THERMAL CONDUCTIVITY
International Advanced Research Workshop

НФДУ

STAND WITH UKRAINE

2nd International Workshop

THERMAL CONDUCTIVITY OF SOLID STATES AT LOW TEMPERATURES

8-9 November 2022

online

to support peace and stand progress in Ukraine

Thermal Conductivity
International Advanced Research Workshop

2nd International Advanced Research Workshop "Thermal Conductivity of solid states at low temperature"

8-9 November 2022
|Kharkiv, Ukraine
ONLINE

Workshop Program

Book of Abstracts

Kharkiv 2022

UDK 536.48; 538.9

Scientific Edition
Workshop Program and Book of Abstracts

2nd International Advanced Research Workshop "Thermal Conductivity of solid states at low temperature", Kharkiv (online), Ukraine, 8-9 November 2022

Organised by B. Verkin Institute for Low Temperature Physics and Engineering (ILTPE) of NAS of Ukraine
8 – 9 November 2022 | Kharkiv, Ukraine

The aim of the Workshop

Traditionally, B. Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine hold the wide-scope meeting in the field of condensed matter and low temperature physics. This year we have planned to organize in Kharkiv the 2nd Workshop "**Thermal Conductivity of solid states at low temperature**" in the frame of traditional International Conference "Condensed Matter & Low-Temperature Physics CM&LTP 2022. Unfortunately the Russian military aggression and invasion in the Ukraine territory significantly complicates the organization of this event as well the research investigations. The experimental studies in the frame of NRFU project № 2020.02/0094 "Quantum tunneling of vibrational excitations in thermal conductivity of crystalline and amorphous materials and composites" are postponed to the better days. The Infrastructure of our institute was locally damaged. In general, now, the electricity and internet connection in Ukraine is limited due to the military aggression. Nevertheless, we continue the research studies using our limiting possibilities during wartime. This event has the aim to save communication and collaboration with our friends and colleagues that support us, our vision about the Ukraine's independence, integration to the European and International Research Network.

International Advanced Research Workshop "Thermal Conductivity of solid states at low temperature" (8-9 November 2022, Kharkiv (online)): Workshop Program and Book of Abstracts / Edited by Dr.Maksym Barabashko and Dr. Razet Basnukaeva. – Kharkiv: FOP Brovin O.V., 2022. – 31 p.

This book contain the abstracts of studies presented at the 2nd International Advanced Research Workshop "**Thermal Conductivity of solid states at low temperature**". The Workshop was planed in the frame of the 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.

https://ilt.kharkiv.ua/bvi/info/IInd-ITCW-22/

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FOREWORD

Dear Participants of the Workshop,

On behalf of the Organizing Committee I am glad to welcome you to the IInd International Advanced Research Workshop "**Thermal Conductivity of solid states at low temperature**" organized online by the B.Verkin Institute for Low temperature Physics and Engineering (ILTPE) of the National Academy of Sciences of Ukraine (NASU), Kharkiv, Ukraine.

The aim of the Workshop is to create a platform for establishing communication between leading researchers engaged in the study of both theoretical and experimental results of thermal conductivity of solids. This scientific seminar has an international status, as its participants are not only leading Ukrainian scientists, but also representatives of large scientific centers from abroad, in particular Poland, Japan, Spain. We hope that this event will be one of the important steps in the Way of Rebuilding the Ukrainian scientific potential and allow us to increase the opportunities for researchers engaged in academic and research institutions for exchanging information and launching cooperation. The results of the Workshop will be also published as the full manuscripts in the special issue of the peer-reviewed scientific journal Fizika Nizkikh Temperatur (English version of the journal Low Temperature Physics published by American Institute of Physics).

On behalf of the Organizing Committee, I would like to say thanks for all participation in this event. I hope it will be fruitful and interesting for you. **#StandWithUkraine!**

Prof. Alexander Dolbin
Deputy director of B.Verkin Institute for Low Temperature
Physics and Engineering of the National
Academy of Sciences of Ukraine

PROGRAM COMMITTEE
THERMAL CONDUCTIVITY WORKSHOP – 2022

Chair: Prof. Alexander Dolbin, ILTPE NASU (Kharkiv, Ukraine)
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Dr. Yulia Horbatenko, ILTPE NASU (Kharkiv, Ukraine)
PhD Diana Hurova, ILTPE NASU (Kharkiv, Ukraine)

ABOUT IInd 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 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 8 -9 November 2022 in Kharkiv(online). The Workshop was planned with the support of NRFU project № 2020.02/0094 "Quantum tunneling of vibrational excitations in thermal conductivity of crystalline and amorphous materials and composites" but the War made changes. We hope that this event will be useful for future collaboration for the aim of the increase the potential of Ukrainian research community in the field of the low temperature physics and condensed matter.

These abstract book 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, Ukraine, Poland, Slovakia and Spain.

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

ONLINE (UTC+2, EASTERN EUROPEAN TIME, KHARKIV) 8 NOVEMBER 2022

Co-chairs: Prof. Alexander Dolbin, Prof. Alexander Krivchikov
Secretary: Dr. Maksym Barabashko

10:00 -10:15 **Opening Ceremony**

10:15-10:40

Detonated nanodiamond ceramics: thermal properties at low temperatures

D. Szewczyk[1,2], M. A. Ramos[2,3]
[1]*Low Temperature and Superconductivity Department, Institute of Low Temperature and Structure Research, Wroclaw, Poland*
[2]*Low Temperature Laboratory, Condensed Matter Physics Department, Universidad Autónoma de Madrid, Madrid, Spain*
[3]*Centro de Microanálisis de Materiales (CMAM), Universidad Autónoma de Madrid, Madrid, Spain*

10:40-11:05

Low-temperature thermal properties of ultrastable glasses

M. Moratalla[1], M. Rodríguez-López[2], C. Rodríguez-Tinoco[2], J. Rodríguez-Viejo[2], D. Szewczyk[1,3], M. A. Ramos[1]
[1] *Departament of Condensed Matter Physics, Condensed Matter Physics Center (IFIMAC), and Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, 28049 Madrid, Spain*
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11:05- 11:30

