Thermal Conductivity
International Advanced Research Workshop

International Advanced Research Workshop
"Thermal Conductivity of solid states
at low temperature"

in the frame of the II International
Advanced Study Conference
CONDENSED MATTER & LOW TEMPERATURE PHYSICS

CM&LTP – 2021
8 June 2021 | Kharkiv, Ukraine

Workshop Program

Book of Abstracts

Kharkiv 2021

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International Advanced Research Workshop "Thermal Conductivity of solid states at low temperature" in the frame of the II International Advanced Study Conference Condensed Matter and Low Temperature Physics 2021
CM&LTP 2021

Organised by B. Verkin Institute for Low Temperature Physics and Engineering (ILTPE) of NAS of Ukraine
8 June 2021 | Kharkiv, Ukraine

Official Partners NRFU

National Research Foundation of Ukraine is a state budgetary institution established by the Government of Ukraine in 2018 in accordance with the Law of Ukraine "On Scientific and Scientific-technical Activities". According to the legislation, the Foundation is a special instrument for the implementation of state policy. The Foundation funds the activities aimed at the all-round development of Ukrainian science as a major factor in the economic growth of the state. The activity of the Foundation is aimed at creating favorable conditions, that help citizens to realize their intellectual potential in the field of scientific and scientific-technical activity. The basic principles of funding and supporting grant-holders are competitiveness and scientific leadership.

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This book contain the abstracts of studies presented at the International Advanced Research Workshop "**Thermal Conductivity of solid states at low temperature**" in the frame of International Advanced Study Conference Condensed Matter and Low Temperature Physics 2021. The Workshop was organized with the support of NRFU project № 2020.02/0094 "Quantum tunneling of vibrational excitations in thermal conductivity of crystalline and amorphous materials and composites". These materials present the studies of modern aspects of condensed matter and low temperature physics and focused on the thermal phenomena in the solid states at low temperature including: Low temperature thermal properties of quasi - 1D and 2D crystals, Heat transfer in magnetic materials, . Collective excitations in molecular crystals and glasses, Heat phenomena in nanomaterials and material science, Thermal conductivity and quantum effects in solid states with different disorder.

The Workshop proceeding is published as a printed edition.

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FOREWORD

Dear Participants of the Conference,

On behalf of the Organizing Committee I am glad to welcome you to the II International Advanced Study Conference "Condensed Matter and Low Temperature Physics 2021" (CM&LTP – 2021) organized at the B.Verkin Institute for Low temperature Physics and Engineering (ILTPE) of the National Academy of Sciences of Ukraine (NASU), Kharkiv, Ukraine.

The CM&LTP – 2021 has evolved from the previous International Conference for Professionals and Young Scientists "Low Temperature Physics" (ICPYS LTP). Now, for recent 11 years, we have been enjoying the tradition of fruitful contacts among professional experts in the field of condensed matter and low temperature physics and young researchers – all this owing to the international conferences organized by the ILTPE.

The program of CM&LTP – 2021 covers all presently important experimental and theoretical aspects of condensed matter physics, including low temperature physics, superconductivity, magnetism, optics, nanophysics, biophysics, materials science and related areas. CM&LTP – 2021 is intended to be a platform for scientists to share their knowledge, to exchange new information and ideas, and to find collaborators and co-partners.

This scientific event offers broad opportunities for researchers engaged in academic and research institutions, as well as in industrial companies for exchanging information and launching cooperation. This will attract the attention of the young scientists of the region to multifaceted present-day solid state physics and its applications – this will encourage them to start a career as a researcher. A special lecture will be delivered concerning the problems of career promotion.

The Conference will host over 200 scientists from 25 countries, in particular from Austria, Algeria, China, Finland, France, Georgia, Germany, Israel, India, Japan, Kazakhstan, Latvia, Poland, Republic of Belarus, Romania, Russian Federation, South Africa, South Korea, Slovak Republic, Spain, Turkey, Ukraine, United Kingdom, United Arab Emirates and USA.

I hope you will gain unforgettable impression of our conference – its interesting high-quality scientific program, offered opportunities of meetings and discussions. And may the meetings be fruitful. Get the most of them!

Prof. Yurii Naidyuk
Director of B.Verkin Institute for Low Temperature
Physics and Engineering of the National
Academy of Sciences of Ukraine

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Co-chairs: Dr. Razet Basnukaeva & Dr. Maksym Barabashko
Secretary/Coordinator: Dr. Maksym Barabashko

Prof. Krivchikov A.I.
Prof. Konstantinov V.A.
Dr. Horbatenko Yu.V.
PhD Hurova D.E.

ABOUT INTERNATIONAL ADVANCED RESEARCH WORKSHOP "THERMAL CONDUCTIVITY OF SOLID STATES AT LOW TEMPERATURE"

Traditionally, B. Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine holds the wide-scope meetings in the field of condensed matter and low temperature physics. International Advanced Research Workshop "Thermal Conductivity of solid states at low temperature" – will be held on Tuesday 8 June 2021 in Kharkiv, Ukraine in the frame of the International Advanced Study Conference Condensed Matter and Low Temperature Physics 2021. The Workshop was organized with the support of NRFU project № 2020.02/0094 "Quantum tunneling of vibrational excitations in thermal conductivity of crystalline and amorphous materials and composites". These materials present the studies of modern aspects of condensed matter and low temperature physics and focused on the thermal phenomena in the solid states at low temperature including: Low temperature thermal properties of quasi - 1D and 2D crystals, Heat transfer in magnetic materials, . Collective excitations in molecular crystals and glasses, Heat phenomena in nanomaterials and material science, Thermal conductivity and quantum effects in solid states with different disorder.

The main aim of this event to create a platform for discussion and popularization of knowledge of theoretical and experimental results of the thermal conductivity of solids with the communication between the leading experts and researchers in this research field.

The B. Verkin ILTPE of NASU have a long history of study the thermal properties of molecular crystals since 1962. Unique experimental setups for the study of thermal properties, in particular, isochoric and isobaric thermal conductivity of solids was created in the Department of thermal properties and structure of solids and nanosystems. Scientific school of academician V.G. Manzheli of studing the thermal properties of solids states and nanomaterials was grew up and have achieved the significant scientific results during this long-term experimental investigations of low-temperature thermal properties and structure of solids.

Communication beetween researchers from different scintific centers and schools is the key point of the developing the successful colaboration network and exchange knowledge, search the new opportunities and strong integration of science and practical applications. The leading experts that take part in this event present the scintific centers from the next countries: Japan, Russia, Ukraine, Poland and Spain.

THE MISSION AND PURPOSE OF THE NATIONAL RESEARCH FOUNDATION OF UKRAINE

The National Research Foundation of Ukraine (hereinafter – the Foundation) is a state budgetary institution established by the Government of Ukraine in 2018 in accordance with the Law of Ukraine "On Scientific and Scientific-technical Activities". According to the legislation, the Foundation is a special instrument for the implementation of state policy. The Foundation funds the activities aimed at the all-round development of Ukrainian science as a major factor in the economic growth of the state. The activity of the Foundation is aimed at creating favorable conditions, that help citizens to realize their intellectual potential in the field of scientific and scientific-technical activity. The basic principles of funding and supporting grant-holders are competitiveness and scientific leadership.

THE MAIN OBJECTIVES OF THE FOUNDATION ARE:

1. stimulation of fundamental and applied scientific researches, development of the national research area and its integration into the world research area;
2. development of research infrastructure in Ukraine and its integration into the world research infrastructure;
3. promotion:
1) establishing scientific and technical cooperation between scientific institutions, higher education institutions and representatives of the manufacture and service sectors;
2) international exchange of information and scientists, involvement of student and student youth in scientific and scientific and technical activities;
3) production-oriented (branch) scientific institutions by organizing competitions at the request of central executive bodies or other customers, provided that such central bodies of executive power or the customers of the corresponding funds are allocated;
4. popularization of scientific and scientific-technical activity.

