temperature define the regions of ice, softened ice, and their mixture. The domain of ice friction is shown to be bounded by relatively small background ice temperatures and fluctuations intensities of the stress and temperature. The growth of ice film's temperature noise can lead to increase or decrease rubbing dependently on the initial conditions, but the ascent of shear stress fluctuations results to growth of the premelting domain only. The ice layer softens with increase in the stress noise intensity even at small thermostat temperatures. Thus, regarded fluctuations cause the complication of softening process [6]. Besides, the offered model predicts opportunity to operate process of friction by means of creation of artificial mediums.

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# MAGNETIC AND MAGNETOCALORIC PROPERTIES OF FRUSTRATED SPIN CLUSTERS OF REGULAR TETRAHEDRA

**M. Mohylna[1,2], M. Žukovič [2]**

*[1] V. N. Karazin Kharkiv National University, Svobody sq., 4, 61022 Kharko ,Ukraine*
*[2]Institute of Physics, P.J. Šafárik University, Park Angelinum 9, 041 54 Košice, Slovakia*
*e-mail: mmogylnaya@mail.ru*

Frustrated magnetic systems have drawn considerable interest in the last decades due to their intriguing and often unexpected behavior. Among others, it has been shown that compared to ordinary nonfrustrated magnets they display enhanced magnetocaloric effect, which is related to the presence of a macroscopic degeneracy below the saturation field [1]. In particular, out of the studied systems the largest magnetocaloric effect was observed in a pyrochlore lattice antiferromagnet, which was also the system with the highest frustration.

More recent studies focused on investigations of the frustration effect in antiferromagnetic spin clusters, consisting of a finite number of spins [2-4]. Such spin clusters are useful in modeling of molecular nanomagnets and have the advantage of the possibility of the exact treatment. Those studies revealed various interesting aspects including the intriguing magnetocaloric properties that turned out to be rather sensitive to the cluster shape and size but in many cases superior to their thermodynamic limit counterparts in terms of the enhanced magnetocaloric effect.

In the present study we consider antiferromagnetic Ising spin clusters composed of a finite number of regular tetrahedra. The regular tetrahedra are building blocks of the pyrochlore lattice if arranged in a proper corner-sharing fashion but other packings in the three-dimensional space are also possible. Our aim is to study the effect of the cluster topology on thermodynamic and magnetocaloric properties of the system by considering clusters comprising a varying number of corner-sharing, edge-sharing and face-sharing tetrahedra.

Our results suggest that the cluster topology has a considerable influence on the magnetization and entropic processes in an applied magnetic field. The latter are studied both in the ground state as well as at finite temperatures by exact enumeration of density of states. In the ground state both the magnetization and entropy show cluster-size- and cluster-topology-dependent multiple plateaux of different heights and widths as functions of the applied magnetic field. At finite temperatures, isothermal entropy changes are found to be particularly pronounced and thus the magnetocaloric effect enhanced in the vicinity of the magnetization jumps at sufficiently low temperatures. Remarkably, for some clusters the entropy plateaux heights are not necessarily a non-increasing function of the field, as one might expect. We identify the spin-cluster systems that are promising for practical applications as magnetic refrigerators, based on their displayed magnetocaloric characteristics, such as the isothermal entropy and adiabatic temperature changes.

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# WEAK LOCALIZATION AND INTERACTION EFFECTS IN ACCEPTOR GRAPHITE INTERCALATION COMPOUNDS

**O. I. Prokopov[1], I. V. Ovsiienko[1], L. Yu. Matzui[1], T. A. Len[1], O. A. Brusylovets[2]**

*Taras Shevchenko National University of Kyiv, Departments of Physics[1] and Chemestry[2], Volodymyrska Str., 64/13, 01601 Kyiv, Ukraine*

Graphite intercalation compounds (GICs) are natural two-dimensional electronic systems in which carriers move mainly parallel to graphite layers. Possibility to change crystal structure and ordering degree of GICs with using different types of graphite matrix, different intercalates and different synthesis conditions makes the GICs an ideal model material for studying the physical properties of two-dimensional structures. The presented work is devoted to investigations of manifestation of quantum effects of weak localization and interaction in electrical conductivity of acceptor CICs.