Low-temperature properties of pentachlorobitrobenzene and p-chloronitrobenzene

J. Ll.Tamarit
[1]*Grup de Caracterització de Materials,Departament de Física, EEBE and Barcelona Research Centerin Multiscale Science and Engineering, Universitat Politècnica de Catalunya, Barcelona 08019, Catalonia, Spain*

Glasslike thermal properties caused by a structural quantumcritical point

Y. Ishii[1], A. Yamamoto[2], N. Sato[3], Y. Nambu[4], S. Ohira-Kawamura [5], N. Murai[5] , K. Ohara[6],S. Kawaguchi[6] , T. Mori[3], and S. Mori[1]

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[6]*Japan Synchrotron Radiation Research Institute, SPring-8, Sayo, Hyogo 679-5198, Japan*

11:30-11:50

Quantum Features around the Mott Boundary in Organic π-electron Compounds

Y. Nakazawa[1], E. Yesil[1], Y. Matsumura[1], S. Imajo[2], S. Yamashita[1], and H. Akutsu[1]

[1]*Dept. of Chemistry & Research Centre for Thermal and Entropic Science, Osaka University, Toyonaka/Osaka, JAPAN*
[2]*Institute for Solid State Physics, the University of Tokyo, Kashiwa/Chiba, JAPAN*

11:50-12:15

Thermal conductivity of the As_xS_{100-x} glass system at low temperatures

Pavlo Baloh[1], Vladimír Tkáč[1], Róbert Tarasenko[1], Martin Orendáč[1], Alžbeta Orendáčová[1], Oleksandr Mitsa[2], Vladimir Mitsa[2], Roman Holomb[2,3], Alexander Feher[1]

[1]*Pavol Jozef Šafárik University in Košice, Park Angelinum 9, Košice 040 01, Slovakia.*
[2]*Uzhhorod National University, Voloshin str. 64, Uzhhorod 88 000, Ukraine.*
[3]*Wigner Research Centre for Physics, Konkoly-Thege Miklós str. 29-33, Budapest 1123, Hungary.*

12:15-12:40

Influence of MWCNTs additives on the thermal conductivity of HA-MWCNTs composite

Barabashko M.S.[1], Basnukaeva R.M.[1], Dolbin A.V.[1], Drozd M[2]., Bezkrovnyi O.[2], Tkachenko M.V. [3]

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12:40-13:00

Coffe Break /Lunch Time

Hopping mechanism of heat transfer in cyclic hydrocarbons

V.A. Konstantinov**,** A.I. Krivchikov, V.V. Sagan, A. Karachtvtseva

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

14:00-14:20

Thermal conductivity in graphene-anatase epoxy nanocomposites

A.B. Nadtochiy[1], O.O. Korotchenkov[1], S.V. Shulga[2], B.M. Gorelov[2], A.M. Gorb[1], O.I. Polovina[1]

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[2]*Chuiko Institute of Surface Chemistry, NAS of Ukraine, 17 General Naumov Str., Kyiv 03164, Ukraine*

14:20-14:40

Evolution of thermal properties in ferrielectric $CuInP_2S_6$ and $Ag_{0.1}Cu_{0.9}InP_2S_6$ layered crystals by means of *ac* photopyroelectric calorimetry

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

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[2.]*Departamento de Física Aplicada, Escuela de Ingeniería de Bilbao,Universidad del País Vasco UPV/EHU, Bilbao, Spain*

14:40-15:00

Non-stationary thermophysical characterization of exfoliated graphite with carbon nanotubes composites

N. V. Morozovsky[1], Yu. M. Barabash[1], Yu. V. Grebelna[2], M. T. Kartel[3], Yu. I. Sementsov[3,4], G. I. Dovbeshko[1]
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15:00-15:20

[2]*TM Spetsmash ltd., 02094, Viskozna str., 5, Kyiv, Ukraine*
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[4]Ningbo Sino-Ukrainian New Materials Industrial Technologies Institute,
Kechuang building, N777, Zhongguan road, Zhenhai district, Ningbo, 315211, China

Triphenyl phosphite: thermal conductivity of glass and glacial state

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15:20-15:40

[2]*Department of Physics, Umeå University, 901 87 Umeå*
[3]*Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, 20018 Donostia - San Sebastian, Spain*

Thermal conductivity analysis of different clathrate-type crystals

15:40-16:00

Yu.V. Horbatenko, O.O. Romantsova, A.I. Krivchikov, O.A. Koroluyk
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Thermophysical properties of the Al_2O_3-SiC nanocomposite

O.M. Morozova[1], M.V. Kislitsa[2], E. S. Gevorkyan [1]

16:00-16:20

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[2]*V. N. Karazin Kharkiv National University, 4 Svobody Sq., 61022 Kharkiv, Ukraine*

1D chains of Xe atoms: contributions of vibrations and spatial redistribution of atoms to the heat capacity and thermal expansion

16:20-16:40

M.I. Bagatskii, M.S. Barabashko, A.V. Dolbin, V.V. Sumarokov
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Phonon flux formation by concurrent specular and diffusion scattering in nanoribbons

16:40-17:00

J. Amrit[1], T. Medintseva[2], K. Nemchenko[2], T. Vikhtinskaya[2]
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About the regularities and singularities of nanostructured material thermal conductivity

17:00-17:30

A.I. Krivchikov[1,2]
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Workshop will be on the ZOOM platform online by the next link:

https://us02web.zoom.us/j/88114489891?pwd=STZ3enUvNERSVDJhd0xSaUxFSUl4UT09

ZOOM Meeting: 881 1448 9891
Password: 443247

Hopping mechanism of heat transfer in cyclic hydrocarbons.

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Abstract

The increase in thermal conductivity with temperature in the dynamically orientationaly disordered (DOD) phases of cyclic hydrocarbons is explained by the recently proposed thermal activation mechanism of heat transfer. It is shown that high-temperature thermal conductivity is well described by the Arrhenius dependence. Activation energies and pre-exponential factors are determined. It is shown that the activation energies do not depend on the sample density. The dependence of the pre-exponential factor on the activation energy of a number of cyclic hydrocarbons was analyzed.