Using such kind of approach for science promoting as a science grants helps to concentrate an active and productive part of researchers and scientists around the most important and actual tasks of modern science.

https://nrfu.org.ua/en/about-us/the-mission-and-purpose-of-the-foundation/

INTERNATIONAL ADVANCED RESEARCH WORKSHOP "THERMAL CONDUCTIVITY OF SOLID STATES AT LOW TEMPERATURE"

CONFERENCE HALL **8 JUNE 2021**

Co-chairs: Dr. Razet Basnukaeva & Dr. Maksym Barabashko

9:00 -9:15 **Opening Ceremony**

9:15 -9:45 **Keynote talk: Heat transfer in molecular crystals and their solutions above or of the order of Debye temperature**
V.A. Konstantinov
B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,47 Nauky Ave., Kharkiv, 61103, Ukraine **11**

9:45-10:00 **Thermal activation heat transfer in dynamically disordered phases of molecular crystals. Ethane series freons.**
A.V. Karachevtseva, V.A.Konstantinov, A.I. Krivchikov, V.V. Sagan.
B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,47 Nauky Ave., Kharkiv, 61103, Ukraine **12**

10:00-10:15 **Features of transport processes in an electroconsolidated FeNi composite**
G. Ya. Khadzhay[1], S. R. Vovk[2], R. V. Vovk[1], E. S. Gevorkyan[1], N. S. Zubenko[1], M.V. Kislitsa[1], V. O. Chishkala[1], A. Feher[2], P. Kollar[2], J. Fuzer[2]
[1] V.N. Karazin Kharkiv National University, Kharkiv 61022, Ukraine
[2] Centre of Low Temperature Physics, Faculty of Science, P.J. Šafárik University, Košice 04154, Slovakia **13**

10:15-10:45 **Keynote talk: Thermal Conductivity of Organic Charge Transfer Complexes with Strong Correlation in 2D π-Electrons Layers**
Y. Nakazawa, T. Nomoto, L. Zhang, S. Yamashita and H. Akutsu
Dept. of Chemistry, Graduate School of Science, Osaka University, Machikaneyama 1-1, Toyonaka, Osaka 560-0043, Japan **14**

10:45-11:00 **Thermophysical and electrophysical characterization of exfoliated graphite - carbon nanotube composites**
N.V. Morozovsky[1], Yu.M. Barabash[1], G.I. Dovbeshko[1], Yu.V. Grebelna[2], M. T. Kartel[3], Yu.I. Sementsov[3], J. Macutkevic[4], J. Banys[4]
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[2]TM Spetsmash ltd., 02094, Viskozna str., 5, Kyiv, Ukraine
[3]O. Chuiko Institute of Surface Chemistry, NAS of Ukraine, 03164, Kyiv, Ukraine
[4]Faculty of Physics, Radiophysics Department, Vilnius University,Sauletekio 9/3, 10022, Vilnius, Lithuania
15

11:00-11:15 **Calculations of thermal gradients in hydroxyapatite composite with the additives of multi-walled carbon nanotubes**
A.E.Rezvanova[1], A.N.Ponomarev[1], M.S.Barabashko[2], M.V.Tkachenko[3], B.S.Kudryashov[4]
[1]Institute of Strength Physics and Materials Science of SB RAS, 2/4 Akademichesky Ave., Tomsk, 634055, Russia
[2]B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,47 Nauky Ave., Kharkiv, 61103, Ukraine
[3]V.N. Karazin Kharkiv National University, 4 Maidan Svobody, Kharkiv, 61077, Ukraine
[4]National Research Tomsk Polytechnic University, 30 Lenin Ave., Tomsk, 634050, Russia **16**

11:15-11:45 **Keynote talk: The influence of diffusive phonon boundary scattering on the thermal conductivity of a two-dimensional sample**

J. Amrit[1], K. Nemchenko[2], T. Vikhtinskaya[2]
[1]*LIMSI-CNRS, Université Paris Saclay, 91405, Orsay, France*
[2]*V.N.Karazin Kharkiv National University, 61022, Kharkiv, Ukraine*

17

11:45-12:00 **Disorder-induced localized low-energy tunneling states in the carbon nanomaterials**

A.N. Ponomarev[1], A.E. Rezvanova[1], M.S. Barabashko[2]
[1]*Institute of Strength Physics and Materials Science of SB RAS, Tomsk, 634055, Russia*
[2]*B.Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,47 Nauky Ave., Kharkiv, 61103, Ukraine*

18

12:00-12:15 **Resonance levels in electron and phonon spectra of graphene nanostructures: formation, decay, possibility of HTS appearance**

S. Feodosyev[1], **I. Gospodarev**, V. Sirenko[1], E. Syrkin[1], I. Bondar[1] and K. Minakova[2]
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[2] *National Technical University "Kharkiv Polytechnic Institute", 2 Kyrpychova str., Kharkiv, 61002, Ukraine*

19

12:15-12:30 **Thermally activated conductivity of molybdenum disulfide MoS_2 nanopowder**

R.M. Rudenko[1], O.O. Voitsihovska[1], G.I. Dovbeshko[1], V.M. Poroshin[1]
[1]*Institute of Physics, NAS of Ukraine, 46 avenu Nauky, 03680, Kyiv, Ukraine*

20

12:30-13:00 **Cofe-break/Lunch Time**

13:00-13:30 **Keynote talk: Thermal conductivity of solid state laser materials: ceramics of YbAG and GAGG**

Daria Szewczyk
Institute of Low Temperature and Structure Research PAS, Division of Low Temperature and Superconductivity, Okólna 2, 50-422 Wrocław, Poland

21

13:30-13:45 **Temperature Dependence of the Thermal Conductivity in SiO_2 with Disorder Due to Embedded Ge Nanoparticles**

V. Shmid, V. Kuryliuk, A. Nadtochiy, O. Korotchenkov
Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Street, 01601 Kyiv, Ukraine

22

13:45-14:00 **Electronic thermal conductivity of single and bilayer graphene with disorder**

N. Bobenko[1], V. Egorushkin[1], N. Melnikova[2]
[1]*Institute of Strength Physics and Materials Science of SB RAS, 2/4 Academichesky Avenue, Tomsk 634021, Russia*
[2]*National Research Tomsk State University, Lenin street, 36, Tomsk 634050, Russia*

23

14:00-14:30 **Keynote talk: Low Thermal Conductivity and the Evidence of the Glassy Behavior in $(Pb_{0.7}Sn_{0.25}Ge_{0.05})_2P_2S_6$ and $(Pb_{0.7}Sn_{0.25}Ge_{0.05})_2P_2Se_6$ Mixed Crystals**

I. Zamaraite[1], V. Liubachko[2,3], R. Yevych[2], A. Oleaga[3], A. Salazar[3], A. Dziaugys[1], J. Banys[1], Yu. Vysochanskii[2]

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[3]*Departamento de Fisica Aplicada I, Escuela de Ingenieria de Bilbao,Universidad del Pais Vasco UPV/EHU, Plaza Torres Quevedo 1, 48013 Bilbao, Spain*

24

14:30-14:45 **Influence of Chemical Substitution on the Thermal Transport Properties in 2D layered $M^{1+}M^{3+}P_2X_6$ (M^{1+} = Cu, Ag; M^{3+} = In, Bi; X = Se, S) Compounds**

V. Liubachko[1], A. Oleaga[2], A. Salazar[2], K. Glukhov[1], A. Kohutych[1], A. Pogodin[1], Yu. Vysochanskii[1]

[1]*Institute for Solid State Physics and Chemistry, Uzhhorod University, Pidgirna Str. 46, 88000 Uzhhorod, Ukraine*

[2]*Departamento de Física Aplicada I, Escuela de Ingeniería de Bilbao, UPV/EHU, Plaza Ing. Torres Quevedo 1, 48013 Bilbao, Spain*

25

14:45-15:00 **Analysis of thermal conductivity for clathrate thermoelectrics**

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

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

26

15:00-15:30 **Keynote talk: Thermal anomalies in ordered and disordered phases**

J.F. Gebbia[1], A.I. Krivchikov[2], C. Cazorla[1], O.A. Koroyuk[2], Y. Miyazaki[3], M. Nakano[3], J. Ll.Tamarit[1]