The GICs based on anisotropic fine crystalline graphite (crystallite size $L_a$~20 nm, interplanar spacing $d_{002}$ = 0.34 nm) with nonmagnetic intercalates, such as iodine chloride, antimony chloride, aluminum chloride and bromine, were obtained with gas-phase manner by standard two-temperature method. The structure of obtained GICs specimens was determined by X-R diffraction. The resistivity of GICs was measured in temperature interval from 4.2K to 293K. Resistivity measurement error was 0.05%.

As shown by studies intercalation leads to a decrease of the resistivity and to change the resistivity temperature coefficient on the positive compared to the initial graphite. At the low temperature for all GICs specimens the minimum in the temperature dependence of resistivity is observed (Figure 1a). This minimum obviously is manifestation of quantum effect of weak localization and interaction of charge carriers. Analysis of low temperature addition to conductivity for all investigated GICs revealed its logarithmic dependence from temperature (Figure 1b). Such logarithmic temperature dependence of addition to conductivity is characteristic for the effects of weak localization and interaction of charge carriers in the case of two-dimensional system [1].

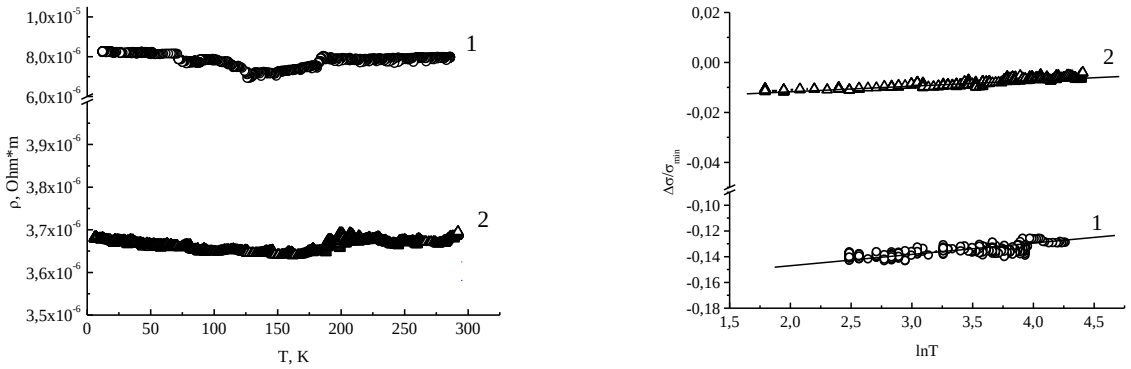



Figure 1. Dependences $\rho(T)$ (a) and $\Delta\sigma/\sigma_{min}$ (b) for GICs with bromine (1) and iodine chloride (2)

In terms of the model of effects of weak localization and interaction for two-dimensional systems temperature dependence of phase relaxation time, localization radius and charge carriers screening constant for all GICs are estimated. It is shown that for CICs based on fine crystalline graphite conductivity addition caused by mainly effects of charge carriers' interaction.

[1] L. Piraux, V. Bayot, J.-P. Michenaud, J.-P. Issi, Phys. Scripta 37(4), 942 (1988).

# INVESTIGATION OF STRUCTURAL AND ELECTRONIC PROPERTIES OF ZNO: A FIRST PRINCIPLES STUDY

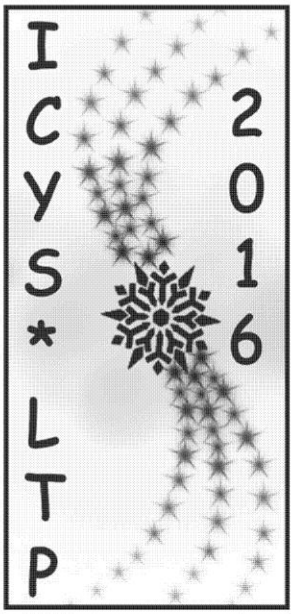
**C. Yamcicier[1], Z. Merdan[2], S. Yamcicier[3]**