Key words: thermal activation mechanism, cyclic hydrocarbons.

Phonon flux formation by concurrent specular and diffusion scattering in nanoribbons

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In this work we investigate the physical mechanisms of phonon scattering at the sample boundaries in the two-dimensional case and their influence on the thermal conductivity of the sample. The main purpose of this work is to generalize the results of Ref. 1, where the establishment of a stationary nonequilibrium state in 2D samples was studied only due to diffuse scattering of phonons at the boundaries. In this work, the specular reflection of phonons from the boundaries is taken into account, and, thus, the results of this work generalize both the results of [1] and the results of classical studies on the thermal conductivity of phonons in a restricted geometry [2, 3].

We study the stationary nonequilibrium state of the phonon system, which is provided only by the interaction of phonons with the lateral boundaries of the samples. In this case, the interaction of phonons between themselves is considered negligible, and the lateral boundaries of the sample are assumed to be thermally insulated.

To consider this problem we introduce the incident $F_{inc}(z, \varphi)$ and reflected $F_{ref}(z, \varphi)$ heat fluxes at the lateral boundary, which are the functions of coordinate and direction, and solve the system of integral equations for these functions:

$$F_{inc}(z,\varphi) = g_h(z,\varphi) + F_{ref}(z - Wctg\,\varphi, \varphi)\eta(0 < z - Wctg\,\varphi < L) \quad (1)$$

$$F_{ref}(z,\varphi) = pF_{inc}(z,\varphi) + \tfrac{1}{2}(1-p)\eta(\pi - \varphi)\int_0^{\pi} F_{inc}(z,\tilde{\varphi})\sin\tilde{\varphi}d\tilde{\varphi} \quad (2)$$

where $g(z, \varphi)$ is the flux of phonons that move directly from the heater and p is the factor of specular reflection. In the case of completely diffusive scattering (p = 0) we get the result obtained in Ref. 3.

This system can be solved both by the iteration method and approximately analytically. The obtained solutions describe the balance of heat fluxes, the temperature distribution in the sample, and the dependence of the effective coefficient of thermal conductivity on the size of the sample.

Thus, the proposed methods accounting successive phonon reflections from boundaries with arbitrary levels of roughness allows us to determine the applicability conditions for the existing models for thermal conductivity of finite dimensions low-dimensional samples.

[1] J. Amrit, K. Nemchenko, T. Vikhtinskaya Journal of Applied Physics, 129 (2021) 085105.
[2] H.B.G. Casimir, Physica V, 6 (1938).
[3] J. M. Ziman, Electrons and Phonons (Clarendon Press, Oxford, 2001).

Acknowledgements

The work of was supported by the to the Ministry of Education and Science of Ukraine (grant No. 0122U001482).

Glasslike thermal properties caused by a structural quantumcritical point

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A quantum critical point (QCP) is a phase transition point at the absolute zero temperature caused by a suppression of an ordered phase. Research of QCPs has been developed over the last decades as one of the leading topics in condensed matter physics, as evidenced by a large number of studies on the novel superconducting phases that appear by suppressing magnetic orders. On the other hand, the *structural* quantum critical point (sQCP) that emerges by suppressing the structural phase transition has received little attention thus far and has been an unexplored research area in materials science.

The focus of this study is to clarify the nature of the sQCP using $Ba_{1-x}Sr_xAl_2O_4$ as the target material. The parent material $BaAl_2O_4$ comprises an AlO_4 tetrahedral network with six-membered cavities occupied by Ba ions. This crystal structure is regarded as a combination of a Ba sublattice and the AlO_4 network. It undergoes a ferroelectric phase transition at T_C=450 K driven by an acoustic soft mode [1], whose vibration pattern is characterized as tilting of AlO_4 accompanied by in-plane rotation of O1 atoms that connect the tetrahedra along the *c* axis. This structural phase transition is rapidly suppressed by substituting Sr for Ba, and the sQCP appears approximately at x = 0.1.

By using synchrotron x-ray diffraction, transmission electron microscopy, pair distribution function analyses, and inelastic neutron scattering, we demonstrate that short-range correlation with a broken translational symmetry is realized in the AlO_4 network at higher concentrations than the sQCP [2]. As *x* increases, the long-range ferroelectric order transformsinto a short-range order. At the sQCP, the periodic atomic arrangement is partially broken in the AlO_4 network, where the Al and O1 atoms form short-range correlation with various Al-O1 bond orientations, giving rise to a sublattice glass state. This glassy state dampens the phonons in the whole energy range and changes the phonon spectra into the broad one resembling those typically observed in glass materials. The glassy phonon spectra significantly affect the physical properties of this material; the lattice specific heat shows an excess at the sQCP, and the thermal conductivity shows a plateau at higher concentrations than the sQCP. In this region, the lattice specific heat even exhibits a characteristic T-linear contribution. Similar excess in the lattice specific heat has also been observed for a strong-coupling superconductor $(Sr_{1-x}Ca_x)_3Rh_4Sn_{13}$ with an acoustic-type sQCP [3]. We believe that the glassy phonon properties shouldbetheessential nature of the sQCP associated with an acoustic soft mode.

[1] Y. Ishii, S. Mori, Y. Nakahira, C. Moriyoshi, J. Park, B. G. Kim, H. Moriwake, H. Tanigushi,and Y. Kuroiwa, Phys. Rev. B **93**, 134108 (2016).
[2] Y. Ishii, A. Yamamoto, N. Sato, Y. Nambu, S. Ohira-Kawamura, N. Murai, K. Ohara,S.Kawaguchi, T. Mori, and S. Mori, Phys. Rev. B (in press).
[3] Y. Terasaki, R. Yamaguchi, Y. Ishii, Y. Tada, A. Yamamoto, and S. Mori, J. Phys. Soc. Jpn.**90**, 113704 (2021).