[1]*Grup de Caracterizació de Materials,Departament de Física, EEBE and Barcelona Research Centerin Multiscale Science and Engineering, Universitat Politècnica de Catalunya, Barcelona 08019, Catalonia*

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

[3]*Research Center for Thermal and Entropic Science, Graduate School of Science, Osaka University, Toyonaka 560-0043, Osaka, Japan*

27

15:30-15:45 **Electrophysical properties of aqueous colloidal solutions of C_{60}**

R.M. Basnukaeva, A.V. Dolbin, N.A. Vinnikov, A.M. Plohotnichenko, V.B. Esel'son, V.G. Gavrilko, S.V. Cherednychenko

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28

15:45-16:00 **Heat capacity and thermal expansion for ordered and disordered crystal materials**

M.S Barabashko, R.M. Basnukaeva, A.I. Krivchikov

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

29

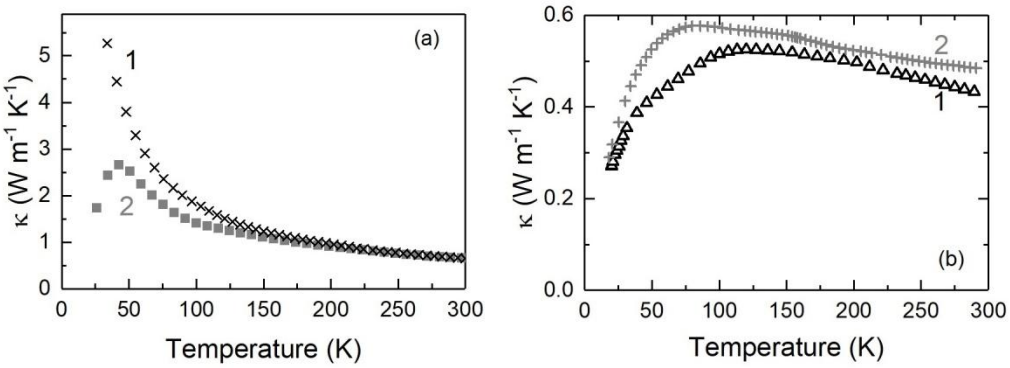
16:00-16:30 **Generalized analysis of thermal conductivity for molecular solids**

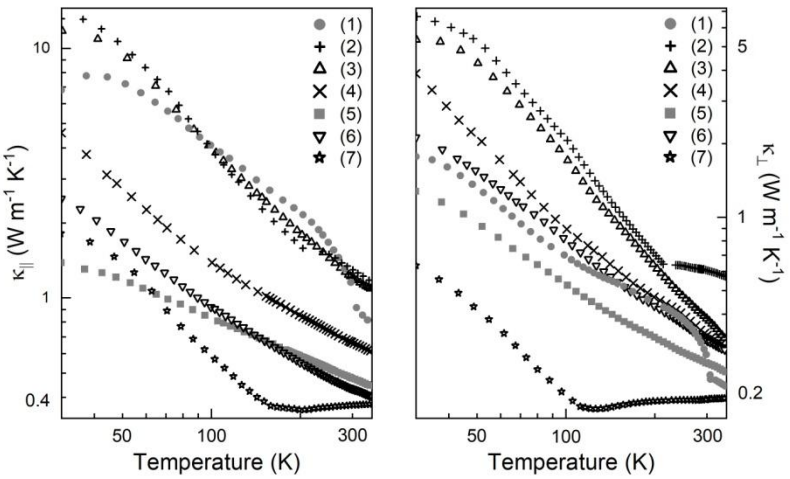
Yu.V. Horbatenko, A.I. Krivchikov

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

30

KEYNOTE LECTURES OF EXPERTS AND RESEARCHERS CONTRIBUTED PAPERS





Heat transfer in molecular crystals and their solutions above or of the order of Debye temperature.

V.A. Konstantinov

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In this short review the specific details of heat transfer in solidified inert gases, simple molecular crystals like N_2, freons of methane and ethane series, simple *n*-alkanes, heterocyclic hydrocarbons, number of another molecular crystals and their solutions at temperatures above or of the order of Debye temperature ($T \geq \Theta_D$) are summarized. It is shown that in orientationally ordered phases of molecular crystals the heat is transferred both phonons and diffusive modes, and thermal conductivity obey the law $\kappa = A/T + B$, where B is constant.

In the dynamically orientationally-disordered (DOD) phases of molecular crystals the isochoric thermal conductivity increases with rise of temperature, similar to how it occurs in amorphous and glass-like substances above the plateau. Earlier the anomalous increase in isochoric thermal conductivity in the DOD phases of molecular crystals was qualitatively explained by the weakening of phonon scattering on rotational excitations of molecules as the correlations of their rotational motion decay [1]. In this review, an alternative mechanism is considered when the effect observed can be described by the hopping thermal activation mechanism, with constant activation energy and a pre-exponential factor depending on the density [2].

The behaviour of isobaric and isochoric thermal conductivity in molecular crystals differs greatly at high temperatures since isobaric thermal conductivity depends on both temperature and molar volume: $\kappa = \kappa(T, V_m(T))$. The Bridgman coefficient $g = -(\partial \ln\kappa / \partial \ln V)_T$, which determines the degree of volume dependence, varies between 4÷8 for most molecular crystals [1].

[1] V.A. Konstantinov, Heat Transfer in Molecular Crystals, in: A. Belmiloudi (Eds.), Heat Transfer - Theoretical Analysis, Experimental Investigations and Industrial Systems, InTech Open Access Publisher (2011) 157-188.
[2] V.A. Konstantinov, A.I. Krivchikov, A.V. Karachevtseva, V.V. Sagan, Solid State Comm. 329, 114241 (2021).

Thermal activation heat transfer in dynamically disordered phases of molecular crystals. Ethane series freons.

A.V. Karachevtseva, V.A.Konstantinov, A.I. Krivchikov, V.V. Sagan.

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The intensive development of the physics of disordered state leads to reconsidering crystalline state concepts. A wide range of practical applications characterizes such disordered states of molecular crystals. One of the most sensitive tools for studying the nature and character of disorder in solids is isochoric thermal conductivity. This method make possible to obtain the dependence of thermal conductivity on temperature for samples with various densities at constant volume.

This work is dedicated to experimental investigation of isochoric thermal conductivity of a molecular crystal of 1,1-difluoroethane (Freon F-152a). Isochoric thermal conductivity was studied for three samples with different molar volumes (V_m = 49.2, 50.25, and 51.5 cm^3/mole) in a dynamically oriented disordered phase.

The thermal conductivity increased with temperature, similar to how it occurs in amorphous and glass-like substances above the plateau area. It is found that this behavior can be described by a thermo-activation mechanism with constant activation energy and density-dependent pre-exponential factor.

The Bridgman coefficient , which characterizes the degree of dependence on the molar volume is determined by the coefficient, is 6.0 ± 0.5 was found from experimental data.

Moreover, a comparison is made with thermal conductivity of other representatives of ethane series freons: F-112, F-113 [1], F-116 [2] and SF_6 [3].It has been found that the thermal conductivity of a number of other molecular crystals with a random disordered orientation can be described in a similar manner.

[1] Jezowski A., Strzhemechny M. A., Krivchikov A. I., Pyshkin O. S., Romantsova O. O., Korolyuk O. A., Zloba D. I., Horbatenko Yu. V.,. Filatova A, AIP Advances. 9, 015121 (2019).
[2] Konstantinov V.A., Revyakin V.P., Sagan V.V., Low Temp. Phys. 33, 1048 (2007).
[3] Konstantinov V.A., Manzhelii V.G., Smirnov S.A., Sov. J. Low Temp. Phys. 18, 902 (1992).