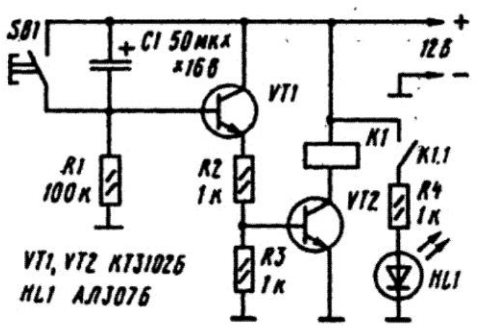
*[1] Gazi University, Institute of Science, Department of Physics, 06500 Ankara, Turkey*
*[2] Gazi University, Science Faculty, Department of Physics, 06500 Ankara, Turkey*
*[3] Ahi Evran University, Vocational School of Health Service, 40100 Kirsehir, Turkey*
*e-mail: cagatay1050@gmail.com*

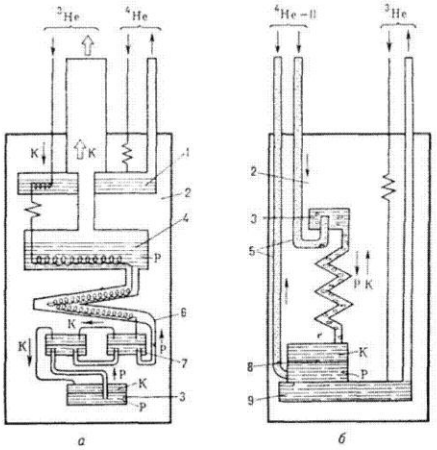
We report a structural study of Zinc Oxide (ZnO) under high pressure. Its crystal structure and electronic properties have been studied theoretically in the generalized gradient approximation (GGA) using density functional theory (DFT) method with the Perdew-Burke-Enzerhof (PBE) functional. We found that the phase transition sequence is wurtzite structure with space group $P6_3mc$ $\rightarrow$ cubic structure with space group $Fm\bar{3}m$ $\rightarrow$ another cubic structure with space group $Pm\bar{3}m$. This results obtained from our study are in good agreement with the results of Maouche et al. [1]. These phase transitions are also studied by total energy and enthalpy calculations.

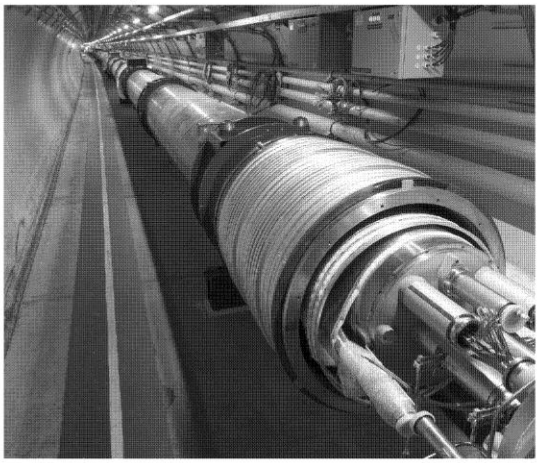
[1] D. Maouche, F. Saad Saoud and L. Louail, Materials Chem. and Phys. **106**, 11 (2007).

# Technologies and Instrumentation for Physical Experiments



# USING OPEN-HARDWARE FOR SCIENTIFIC RESEARCHES AUTOMATION

**A. V. Semchenkov[1], R. Vydro, P. Dmitryev[2]**

*[1] http://web-manufacture.net, Technical incubator,*
*30 Kamycheva, ap 14, Kharkiv 61038, Ukraine*
*[2]BoostLab.org, startup, laboratory equipment for education*
*e-mail: Azzzooo@gmail.com*

To automate the processing of the results of scientific experiments used a lot of private solutions, that are often poorly integrable among each other. In our country also imposed the problem of a lack of funding for the automation and integration with existing equipment. Developed in the Soviet Union automation systems are not widely spread, do not support common standards and are not always compatible with each other.

Many researchers continue to operate the most part of the work by hand. The use of automation would allow them to perform more experiments, to obtain more accurate results and spend less time on routine work.