Quantum Features around the Mott Boundary in Organic π-electron Compounds

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We discuss feature of quantum phase transitions in molecule-based compounds studied by thermodynamic measurements using single crystal samples weighing in orders of 10^1-10^2 μg. The compounds we study in this work are charge transfer complexes with chemical formula of κ-(BEDT-TTF)$_2$X, β'-Y[Pd(dmit)$_2$]$_2$ (X: counter anions, Y: counter cations) where BEDT-TTF denotes bis(ethylenedithio)tetrathiafulvalene and dmit is 1,3-dithiole-2-thione-4,5-dithiolate. These compounds are known as dimer-Mott π-electrons system in which Mott insulating future is competed with metallic/superconductive properties and some other electronic ground states. We show heat capacity data of the spin-liquid (SL) systems such as κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$, β'-EtMe$_3$Sb[Pd(dmit)$_2$]$_2$ and their alloying system in which gradually changes of their ground states from SL to AF, CO, and Fermi liquid occurs by chemical pressure. Although we discuss that the SL state exists as a distinct phase and thermodynamic feature of SL resembles well with that of the Fermi liquid state, the alloying of the molecules induces continuous variation in electronic state across several types of boundaries shown in Fig.1. By comparing the low temperature thermodynamic data, we discussed how the SL state varies to the other ground state in the dimer-Mott phase diagram [1,2]. We especillay foucus on the genuine Mott transition due to the openig/disapperance of charge gap by keeping frustrated structures with BEDT-TTF and BEDT-STF substitution which is denoted by green arrow in Fig.1. The possibility of the quantum chritical behavior is discussed.

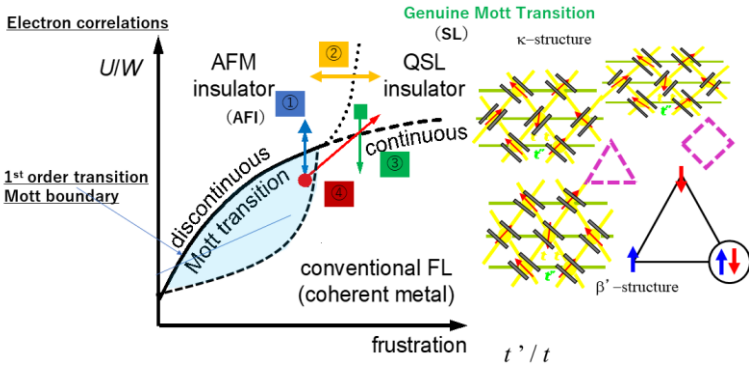

Fig.1 Possible ground states of the dimer-Mott charge transfer complexes. U/W and t'/t demonstrate the magnitude of electron correlation and geometric frustration, respectively.

[1] S. Imajo et al. PhysRev B.**105**,125130 1-7(2022).
[2] E. Yesil et al. *J. Phys. Soc. Jpn.* **89**, 073701 1-5 (2020).

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The work of was supported by the JSPS KAKENHI Grant. No. 19K22169 and 20H01862.

About the regularities and singularities of nanostructured material thermal conductivity

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Theoretical and empirical knowledge about the thermal conductivity of substances is important for the development of nanoelectronic devices and for the creation of the newest composite functional materials, etc. In particular, low thermal conductivity substances are required for thermoelectric generation devices. The designing of systems based on such materials is difficult due to the absence of descriptive data. The key component of the new understanding [1] is the concept that vibrational excitations can propagate not only as quasiparticles but also quantum tunnel between coupled energy states. In nanostructured material, the contribution of such tunneling to thermal conductivity increases with temperature increasing becomes significant, and in some cases becomes dominant. This review presents the advanced understanding of some emerging phonon phenomena in nanostructured materials: silicon ultra-thin films, nanowires, individual silicon nanoribbons and etc.

A working formula for describing the temperature dependence of the diffusion contribution (coherence-channel) due to quantum tunneling of vibrational excitations of the phonons is proposed, which has the exponential form [2] $\kappa(T) = \kappa_0 exp(-E/\hbar T)$, where κ_0 is a high limit of thermal conductivity and E is characteristic energy of dominant excitations.

It was established that the specified working formula describes the diffusion contribution well and is the result of the generalization of the model of the minimum thermal conductivity of solids [3].

[1] M. Simoncelli, N. Marzari and F. Mauri, Nature Physics, **15**, 809 (2019).
[2] V.A.Konstantinov, A.I.Krivchikov, A.V.Karachevtseva, V.V.Sagan, Solid State Communications **329**, 114241 (2021).
[3] D. G. Cahill, S. K. Watson, R. O. Pohl, Physical Review B, **46**(10), 6131(1992).

Acknowledgements

The work of was supported by the National Research Foundation of Ukraine (Grant No.197/02.2020).

1D chains of Xe atoms: contributions of vibrations and spatial redistribution of atoms to the heat capacity and thermal expansion

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The formation of quasi-1D and -2D physically adsorbed atomic and molecular structures is possible due to the unique structure of (c-SWCNTs) bundles of single-walled carbon nanotubes. The length of nanotubes is several orders of magnitude larger than the diameter. The experimental heat capacity of 1D chains of Xe atoms was obtained using an adiabatic calorimeter in the temperature range of 2–75 K [1, 2].

In this temperature range, detailed analysis and comparison were performed for: (i) experimental $C_{P\_Xe}(T)$ and theoretical $C_{V\_Xe}(T)$ heat capacity data for 1D chains of Xenon atom that adsorbed in grooves on the outer surface of bundles of single-walled carbon nanotubes with closed ends (c-SWNTs); (ii) experimental $C_{P\_Xe}(T)$ and contribution of Xe $(\alpha_{R\_Xe}(T)$ to the experimental radial thermal expansion of the c-SWNTs-Xe system. For the first time, a feature in the character of $C_{P\_Xe}(T)$ near 60 K was found. It is associated with the processes of spatial redistribution of xenon atoms from the grooves to the nearest energetically favorable positions on the outer surface of the c-SWNTs bundle. It was found that the dependences of $C_{P\_Xe}(T)$ and $\alpha_{R\_Xe}(T)$ are qualitatively similar below 60 K. The anomaly near 60 K indicates the completion of the process of the fragmentation of 1D Xe atomic chains. The obtained result is important for understanding the processes of sorption/desorption of gas impurities by carbon nanomaterials.