Features of transport processes in an electroconsolidated FeNi composite

G. Ya. Khadzhay [1], S. R. Vovk [2], R. V. Vovk [1], E. S. Gevorkyan [1], N. S. Zubenko [1], M.V. Kislitsa [1], V. O. Chishkala [1], A. Feher [2], P. Kollar [2], J. Fuzer [2]

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The production of new polyfunctional materials with specified magnetoresistive characteristics is one of the main areas of research in modern solid-state physic [1, 2]. Transport properties of these materials, such as electrical and thermal conductivity, are especially interesting, particularly at low temperatures, where the temperature dependence of the electrical resistivity is determined by the scattering of electrons by phonons, defects, electrons and magnons, while the temperature dependence of thermal conductivity is primarily determined by the scattering of heat carriers – electrons and phonons – on defects and on each other.

This article is devoted to the study of electrical and thermal conductivity of a Fe–Ni metal composite obtained by the electroconsolidation, in the range 4.2–300 K.

The samples were obtained from nickel and iron powders by a 10 min electroconsolidation at temperature of 1100°C, pressure 35 MPa and current ~5 kA. Such technologies are effective for compacting powders, especially difficult-to-sinter materials and compounds. This approach provides a high-density and finely dispersed structure of the resulting material [3].

It was found that the electrical and thermal conductivity of the electroconsolidated sample is significantly higher than that of samples with the same composition, obtained by melting. The thermal conductivity in the residual resistivity region ($T \leq 25$ K) is proportional to temperature, $\lambda_e(T) \sim T$. This behavior of the studied quantities indicates electronic heat transfer, which is characterized, in this temperature range, by the elastic scattering of electrons by impurities and other defects. In this case, the Wiedemann–Franz–Lorentz law [4] is satisfied. At high temperatures elastic scattering of electrons by phonons is predominant, $\rho(T) \sim T$, $\lambda_e(T) \approx$ const. The resistivity as a function of temperature for the equiatomic Fe–Ni system and Fe and Ni metals can be approximated with a high degree of accuracy ($\Delta\rho/\rho \leq 1\%$) by (1), over the entire investigated range of 4.2–300 K.

$$\rho(T) = \rho_0 + \rho_{ph}(T) + b_0 T^2 \quad (1)$$

here, ρ_0 is the residual resistivity associated with electron scattering on defects and $\rho_{ph}(T)$ is the resistivity due to the scattering of electrons by phonons (intraband s-s scattering of electrons and the interband s-d scattering characteristic of transition metals, their alloys, and compounds [5, 6]). The term $\sim T^2$ in the Fe–Ni system is caused by the interference between inelastic scattering of electrons by phonons and elastic scattering of electrons on boundaries and defects.

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Thermal Conductivity of Organic Charge Transfer Complexes with Strong Correlation in 2D π-Electrons Layers

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To measure temperature and magnetic fields dependences of the thermal conductivity is widely required in the field of physics and chemistry of condensed matters, since heat transport phenomena are related to the micrscopic features and interaction of mobile electrons and phonons. The novel quantum mechanical features occurs in materials with complicated structures and electronic properties are discussed extensively in terms of heat transport experiments. It is especially the case for molecule-based compounds such as donor/acceptor charge transfer salts, metal assembly complexes, coordinated polymer compounds, since they usually obtained as multi-components and grown as small pieces crystals or powder from chemical solutions. With the aim at perfoming tiny single crystal thermal conductivity measurements for these compounds, we have newly constructed a thermal conductivity measurement system consisiting of a small chip type sensor, heater and thin wires. [1] The steady state tecnnique to get thermal gradient in the single crystalline samples was used to determine absolute values of κ with high precision. The system enables us to measure the thermal conductivity κ(T) of a sample with the length of 0.5mm or less in the wide temperature range between 250K and 0.5K.

By using this system, we have performed systematic thermal conductivity measurements for small single crystals of charge transfer complexes consisting of organic donors/ acceptors with their counter-ions. Firstly, we report the results of well-known organic conductor α-(BEDT-TTF)$_2$I$_3$ which show metal-insulator transition due to electron correlations of π-electrons. Rather large change of thermal conductivity was detected as the sudden drop of κ(T) at TMI=135K. Below the TMI, the temperature dependence of κ(T) follows the temperature dependence of typical insulators and forms the peak structure around 20K. Furthermore, in the measurement of an organic conductor κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br and θ-(BEDT-TTF)$_2$I$_3$, we succeeded in detecting the superconductor transition as increment of κ(T) at the critical temperature Tc=11.4 K. We also report a drastic magnetic-field dependence of thermal conductivity due to the suppression of the superconducting state by external magnetic fields applied perpendiculary to the conducting layers. [1] The effects due to the coupling of charge and lattice degrees of freedom can be considered as the origin. The discussion on the phonon structures of charge transfer complexes is extended to the systems whcih shows anomalous quantum liquid like features due to the strong charge fluctuations and spin fluctuations [2]. In these systems, we have observed that the charge-phonon and spinphonon couplings at low energy region induce a kind of disorder feature in the acoustic phonon modes even in the periodic crystals and glassy states of phonon are induced by the strong electron correlation mechansim.We discuss the possible origin of these glass formers and a tuning possiblity of low energy phonon states through chemical substitution or external pressures.

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Thermophysical and electrophysical characterization of exfoliated graphite - carbon nanotube composites

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Nowadays the carbonaceous materials possess a large application area – from nano-technologies (e.g. as high conductive AFM-tip), thermal imaging (e.g "black coatings" of IR-detectors), bio-sensorics and medicine (as gas adsorbents) to chemical industry (sensors and reaction nano-vessels) and thermal management, including aerospace and spacecraft.

The exfoliated graphite (EG) - carbon nanotubes (CNT) composites (EG-CNT) were synthesised by persulphate oxidation method using chemical and electrochemical (anodic) oxidation, and sheet samples were obtained by roll rolling of prepared EG-CNT powder [1].

For EG-CNT, the heat pulse (500 ms) and thermo-wave (20 Hz modulation) methods were applied to estimate the effective values of diffusivity $a_T = k_T/C_T$ and effusivity $b_T = (k_T C_T)^{1/2}$ (k_T is the thermal conductivity, C_T is the volume heat capacity).

Obtained a_T values are ~ (10^{-5} - 10^{-4}) m^2/s and b_T values are ~ (10^3 - 10^4) $Ws^{1/2}/m^2K$. The a_T values for EG-CNT are less than a_T values for CNT-rope (~ 10^{-3} m^2/s) [2] and are higher than a_T values for the bulk CNT-mats (≈ $10^{-6}\cdot m^2/s$) estimated using the data [2], and lie in the range limited by a_T values known for multiwall CNT sheets [3] in the directions perpendicular (~$\cdot 10^{-5}\cdot m^2/s$) and parallel (~$\cdot 10^{-4}\cdot m^2/s$) to the CNT alignment in the sheets. Such ratios of the values of a_T are associated with different values of thermal resistance in the areas of point and extended thermal contacts of various types of components in carbon-carbon composites.

For TEG-CNT, in the range of sound (SF) and low radio frequencies (RF) 10 Hz ≤ f ≤ 1 MHz, the frequency dependences of the electrical conductivity σ(f) were obtained and in the microwave frequency (MWF) range 24 ≤ ν ≤ 40 GHz the frequency dependences of the real ε'(ν) and imaginary ε"(ν) components of the complex permittivity ε* = ε - iε" were obtained.

In the SF range, with a frequency increase from 10 Hz to 10 kHz, the dependences σ(f) are almost flat and σ value lies between ≈ 60 S/m and ≈ 130 S/m for different EG-CNT samples. In the RF range, for f > 100 kHz the value of σ decreases significantly (by ≈ 30%), and the dependences of σ(f) are approximated by an exponential decrease slightly better than a polynomial one. In the MWF range, with increasing v there is a close to linear decrease of ε' from 40 to 20, and ε" decreasing from 4 to 1 has a minimum (≈ 2) near 27 GHz and a maximum (≈ 2.8) near 29 GHz and looks as Fano-type antiresonance-resonance.

The noted features of the behaviour of σ(f) in the SF and RF ranges, as well as ε'(v) and ε"(v) in the MWF range, can be associated with the specificity of the electrical transport between the EG-CNT species and particularity of their point and extended defects.