Open-Source and Open-Hardware technologies have changed the general approach to automation and can be used to create an modern, integrated systems. We will talk about platforms Arduino, STM32 (ARM cortex), Raspberry PI, as well as projects based on them: RepRap, EasyCNC, RoboPlatform, etc. We will look how their use can simplify the daily work, and also will touch the possibility of integration with external systems.

The project RoboPlatform developed as part of our initiative http://web-manufacture.net that will allow you to use electronic management systems (on the basis of the decisions above), particularly without touching the programming, or using a modern development system in JavaScript and Python.

All solutions within the RoboPlatform have quite a low price that allows to use them in conditions of low funding. The project based on the principle of open source technology that makes it maximum cost effective for you.

On one of our installations, we carry out a study of the electric field anisotropy in the sample by mapping voltages with an accuracy of 0.01 mm without the participation of the experimenter.

# THE MAIN MECHANISMS OF THE CUTTING CBN TOOL WEAR

**K. V. Slipchenko**

*V.N. Bakul Institute for Superhard Materials of NAS of Ukraine,*
*Avtozavodskaya Str., 2, Kyiv 04074, Ukraine*
*e-mail: kateslipchenko@gmail.com*

The finish quality and cost of any product are closely related to the expenses on cutting tools, so the problem of increasing the tools service life has always been interesting for materials scientists. The cBN effectively works at high temperatures in the cutting zone, which define the allowable cutting speed, and has become widespread as a tool material for steel and alloys processing. Superhard cBN materials are obtained by synthesis at high temperatures and pressure. Among the main disadvantages of cBN tools are their bad resistance to oxidation and a strong chemical interaction with the processed material during cutting. The question of stability of the cutting tools with cBN, which affects the instrument lifetime and the cost of parts manufacturing, is of great interest for further investigation.

The cBN tools are used mainly for turning, drilling and milling of the hardened steel with a hardness of 55-68 HRC, speed steel, gray cast iron and high-temperature nickel- or cobalt-based alloys, the materials that are very difficult to process by hard alloys. The cBN is inert to iron and thermally stable at high temperatures [1], which makes it suitable for cutting materials in the situations where a cutting tool from diamond would start to react with the workpiece. In most applications a polycrystalline cubic boron nitride (PCBN), a composite of cBN and several other substances, is used. The PCBN materials are conventionally divided into two groups: high-cBN (more than 70%, BH group) and low-cBN (40-70%, BL group). The BH group materials are obtained by sintering the mixture of cBN with aluminum or transition metals under ultrahigh pressure conditions (more than 4 GPa) and characterized by a strong cBN frame.

During cutting, the processes of deformation, separation and friction are present in the cutting edge area. The main mechanisms of the cutting tool wear are adhesion, oxidation, abrasion, tribochemical reaction and surface damage. The tribochemical wear mechanism involves diffusion wear, dissolution wear, chemical wear and oxidation wear. High cutting temperatures stimulate rapid oxidation of the metallic transfer layers, the latter may be covered by a layer of surface oxide. When different types of oxides are present or forming, chemical reactions between them can occur, which leads to the formation of complex oxides, usually a spinel. Oxidation wear of fragments or irregularities can also result in the formation of solid oxide fragments that increase abrasion wear [2]. In 2007, French scientists from ENSAM compared the wear rate of the cutting tools made from known composites during finishing processing of superalloy Inconel 718.The results of this research indicate that the tools with ceramic binders (TiC, TiN or Ti) and cBN content below 65% have a longer lifetime, whereas combination of ceramic binders and high content of cBN (above 80%) has no positive influence on the service life of the tools. It is also found that the dominant mechanisms of wear during the cutting process are adhesion and diffusion due to a chemical affinity of the elements of workpiece and cutting tool [3]. At present time found of new binders such as nitrides and / or carbides of transition metals which can slow down diffusional wear and to prolong tool life. Experimental data will be presented on the conference