1. M.I. Bagatskii, V.G. Manzhelii, V.V. Sumarokov, M.S. Barabashko, Fiz.Nizk.Temp. **39**, 801 (2013).
2. M.S. Barabashko, M.I. Bagatskii, and V.V. Sumarokov, in: Nanotechnology in the Security Systems, ed. by J. Bonča, S. Kruchinin (Springer, The Netherlands, 2015), p.121−130, doi:10.1007/ 978-94-017-9005-5_11

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Thermal conductivity of the As_xS_{100-x} glass system at low temperatures

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Thermal conductivity $k(T)$ and specific heat C_p measurements of the As_xS_{100-x} glass system were performed down to 1.8 K in a wide range of various (x = 20, 28.6, 40, 45, and 50) compositions. The universal glass anomalies, boson peak, and plateau were detected in C_p/T^3 and $k(T)$, respectively. Room temperature Raman spectra of As_xS_{100-x} glasses were measured in the frequency range of 10 – 600 cm^{-1}. Cluster modeling and DFT calculations were performed in order to facilitate spectra interpretation and to determine the boson peak position as well as sample structures at nanometric scales.

The boson peak in C_p/T^3 of As-S glasses is found to depend on sample composition and is located in the temperature range between 4 and 5 K. The Raman spectroscopy of As-S glasses revealed the boson peak between 22 and 27 cm^{-1} together with additional contribution in the ultra-low (~10 cm^{-1}) frequency region (quasielastic scattering). Both spectroscopically and thermodynamically determined boson peak positions show nonlinear dependence on As concentration. Simultaneously, the plateau in $k(T)$ dependencies was observed from 2 to 15 K.

The k and C_p temperature dependences were analyzed in the frame of the Soft-Potential Model (SPM) [1,2], and the critical parameter W responsible for the transition between scattering on quantum tunneling states' contribution and a soft modes contribution was determined. The DFT calculation shows that ultra-low frequency vibrations could originate from larger "soft" ring- and branchy-like nanoclusters [3,4]. The parameter W was calculated from suitable types of nanoclusters identified by Raman spectroscopy and DFT investigation.

The combination of the SPM and "soft" nanocluster approach can serve as a helpful tool for identifying nanoclusters responsible for $k(T)$ plateau creation and interpretation of quasielastic scattering in Raman spectra. The plateau region in $k(T)$ of sulfur-rich As_2S_5 ($As_{28.6}S_{71.4}$) glass could be a consequence of the S_8 ring and "soft" $As_{2+4/5}S_5$ nanoclusters vibrations. Additionally, k-plateau in As-rich composition ($As_{50}S_{50}$) could be the outcome due to clusters vibrations, with homopolar As—As bonds. The stoichiometric composition As_2S_3 ($As_{40}S_{60}$) combines all the different cluster vibrations, mainly of pyramidal-based ring structures.

[1] D. A. Parshin, Phys Rev B **49**, 9400 (1994).
[2] M. A. Ramos and U. Buchenau, Phys Rev B **55**, 5749 (1997).
[3] R. Holomb, V. Tkáč, V. Mitsa, A. Feher, M. Veres, Physica Status Solidi (b) **257**, 1900525 (2020).
[4] R. Holomb, P. Ihnatolia, O. Mitsa, V. Mitsa, L. Himics, M. Veres, Appl. Nanosc. **9**, 975 (2019).

Acknowledgments

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Detonated nanodiamond ceramics: thermal properties at low temperatures

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Comprehensive investigations of the thermal properties in detonated nanodiamond ceramics were carried out on specially designed experimental systems (one implementing the uniaxial stationary heat flow method and second the thermal relaxation method for thermal conductivity and heat capacity respectively) and a commercial Physical Properties Measurement System. Two types of samples were considered, of varying sintering temperatures (either 1000°C or 1600°C) and sintering time (11 – 25s), all were sintered at high pressures (6 – 7 GPa). The effect of different sintering conditions on resulting thermal transport is examined. In thermal conductivity $\kappa(T)$, an improvement up to a factor of 3 of heat flow at room temperature is observed, when we increase both the sintering time and temperature. The temperature dependence of $\kappa(T)$ exhibits a typical polycrystalline character due to hindered thermal transport stemming from the microstructure of ceramic material, but with values around 1 – 2 W/mK. At the lowest temperatures, the thermal conductivity is very low and increases only slightly faster than linear with temperature, proving the significant contribution of the scattering due to multiple grain boundaries. The heat capacity data did not show a substantial difference between detonated nanodiamond ceramics obtained at different temperatures unlike for $\kappa(T)$ results. For both samples, an unexpected upturn at the lowest temperatures is observed – most likely reminiscent of a low-T Schottky anomaly inherited most likely in the fabrication process. A linear contribution to the specific heat is also present, with a value of 20 μJ/K, one order of magnitude higher than in canonical glasses. The determined Debye temperature is 482 (±6) K. The data analysis is supplemented by the phonon mean free path considerations.

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Low-temperature thermal properties of ultrastable glasses

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Much has been discussed about the possible existence of an "ideal glass" which should correspond to the best and most stable glass achievable, associated with the lowest relative minimum within the potential energy landscape of the substance. In the last years, the existence of glasses with very high thermodynamic and kinetic stability has been realized experimentally. So-called *ultrastable glasses*, usually prepared through physical vapor deposition (PVD) under optimized deposition rates and temperatures, represent a unique class of materials with remarkable properties, including low enthalpies and high kinetic stabilities [1]. These glasses offer unprecedented opportunities for practical applications, as well as to understand many aspects of the glassy state.