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Calculations of thermal gradients in hydroxyapatite composite with the additives of multi-walled carbon nanotubes

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Calculations of thermal diffusivity and the analysis of temperature gradients in composite ceramics based on hydroxyapatite (HA) with additives of multi-walled carbon nanotubes (MWCNTs) is carried out. The concentration of nanotubes was varied in the range 0 - 0.5 wt%. HA is a bioactive matrix, while MWCNTs additives can improve the mechanical properties of ceramics. In particular, the additives of MWCNTs lead to the unique electrical, thermal, and mechanical properties of composite materials [1,2]. X-ray diffraction studies of ceramics indicate that the presence of macrostresses in the sample of HA ceramics due to its low thermal diffusivity. MWCNT additives reduce temperature gradients during sintering of the composite due to the better thermal diffusivity of composite with additives of MWCNTs.

The dependence of the temperature difference between the surface Ts and the center of the sample Tc are calculated by eq:

$$\Delta T = T_s - T_c \approx 0.25 \frac{R^2}{\alpha} \frac{\partial T}{\partial \tau},$$

where R is radius of cylindrical samples and α – thermal diffusivity.

Increase of the temperature difference between the surface and the center of the HA ceramic sample occurs during heating of the ceramic on the first stage of sintering. It is observed due to the change of thermal diffusivity of HA with increasing the temperature [3]. The surface of the samples is heated faster than the central part. Therefore, the surface of the material expands faster and experiences compressive stresses.

It was found that HA ceramics has higher macrostresses than in the case of HA ceramics with the additives of MWCNTs. HA ceramics have low thermal diffusivity and the temperature gradients occur during heterogeneous heating/cooling of different parts of ceramics at sintering. The additives of MWCNTs allow to increase the thermal diffusivity and reduce internal residual macrostresses in the HA-MWCNTs ceramics.

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The influence of diffusive phonon boundary scattering on the thermal conductivity of a two-dimensional sample

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The various physical mechanisms of phonon scattering at the boundaries of a finite-size sample in the two-dimensional case and their effect on the thermal conductivity of the sample are studied. An analytical model of the thermal conductivity of a two-dimensional phonon gas in two-dimensional samples of finite sizes is proposed. The model is presented for so-called, ballistic regime [1 – 3], when only interaction of phonons with lateral sides of the sample are taken into account.

A number of physical mechanisms that ensure the transition from specular boundary conditions to completely diffusive are considered. In particular, the models of absolutely absorbing and specular boundaries, the finite numbers of reflections, the model of finite probability of specular reflection and the weak diffusive scattering are considered. The latter model is proposed for the effective accounting of roughness for the limiting cases of weak diffuse scattering, and a comparison is made with existing models. For every case the explicit analytical expression is presented and experimental conditions for definite models are proposed.

In each model the spatial dependence of temperature and heat flow inside the sample are derived and the dependence of effective coefficient of thermal conductivity on sample sizes is discussed. The comparison with experimental data [4 – 6] and another models [7] for two-dimensional nanosamples of various materials are carried-out.

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Disorder-induced localized low-energy tunneling states in the carbon nanomaterials

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Low-temperature heat capacity of low-dimensional carbon materials, in particular, fullerite C_{60} and carbon nanotubes(CNTs) was theoretically described. The temperature dependences of the speed of sound and the low-temperature heat capacity of fullerite C_{60} were calculated in the frame of the model of dynamic configuration excitations. The dynamics of short-range order cluster formations in fullerite C_{60} was considered b, taking into account the contribution to the heat capacity of excitations of both atomic and electronic subsystems. It was shown that the low-energy tunneling states located at the boundaries of the C_{60} domains make a dominant contribution to the linear term of the heat capacity and plateau in the speed of sound of C_{60} [1].

The equation for the contribution of the electronic heat capacity of nanotubes with structural defects was obtained taking into account multiple elastic scattering of electrons on impurities and structural defects. The relationship between the value of the electronic contribution to the heat capacity and the value of the nanotube diameter, impurity concentration, short-range order parameters (structural inhomogeneity) has been proposed [2].

In the frame of this study, electronic nature of the low-temperature features in the heat capacity in low-dimensional carbon structures was considered. It was proposed that features at low temperatures in the low temperature heat capacity can be determined by electrons scattered on the point defects and short-range order inhomogeneity.

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Resonance levels in electron and phonon spectra of graphene nanostructures: formation, decay, possibility of HTS appearance

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In electron spectra of the graphene monolayer and superthin graphene nanofilms (bigraphene, thrigraphene), some of the local and extended crystal imperfections, like vacancies and vacancy arrangements, zig-zag boundary, facilitate a formation of resonance levels nearby the Fermi energy [1,2]. Such levels are manifested by resonances in local densities of states (LDOS) of the atoms in the defect vicinity. No the worthy to mention, that these resonances appear only in the LDOS of atoms, pertained to sublattice, revealing the atomic bonds breaking at the defect formation. It means that decay of the resonance with a distance from defect is accompanied by strong oscillations. Therefore, these types of defects result in the enrichment of electron spectrum near Fermi level.

In the phonon spectra of both the graphite and carbon nano-formations under consideration, from frequencies $\sim$ 1 THz the splitting occurs in the vibrational modes, polarized in graphene monolayer and in normal to it direction. It means, that at higher frequencies these modes are practically independent. Consequently, spectral density of states for the vibrations, polarized normally to the layer, the so-called quasi flexural modes, takes a form of density of vibrational states in scalar model of a two-dimensional honeycomb lattice, i.e. similar to electron DOS of graphene. For this reason, such DOS at the frequency corresponding to K-point of first Brillouin zone is featured by V- type singularity likewise Dirac singularity in electron DOS of graphene. Thus, the defects relevant to formation of sharp resonances in electron LDOS should facilitate a formation of their analogues in phonon LDOS, enriching the vibrational spectrum by the high-frequency, $\sim$600 K, phonons.

In this way, vacancies, some of their arrangements and extended defects like zigzag boundary, significantly increase electron population in the energy range near Fermi level, and at the same time enrich phonon spectrum with the high-energy fast phonons, which are able to assist efficiently the Couper pairing of these electrons. All that provides opportunity to observe HTS in relevant structures.

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Thermally activated conductivity of molybdenum disulfide MoS_2 nanopowder

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Molybdenum disulfide MoS_2 is a very attractive material with the potential for multifunctional application [1-2]. The layered 2D structure of molybdenum disulfide is an inorganic analogue of graphene [3]. MoS_2 hold specific advantages over graphene, including the presence of a bandgap that is critical for electronic and optoelectronic devices. Integrating of semiconductor molybdenum with graphene opens up new possibilities for the development of next-generation, ultrathin, flexible, transparent, light emitting, light-harvesting and light-detecting devices.

This paper goal is to study the electrical properties of MoS_2 nanopowder in a wide temperature range. To understand the nature of the electrical transport in molybdenum disulfide nanopowder, temperature dependence of electrical resistance and current-voltage characteristics measurements were carried out in a wide temperature range of 60−300 K (Fig. 1) in the cryostat in a helium atmosphere. Current-voltage characteristics are symmetrical and linear, that indicates the ohmic regime of conductivity. Molybdenum disulfide MoS_2 nanopowder purchased from Aldrich-Sigma (N 804169) exhibits semiconducting behavior ($dR/dT < 0$). The analysis of the temperature dependence of the resistance indicates that thermally activated transport of charge carriers occurs in the temperature range of 200–300K. At temperatures below, hopping conduction is likely to be realized [3]. Thermal activation energy of the carriers E_a could be obtained using the Arrhenius plot $R \sim exp(E_a/k_BT)$. For the studied MoS_2 nanopowder value of E_a is ~180 meV.