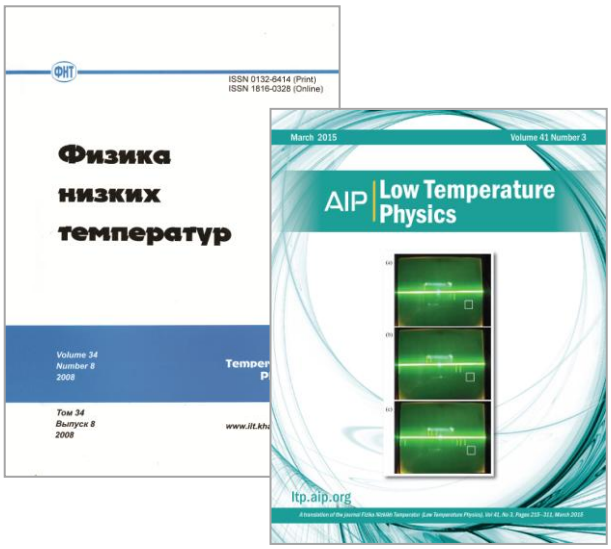
[1] Wentrof, R. H., DeVries, R. C. and Bundy, F. P. Sintered Superhard Materials Science, **208,** 4446, 873, (1980)

[2] Klocke F. Manufacturing processes 1, Sheet Metal Forming. Springer, Berlin, Heidelberg (2011)

[3] Costes J. P. et al. Tool-life and wear mechanisms of CBN tools in machining of Inconel 718 International Journal of Machine Tools and Manufacture, **47**, 1081, (2007)

# AUTHOR INDEX

# «FIZIKA NIZKIKH TEMPERATUR»




The monthly scientific journal Fizika Nizkikh Temperatur is a simultaneous Russian-English publication entitled Low Temperature Physics.
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Тел. (057) 766-47-10, 786-18-60

## Monday, 6 June

| | |
|---|---|
| 8:00-10:00 | Registration |
| 10:00-10:15 | Opening the Conference |
| 10:15-10:55 | **Plenary lectures** |
| 10:55-11:30 | *General photo and Coffee Break* |
| 11:30-13:15 | **Magnetism and Magnetic Materials** |
| 13:15-14:00 | Lunch |
| 14:00-15:20 | **Plenary lectures** |
| 15:20-17:05 | **Theory of Condensed Matter Physics** |
| 17:05-18:00 | Poster Session |

## Tuesday, 7 June

| | |
|---|---|
| 10:00-11:20 | **Plenary lectures** |
| 11:20-11:40 | *Coffee Break* |
| 11:40-12:55 | **Electronic Properties of Conducting and Superconducting Systems**<br>**Biophysics and Physics of Macromolecules** |
| 13:00-14:00 | Lunch |
| 14:00-15:00 | Lab Tour |
| 15:00-15:40 | **Plenary lectures** |
| 15:40-16:55 | **Electronic Properties of Conducting and Superconducting Systems**<br>**Biophysics and Physics of Macromolecules** |
| 17:00-18:00 | Poster Session |

## Wednesday, 8 June

| | |
|---|---|
| 10:00-11:20 | **Plenary lectures** |
| 11:20-11:40 | *Coffee Break* |
| 11:40-12:40 | **Materials Science** |
| 12:40-13:30 | Lab Tour |
| 13:30-14:00 | Lunch |
| 14:00-15:20 | **Plenary lectures** |
| 15:40-16:15 | **Materials Science** |
| 17:00-21:00 | ***Welcome Party*** |

## Thursday, 9 June

| | |
|---|---|
| 10:00-11:20 | **Plenary lectures** |
| 11:20-11:35 | *Coffee Break* |
| 11:35-13:20 | **Quantum Liquids and Quantum Crystals, Cryocrystals** |
| 13:20-14:30 | **Young Scientists Workshop** |
| 14:30-19:00 | Excursion to FELDMAN EcopArk |

## Friday, 10 June

| | |
|---|---|
| 10:00-11:20 | **Plenary lectures** |
| 11:20-11:40 | *Coffee Break* |
| 11:40-13:10 | **Optics, Photonics and Optical Spectroscopy**<br>**Nanophysics and Nanotechnologies** |
| 13:30-14:00 | Closing the Conference |
| 14:00-15:00 | Lunch |
| 15:00-16:00 | *Concert of Classical Music* |