Specifically, it is well known that glasses exhibit thermal, vibrational and acoustic properties at low temperatures anomalously different from those found in crystalline solids, and with a striking degree of universality. The question has naturally arisen as whether these peculiar low-temperature "glassy anomalies" persist or vanish in these highly-stable glasses. Interestingly, our earlier low-temperature specific-heat measurements on (highly anisotropic) ultrastable glasses of indomethacin [2] prepared by PVD showed the suppression of the ubiquitous linear term below 1–2 K traditionally ascribed to the existence of tunneling two-level systems (TLS) in glasses. This finding apparently challenged the opposite behaviour found in hyperaged glasses of geological amber [3]. To shed more light on this controversial issue, we will present very recent, unpublished results of low-temperature specific heat on a different ultrastable glass, TPD, whose degrees of anisotropy and stability can be controlled. Future measurements of their low-temperature thermal conductivity are under way.

[1] C. Rodríguez-Tinoco, M. González-Silveira, M. A. Ramos, J. Rodríguez-Viejo, Riv. Nuovo Cim. **45**, 325–406 (2022).
[2] T. Pérez-Castañeda, C. Rodríguez-Tinoco, J. Rodríguez-Viejo, M. A. Ramos, Proc. Natl. Acad. Sci. **111**, 11275 (2014).
[3] T. Pérez-Castañeda, R. J. Jiménez-Riobóo, M. A. Ramos, Phys. Rev. Lett. **112**, 165901 (2014)

Acknowledgments

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Triphenyl phosphite: thermal conductivity of glass and glacial state

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Triphenyl phosphite under normal conditions is a molecular glass-forming liquid; in this substance a polyamorphous transition was first observed by Ha et al. [1]. They observed a new solid exotic phase, which they called glacial, obtained as a result of the transition from a supercooled liquid, this phase is distinct from both the glass and the crystal.

Thermal conductivity κ of triphenyl phosphite in glass and exotic glacial state was measured by the transient hot wire method at pressures up to 0.5 GPa, in the temperature range of 90-270 K. Heat transfer processes in these amorphous states were studied as functions of temperature and pressure.

The thermal conductivity of the glass and glacial states is described well by a term associated with heat conduction of diffusons only, which is one of the heat transfer channels of the two-channel heat transfer theory of dielectric solids including both complex and simple crystalline phases and amorphous states [2]. The thermal conductivity can be represented by an Arrhenius-type function: $\kappa(T, P) = \kappa_0(P) \exp(-E/T)$, where E is the activation energy, and κ_0 is a pre-exponential factor, which varies linearly with pressure, $\kappa_0(P) = a + bP$. The behavior of thermal conductivity as a function of temperature and pressure $\kappa(T, P)$ of glassy and glacial states is compared. It shows that the behavior of the thermal conductivity of these states is strikingly similar in magnitude, showing low values of κ, which increase only slightly with increasing temperature and pressure. This similarity, which suggests a structural relationship between the glass and glacial states, is demonstrated quantitatively by the similar values of the parameters: E, κ_0, a, and b. We note, however, that although κ of a glass is known to be dependent on thermal history, this dependence is smaller than that for the glacial state [3].

[1] A. Ha, I. Cohen, X. Zhao, M. Lee, & D. Kivelson, J. Phys. Chem. **100**, 1 (1996).
[2] M. Simoncelli, N. Marzari, & F. Mauri, Nat. Phys. **15**, 809 (2019).
[3] A. I. Krivchikov, & O. Andersson, J. Phys. Chem. B **120**, 2845 (2016).

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Low-temperature properties of pentachlorobitrobenzene and p-chloronitrobenzene

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Low-temperature thermal properties of translational ordered and minimally orientationally disordered crystals are analyzed. While pentachloronitrobenzene ($C_6Cl_5NO_2$, PCNB) displays a hexagonal structure in which molecules are disordered around six equivalent crystallographic positions with partial site occupation, p-chloronitrobenzene ($C_6H_4ClNO_2$, p-CNB) shows a high-temperature orientationally disordered phase in which molecules occupy two equivalent crystallographic positions orientations. Despite the similar highly anisotropic layered structures (disorder is exhibited only within the parallel planes where the molecules execute large amplitude in plane reorientations), low-temperature properties are revealed to be different as far as the ubiquitous glassy anomalies are concerned. In this talk we will analyze the differences of the glassy anomalies as well as propose the origin of them.

Evolution of thermal properties in ferrielectric $CuInP_2S_6$ and $Ag_{0.1}Cu_{0.9}InP_2S_6$ layered crystals by means of *ac* photopyroelectric calorimetry

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Multiferroics of van der Waals family $CuInP_2S_6$ crystals are very attractive among the scientific community due to the presence in these materials of very unusual features such as a nonlinear dielectric response [1], a giant negative electrostriction [2] or extremely large elastic nonlinearity [3]. A combination of these properties opens the possibility for broader applications of these materials in functional electronics.

The study of the thermal properties of layered $CuInP_2S_6$ ferrielectric crystals has been carried out by obtaining high resolution thermal diffusivity and heat capacity curves using an *ac* photopyroelectric calorimeter in the back configuration. These Wan der Waals crystals are layered structures which are known to undergo a phase transition from a paraelectric to a ferrielectric state, as unusual examples of anticollinear two-sublattice ferrielectric systems. In this study, plane-parallel plates are prepared with surfaces parallel or perpendicular to the crystal structure layers. In the case of $CuInP_2S_6$ the ferrielectric phase transition has been found at about 311 K, signalled by a sharp dip on the thermal diffusivity curve and lambda-like jump on the heat capacity curve (Fig. 1 (a)). On the other hand, completely different shape of the anomalies for $Ag_{0.1}Cu_{0.9}InP_2S_6$ are obtained at about 290 K (Fig. 1 (b)). Such abrupt change of the thermal diffusivity and heat capacity curves in the vicinity of the transition can be explained by the previous theoretical studies [4,5] which predict the appearance of a critical end point (CEP) instead of a tricritical point (TCP) on the phase diagram. Thus, the splitting of the anomaly of the heat capacity in $Ag_{0.1}Cu_{0.9}InP_2S_6$ can be interpreted as a transformation of the ferrielectric first order phase transition into the paraelectric-ferrielectric second order phase transition together with the isostructural first order one with a sharp change of the polarization in the ferrielectric phase.