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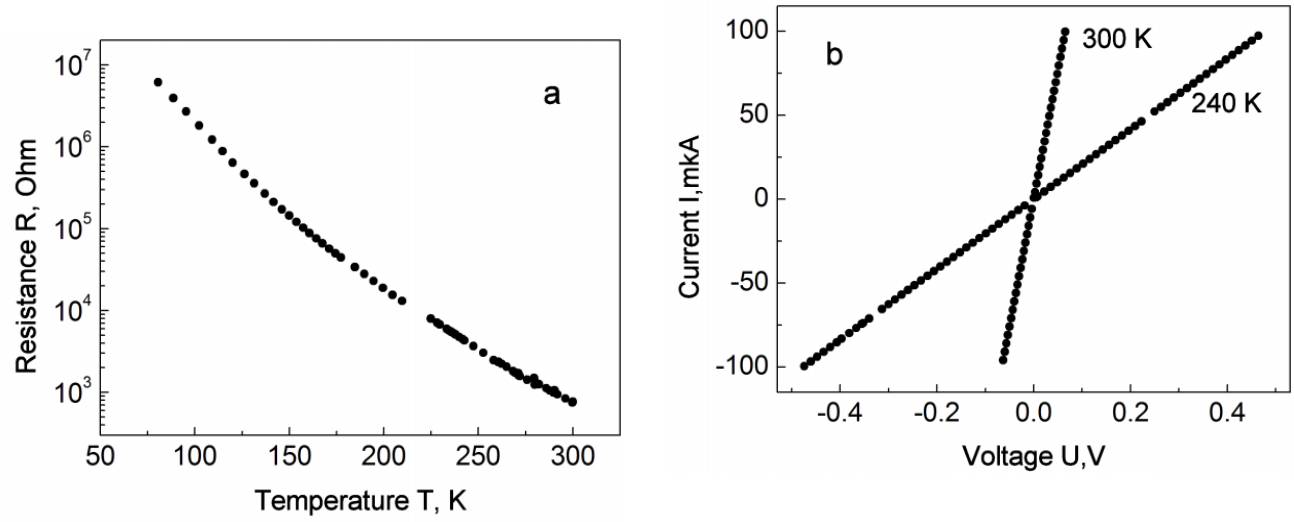

Figure. 1. Temperature dependences of resistance (a) and current-voltage characteristics (b) of molybdenum disulfide MoS_2 nanopowder.

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Thermal conductivity of solid state laser materials: ceramics of YbAG and GAGG

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Garnets are the most common materials used for lightening or other optical applications due to their physical properties like good thermal conductivity, large thermal stability and optical isotropy. One of the most studied garnets are yttrium aluminium garnet $Y_3Al_5O_{12}$ (YAG), ytterbium aluminium garnet $Yb_3Al_5O_{12}$ (YbAG) and gadolinium gallium garnet $Gd_3Ga_3Al_2O_{12}$ (GGAG) because of their unique radiation conversion ability and wide energy band gap. Different type of garnets can be optically active by replacing Y^{3+}/Yb^{3+}/Gd^{3+} ions by others lanthanide ions (e.g. Ce^{3+}, Nd^{3+}, Er^{3+}, Tb^{3+}, Eu^{3+}). An improved understanding of thermal conductivity of the transparent garnet ceramics and its compositional derivatives is important for the practical application. The primary difference in thermal conductivity between single crystals and polycrystalline ceramics is mainly caused by the existence of grain boundary and lattice defects, which work as phonon scattering centers, limiting the phonon mean free path and as a result reducing the thermal conductivity [1,2]. One of the reasons for developing new matrices with various dopants are to achieve a more efficient persistent luminescence [3]. Our approach it to enhance the thermal conductivity of the matrix by additional annealing of the ceramics or by introducing graphene flakes into the structure. The analysis will be demonstrated for the YbAG:Er^{3+} and YbAG:Ho^{3+} annealed and non-annealed ceramics. The addition of the graphene was investigated for the GAGG:Ce and GAGG:Ce, Dy ceramics.

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Temperature Dependence of the Thermal Conductivity in SiO_2 with Disorder Due to Embedded Ge Nanoparticles

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Accurate knowledge of thermal conductivity of amorphous matrices, such as silica (SiO_2), and appropriate mathematical modeling are very important for managing heat dissipation, particularly at the nanoscale. Metallic nanoclusters formed within SiO_2 have numerous applications as thermoelectric materials [1]. A reinvigorated interest have similar multilayered SiO_2/SiO_2+Ge thin film systems [2].

In this study, we report the means for predicting the thermal conductivity of amorphous nanocomposite systems with disorder caused embedded nanoparticles. The thermal conductivity was measured by a differential 3ω method [3]. The measurements were performed in a temperature controlled Lakeshore TTP-6 probe station and a CS_2O_4 (Advanced Research Systems) closed cycle cryostat. The temperature of the heater was obtained by monitoring its resistance and pre-calibrating the temperature coefficient of resistance using the four-point-probe technique. The thermal conductivity was modeled using nonequilibrium molecular dynamics method. The involvements of the interface phonon scattering and strain regions arisen in the vicinity of the interface were taken into account. We show that the conductivity of the SiO_2/Ge system is fairly well described by the model. The comparison of the measured and computed temperature dependence of the thermal conductivity in the Ge/SiO_2 composite is shown in Fig. 1.

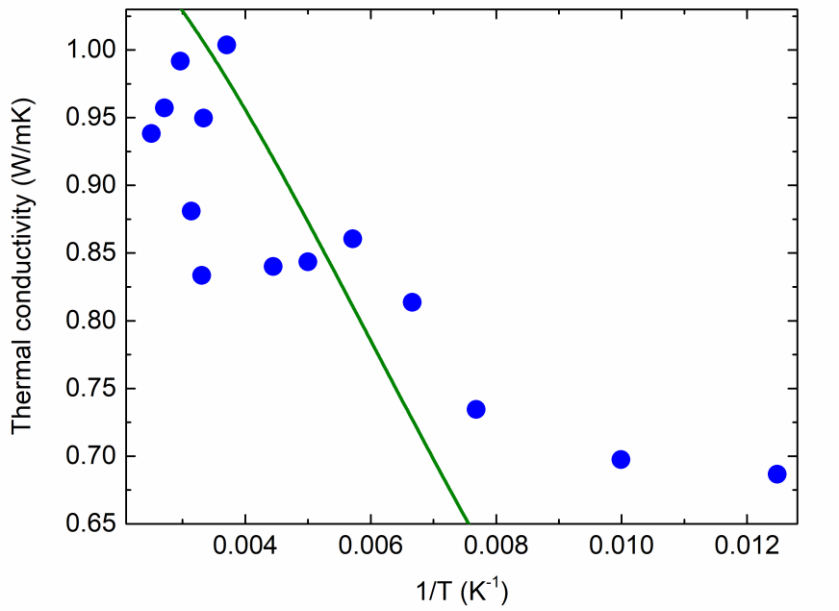

Fig. 1. Thermal conductivity in the Ge/ SiO_2 composite with ≈5 nm Ge particles. Circles – experiment, line – calculation

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Electronic thermal conductivity of single and bilayer graphene with disorder

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Structural disorder exists in any real material, and graphene is no exception. Modification of the graphene structure is observed after annealing, functionalization and other types of post-processing of graphene. The appearance of structural short-range order, as a result of post-processing, can affect the physical properties of one- and two-layer graphene. Therefore, it is important to study this effect in graphene with a different number of layers together.

In the present work, the electron transfer in disordered graphene and bigraphene is investigated taking into account the scattering of electrons by impurities and various structures of the short-range order type [1]. A new expression for electronic thermal conductivity $K_{el}(T)$ in graphene and bigraphene, as a systems in the process of «ordering-stratification» transformation, is obtained.

Contribution to $K_{el}(T)$ from electron scattering by impurities is shown to depend linearly on temperature in single- and bilayer graphene. Contribution to $K_{el}(T)$ from electron scattering by the short-range ordered complexes depends on temperature as $\sim T^2$ in a single-layer graphene and as $\sim T^{1.5}$ in a bigraphene. These results correspond to the experimental data on the total thermal conductivity [2, 3]. The calculated $K_{el}(T)$ in a bigraphene is higher than in a single-layer graphene, but the order of magnitude $K_{el}(T)$ in these systems is the same and amounts to ~ 10–15% of the total thermal conductivity. The electrical conductivity calculated with the help of the Videman-Frantz law via thermal conductivity, is in a good agreement with experimental data [2]. Thus, the effect of electron scattering by structural defects on electron transport properties is shown to be significant in both single and bilayer graphene.