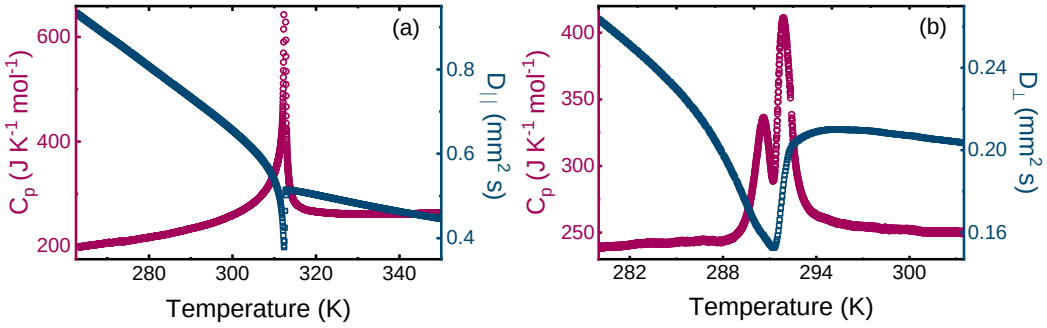

Figure 1. Temperature dependence of thermal diffusivity (blue squares) and heat capacity (dark pink circles) for $CuInP_2S_6$ (a) and $Ag_{0.1}Cu_{0.9}InP_2S_6$ (b) layered crystals in the vicinity of the PT.

[1] A. Dziaugys, I. Zamaraite, J. Macutkevic, et al., Ferroelectrics **569**, 280 (2020).
[2] S. M. Neumayer, E. A. Eliseev, M. A. Susner, et.al., Phys. Rev. Mater. **3**, 024401 (2019).
[3] V. Samulionis, J. Banys, and Yu. Vysochanskii, Ferroelectrics **389**, 18 (2009).
[4] A. N. Morozovska, E. A. Eliseev, S. V. Kalinin, et. al., Phys. Rev. B **104**, 054102 (2021).
[5] Sumedha and S. Mukherjee, Phys. Rev. E **101**, 042125 (2020).

Non-stationary thermophysical characterization of exfoliated graphite with carbon nanotubes composites

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Under operation of any material in the thermal management as an IR-absorber (IR-to-heat energy converting) [1], thermal interface material [2] or as a heat sink [3], the most important are its heat transfer and heat accumulation abilities. These qualities are determined by two thermophysical parameters, thermal conductivity, k_T, and volume specific heat, C_ρ, which determine other two interconnected parameters, thermal diffusivity, $a_T = k_T/C_\rho$, and thermal effusivity, $b_T = (k_T C_\rho)^{1/2} = C_\rho a_T^{1/2}$. The knowledge of a_T and b_T is especially important in the case of operation at the non-stationary conditions, when quick heat exchange (high a_T) and effective heat sink (high b_T) must be realized.

The thermally exfoliated graphite (EG) - multiwall carbon nanotubes (CNT) composites (EG-CNT) were synthesized by persulphate oxidation method [4]. The processes of deagglomeration of CNT and intercalation of natural graphite were united during chemical oxidation (CO) and electrochemical (anode) oxidation (ECO). The thin plate samples of EG-CNT were manufactured by roll rolling of the powder.

For estimation the effective a_T and b_T values, the heat pulse (500 ms) and thermo-wave (20 Hz modulation) methods were applied. The light emitting diode as radiation heater and the pyroelectric detector as heat sensor were used.

For EG-CNT, 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 are within the limits known for sheets of multi-walled CNTs [5] in directions across (~$\cdot 10^{-5} \cdot m^2/s$) and along (~$\cdot 10^{-4} \cdot m^2/s$) the alignment of CNTs in sheets.

The relation $k_T = C_\rho v_p l_p/3 = C_\rho v_p^2 \tau_p/3$ [6], where v_p, l_p and τ_p are the averaged phonon group velocity (~ 10^4 m/s), mean free path and relaxation time, respectively, gives $a_T = v_p l_p/3 = v_p^2 \tau_p/3$. The evaluated $l_p \approx$ (3 - 30) nm and $\tau_p \approx$ (0.3 - 3) ps ranges for EG-CNT are characteristic of phonon scattering in defective graphene layers [7].

It is found that the less dense CO samples have higher values of a_T, b_T, l_p and τ_p than the denser ECO samples, which can be associated with the difference in the state of defects in EG-CNT samples obtained without (CO) and with electrical treatment (ECO).

[1] S. L. Bravina, N. V. Morozovsky, G. I. Dovbeshko, O. M. Fesenko, and E. D. Obraztsova, Nanosystems, Nanomaterials, Nanotechnologies, 7, 137 (2009).
[2] K. M. F. Shahil, and A. A. Balandin, Nano Lett., 12, 861 (2012); doi: 10.1021/nl203906r.
[3] J.-D. Xie, S.-Y. Gu, and H. Zhang, Coatings, 7, 138 (2017); doi:10.3390/coatings7090138.
[4] Yu. I. Sementsov, S. L. Revo, and K. O. Ivanenko, Thermo-Expanded Graphite (Interservis, Kyiv, 2016). (In Ukrainian).
[5] E. Aliev, M. H. Lima, E. M. Silverman, and R. H. Baughman, Nanotechnology, 21, ID 035709 (2010); doi:10.1088/0957-4484/21/3/035709.
[6] R. Berman, Thermal Conduction in Solids (Clarendon Press, Oxford 1976).
[7] T. Feng, X. Ruan, Z. Ye, and B. Cao, Phys. Rev. B, 91, 224301 (2015); doi:10.1103/PhysRevB.91.224301.

Thermal conductivity in graphene-anatase epoxy nanocomposites

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A nanostructured hybrid material consisting of anatase-TiO_2 nanoparticles deposited on multi-layered graphene platelets (MLG), was synthesized and tested as nanofiller for a DGEBA-epoxy polymer matrix. MLG:TiO_2 hybrid material combines the nanoscale structure, large interfacial area, mechanical features of a 2D, layered material, and enhanced thermal properties, properties of ceramic oxides, able for preparing thermal interface composite material or solid electrolyte for proton exchange membrane fuel cell (PEMFC) applications under low-temperature operative conditions.