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Low Thermal Conductivity and the Evidence of the Glassy Behavior in $(Pb_{0.7}Sn_{0.25}Ge_{0.05})_2P_2S_6$ and $(Pb_{0.7}Sn_{0.25}Ge_{0.05})_2P_2Se_6$ Mixed Crystals

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The chalcogenide crystals of the $Sn(Pb)_2P_2S(Se)_6$ system are uniaxial ferroelectrics and also demonstrate the quantum paraelectric state appearance at the variation of chemical composition [1]. The dipole ordering temperature of such materials may be tuned by the chemical substitution realizing a ferroelectric quantum phase transition and quantum glassy or relaxor type phenomena in different parts of the phase diagram. The thermal properties of $(Pb_{0.7}Sn_{0.25}Ge_{0.05})_2P_2S_6$ and $(Pb_{0.7}Sn_{0.25}Ge_{0.05})_2P_2Se_6$ single crystals have been studied by means of measuring their thermal diffusivity D. Thermal conductivity κ has been retrieved by the well-known relation $\kappa = C\,D$, where C is heat capacity.

As it was found [2] for $(Pb_{0.98}Ge_{0.02})_2P_2S_6$ crystal, the value of κ at low temperatures (near 50 K) is bigger than that in the case of a pure $Pb_2P_2S_6$ crystal (see fig. 1 (a)). This is obviously related to the Ge induction of polar clusters of the ferroelectric phase. At presenting of Ge the hardening of the optical branch lowers the population of the optical phonons and increases thermal conductivity of the $(Pb_{0.98}Ge_{0.02})_2P_2S_6$ crystal. In the case of $(Pb_{0.7}Sn_{0.25}Ge_{0.05})_2P_2(S,Se)_6$ mixed crystals the introduction of Ge slightly increases κ. As it shown in fig.1 (b), the thermal conductivity behaves on cooling, like in glassy materials, which demonstrates an effective phonon scattering in solid solutions with sublattice of mixed tin and lead cations. Here, germanium impurity induces the dipole glass state, which is manifested in the complex dielectric permittivity frequency dependence below 100 K. Also, the quantum fluctuations are destroyed in the mixed crystals, which follows from the comparison of the low temperature behavior of the thermal diffusivity and the complex dielectric permittivity at different frequencies [2].

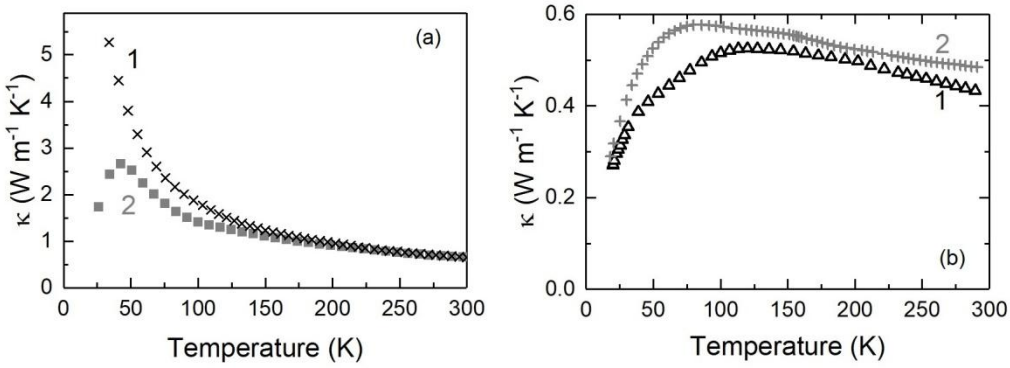

Figure 1. Temperature dependence of thermal conductivity in $(Pb_{0.98}Ge_{0.02})_2P_2S_6$ (1) and $Pb_2P_2S_6$ (2) (a), $(Pb_{0.7}Sn_{0.25}Ge_{0.05})_2P_2S_6$ (1) and $(Pb_{0.7}Sn_{0.25}Ge_{0.05})_2P_2Se_6$ (2) (b) mixed crystals.

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Influence of Chemical Substitution on the Thermal Transport Properties in 2D layered $M^{1+}M^{3+}P_2X_6$ (M^{1+} = Cu, Ag; M^{3+} = In, Bi; X = Se, S) Compounds

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Two-dimensional materials are attracting an increasing interest in the search for materials with correlated magnetic, structural and ferroelectric properties. Metal thio- and selenophosphates are promising candidates as they have an intermediate bandgap which is interesting for new electronic applications [1]. The knowledge of their thermal and ferroelectric properties is relevant for future applications in technological devices. Here, we are focusing our attention on the compounds $CuInP_2S_6$, $CuInP_2Se_6$, $AgInP_2S_6$, $AgInP_2Se_6$, $AgBiP_2S_6$, $AgBiP_2Se_6$ and $CuBiP_2Se_6$, whose thermal diffusivity is measured and combined with theoretically calculated heat capacity to extract their thermal conductivity, paying special attention to the presence or absence of ferroelectric ordering which will leave a characteristic footprint on the thermal diffusivity curve as a function of temperature [2]. Due to their layered character, the anisotropic thermal properties (thermal diffusivity and thermal conductivity) were evaluated in two directions: one contained in the layers and another one perpendicular to them. Thermal conductivity curves for 2D layered $M^{1+}M^{3+}P_2(Se,S)_6$ phosphorus chalcogenides are presented in a temperature range from 30 K till 350 K in fig. 1 in a log-log scale.

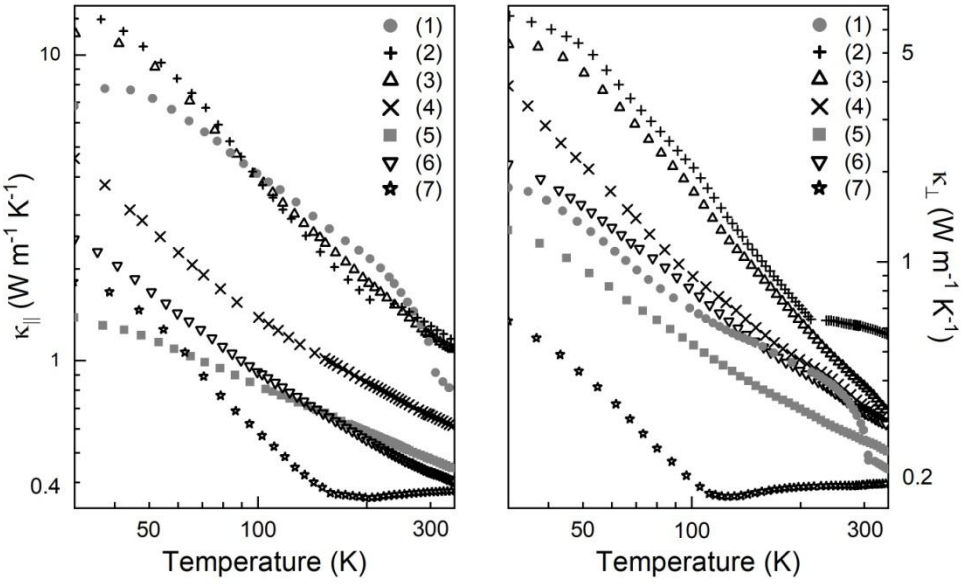

Figure 1. Temperature dependence of thermal conductivity in $CuInP_2S_6$ (1), $CuInP_2Se_6$ (2), $AgInP_2S_6$ (3), $AgInP_2Se_6$ (4), $AgBiP_2S_6$ (5), $AgBiP_2Se_6$ (6) and $CuBiP_2Se_6$ (7) measured in the direction parallel (||) and perpendicular (⊥) to the structural layers.

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Analysis of thermal conductivity for clathrate thermoelectrics

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The purpose of this work is to analyze the temperature dependences of the thermal conductivity of clathrate thermoelectrics based on $Ba_8Ga_{16}Ge_{30}$ (BGG) and $Ba_8Ga_{16}Sn_{30}$ (BGS). In these substances changing the ratio of Ga:Ge or Ga:Sn during crystal growth it is possible to obtain thermoelectrics with n-type or p-type carriers. It is shown for p-type samples in crystals (BGS) and (BGG) the temperature dependence of thermal conductivity shows glass-like behavior, while for n-type samples a maximum of is observed, which indicates crystal-like behavior $\kappa(T)$ [1].

It is shown the temperature dependences of thermal conductivity for n-type crystals can be represented as a sum of two contributions: $\kappa = A/T+B$ which take place in the case of orientational-ordered dielectric molecular crystals. First term is due to phonon–phonon scattering processes: it is inversely proportional to temperature, and it also dominates in ordered crystals at temperatures above the phonon maximum. Second term so called diffusons B at low temperatures it is weakly dependent on temperature, while in the high temperature region it is almost independent of temperature, but it becomes dominant in disordered solids (glass), when there is no translation order. This representation of thermal conductivity data is consistent with the unified theory of thermal transport [2], in particular, that thermal conductivity is the sum of two contributions – quasiparticle and quasi-wave.

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Thermal anomalies in ordered and disordered phases

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Solids made of atomic constituents can only display translational degrees of freedom, in such a way that their structure is fully determined by translation symmetry and excitations are only vibrational. In molecular solids the entities forming the system can display, in addition to internal degrees of freedom, orientational ones, giving rise to a richer variety of phases with different degrees of disorder and thus, showing different rotational and librational excitations. As a consequence, in between a perfectly ordered molecular solid, and its fully disordered counterpart, the liquid state of the same molecular entities, there are mesophases with orientational disorder (plastic phases)[1,2] or with occupational disorder [3.4]. This rich variety of different mesophases showing subtle differences in the long-range translational order as well as in the rotational and librational excitations enables to analyse the influence of them into the thermal properties. In particular, we are interested in comparing the low-temperature anomalies for different mesophases formed by the same molecular entity.

Our presentation will focus on the low-temperature (stable and metastable) phases of normal and deuterated thiophene (C_4H_4S and C_4D_4S, respectively) [5]. We will analyse the specific heat at low-temperature (below 25 K) for fully ordered phases, orientationally disordered phases and phases displaying only occupational disorder. Our study reveals the existence of a large bump (boson leak) in the specific heat for stable and metastable phases regardless the order or disorder character. This system will be compared with some similar molecular materials with similar properties in order to generalize the conclusions.

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Electrophysical properties of aqueous colloidal solutions of C_{60}

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We have performed a number of studies on the influence of fullerenes on the electrophysical properties of water, which is in contact with these nanostructures. The measurements of dielectric losses of liquid samples in the frequency range 100–10^4 Hz were performed to study the effect of nanostructures on water properties. When water comes into contact with fullerenes due to donor-acceptor bonds between water molecules and the surface of C_{60}, boundary spherical layers of water molecules are formed. This process is facilitated by the unique electronic structure of fullerene molecules, which have unpaired π-electrons participating in donor-acceptor bonds between water molecules and carbon nanostructures. Based on the literature data [1], it can be assumed that such interaction involves the surrounding nanostructures of water layers up to a submicron thickness, greatly changing the dielectric characteristics of the liquid - increasing the losses associated with the reorientation of the dipoles, as a result of which the maximum dielectric losses for water in contact with nanostructures (curve 1 on Fig.1) shifts to the region of higher frequencies in comparison with the sample of pure water (curve 2 on Fig.1).

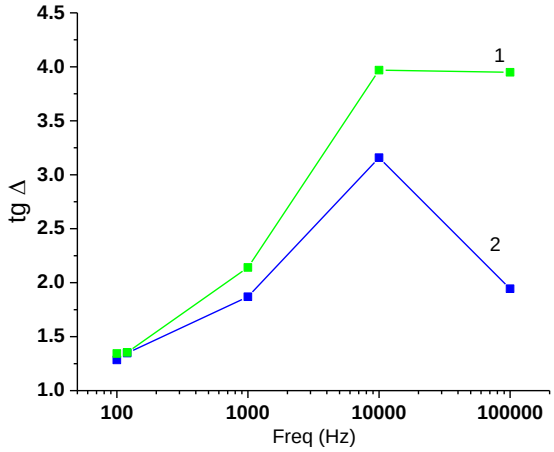

Fig.1 Frequency dependences of the dielectric loss tangent, 1 – aqueous colloidal solution of C_{60}, 2 – control sample of pure water.

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Heat capacity and thermal expansion for ordered and disordered crystal materials

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The study of the heat capacity and thermal expansion are powerful instruments for understanding the lattice vibrations, phase transitions, tunneling and quantum effects in ordered and disordered systems. In the phonon thermodynamics, thermal expansion of solids both like the heat capacity expressed the change of the internal energy U, enthalpy H, Helmholtz free energy F, and the Gibbs free energy. In the present work, universal relations between heat capacity and thermal expansion for crystal and amorphous materials in a wide temperature range were analyzed.

It was found that for the experimental data of the low temperature heat capacity and volume thermal expansion coefficients of rare gas solids such as Xe, Ar, Kr, in the entire range from the lowers measured temperatures up to the temperatures of the classical Dulong and Petit limit (heat capacity $C_v \approx 3R$ are observed the pronounced linear correlation between normalized thermal expansion (β/β^*) and heat capacity normalized to the 3R-limit ($C_v/3R$). For molecular crystals with linear simetry, such as N_2, CO_2, CO, N_2O the kink from the linear dependence of (β/β^*) vs. ($C_v/3R$) observed at the values of the heat capacity below $C_v \approx 5R$. The similar tendence was also found for nanostructures of fullerite C_{60} that has spherical symmetry of the molecules. Its indicates a new possible universal relations between volume themal expansion and heat capacity in the range of the close to constant value of the relative change of the vibrational frequency of atoms with the change of volume.

In the case of materials with structural disorder , such as a-quartz and vitreous silica, the presence of the negative thermal expansion contribution change the dependence of (β/β^*) vs. (Cv/3R). In this case, the positive and negative contributions to thermal expansion lead to a qualitative change of the (β/β^*) vs. (Cv/3R) dependence and and linear corelation is observed is this coordinates at temperatures above apear of domination of positive contribution from phonons to thermal expansion.

Generalized analysis of thermal conductivity for molecular solids

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The investigation of thermal properties of molecular solids, in particular, thermal conductivity, is an important area of modern materials science, since it stimulates the development of new composite functional materials with specified physical and chemical properties. Usually the phonon gas model is used to describe the thermal conductivity of ordered solids, and various phenomenological models are used for disordered and amorphous ones. However, in recently published work [1], it has been presented the fundamentally new theory based on quantum-field approach for thermal transport (also so called Simoncelli-Marzari-Mauri theory), which allows to describe the thermal conductivity for solids in crystalline and also in amorphous states. The main idea of this theory is vibrational excitations can propagate not only as quasiparticles, but they can also tunnel between paired energy states. In complex crystals and amorphous substances, the tunnel contribution to thermal conductivity increases with temperature, and in some cases even becomes dominant. In a sense, this contribution is universal since it does not depend on the crystal structure and on the nature of the material.

This work presents a procedure for processing and further analysis of the thermal conductivity data of molecular solids for experimental verification of the positions and predictions of the new theory based on quantum-field approach or Simoncelli-Marzari-Mauri theory. First of all, this concerns the processing of the available literature data on the thermal conductivity of various crystalline and amorphous materials, such as molecular, semiconductive, organometallic, clathrate compounds, ferroelectrics, quasicrystals, ceramics, polymers, etc. in a wide temperature range. This also applies to experimental data. It is shown that this calculation method provides universal analytical dependences to describe the thermal conductivity of any solid, including systems with ultra-low thermal conductivity within the framework of a unified universal approach. The obtained information has fundamental and applied aspects and it can be used in various fields of material science.

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