MLGs have been prepared from the scales of thermally expanded graphite by using the electrochemical technique described in literature. The nanoplatelets having the specific surface area S_f ~ 790 m^2/g consist of several dozen loosely bound monoatomic graphene layers with an area of about least 5×5 μm^2. MLG-mass-loading ($\varphi_{f,m}$) of the nanocomposites varied from 0.1 % to 5.0 % by weight. The commercially available anatase-TiO_2 nanoparticles, being of about 50 nm in diameter and of S_f ~1500 m^2/g, have been deposited on MLG in mass concentration of 0.5 %, 1 % and 5 %. The commercially available CHS-EPOXY 520 (SpolChemie, a.s. Czech Republic) DGEBA-epoxy resin cured with the diethylenetriamine (DETA) hardener was used as the host polymer matrix for the MLG:TiO_2-nanocomposites (GTNCs). The sample preparation procedure included six subsequent steps: first, simultaneous dilution of both MLG- and TiO_2- fraction in ethyl alcohol; second, 15-minutes-long ultrasonic stirring of the solution; third, the as-prepared MLG+TiO_2-solution was added into initial epoxy-olygomer solution and mixed manually; fourth, the liquid composite have been vacuumized in order to remove the alcohol residue; fifth, the vacuumated composite was mixed manually with the hardener in a ratio of 7 to 1; and, sixth, cured at a room temperature during 72 hours.

Thermal conductivity (k_C) of the GTNCs has been determined within temperature range 50-300 K by using a traditional technique to measure temperature gradient across the sample provided that the thermal flux is given.

It was proved that k_C-values increase as compared to those obtained for pure epoxy. The Su-Li-Weng approach [1] has been adapted for to calculate loading-temperature dependence of k_C for a three-phase polymer nanocomposite taking interphase layers surrounding every constituent phase into account. Numerical calculations showed that a plausible explanation of k_C-enhancement is decreasing the Kapitza thermal boundary resistance (R_K) at MLG:TiO_2-epoxy interface. In turns, decreasing R_K is accompanied with increasing thermal conductivity of interphase layers surrounding MLG:TiO_2 hybrid nanoparticles embedded into a polymer matrix. A decrement in R_K may be caused with an enhanced impact of MLG:TiO_2-hybrid nanoparticles on epoxy's molecular structure within the interphase layers as compared to an impact of bare MLG-nanoplatelets. It may be suggested that the interphase molecular interaction will be enhanced due to forming the double electric layer [2] around the hybrid nanoparticles as a consequence of relatively high dielectric permittivity of anatase particles.

[1] Yu Su, J.J. Li, G.J. Weng, Carbon **137**, 222 (2018).
[2] T. Tanaka, M. Kozako, N. Fuse, Y. Ohki, IEEE Trans. Dielectr. Electr. Insul. **12**, 669 (2005).

Thermophysical properties of the Al_2O_3-SiC nanocomposite

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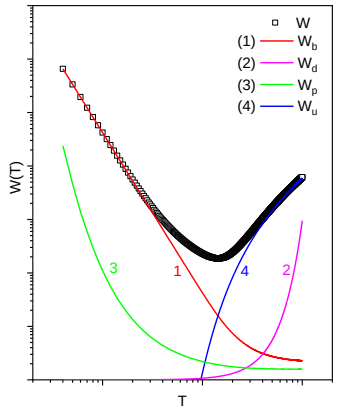
In this work, the effect of contribution of various scattering's mechanisms on W(T)&T are studied. The composite Al_2O_3-SiC has been sintered via electroconsolidation method by hot pressing in a vacuum chamber [1].
Phonon heat transfer has been considered due to dielectric properties of the Al_2O_3-SiC composite. During heat transfer any elementary excitations experience scattering that results in dissipation of the heat flux. Electrons are not involved either in the heat transfer process or in the scattering. The expression of the thermal resistance of the sample takes the form

$$W = W_b + W_d + W_p + W_u$$

where the right-hand side of the equality is the sum of thermal resistances due to phonon scattering on boundaries, point defects, plane defects and on phonons respectively.
The figure shows the temperature dependences of the total thermal resistance of the Al_2O_3-SiC sample and its terms. It can be seen that at low temperatures the boundary scattering (curve 1) is dominating, and at high temperatures the phonon-phon scattering leading to $W \sim T$ dependence dominates. In the region of minimum $W(T)$ the scattering at defects is also important.



Pic 1. Qualitative temperature dependence of the thermal resistance of the Al_2O_3-SiC sample, as well as contributions from various scattering mechanisms: on boundaries (1), point (2) and plane (3) defects, on phonons (4).

This behaviour of the thermal resistance at low temperatures (presence of a minimum) is characteristic of solids that do not contain conduction electrons.
In conclusion, the effect of scattering's mechanisms on the thermal resistance of the Al_2O_3-SiC sample has been studied. The scattering mechanism on boundaries, point defects, plane defects and on phonons contributes on the thermal resistance of Al_2O_3-SiC nanocomposite.

[1] Gevorkyan, E., Nerubatskyi, V., Chyshkala, V., Gutsalenko, Y., & Morozova, O. (2021). Determining the influence of ultra-dispersed aluminum nitride impurities on the structure and physical-mechanical properties of tool ceramics . Eastern-European Journal of Enterprise Technologies, **6**(12) (114), 40–52. https://doi.org/10.15587/1729-4061.2021.245938.

Thermal conductivity analysis of different clathrate-type crystals

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Analysis of the temperature dependences of the thermal conductivity of various complex crystals with a clathrate structure were made. It was shown that both crystal-like and glass-like behaviour of $\kappa(T)$ of these crystals [1-3], is possible to describe in terms of the unified theory of thermal transport [4], where thermal conductivity is the sum of two contributions – quasiparticle (phonon`s) and quasi-wave (coherence): $\kappa = \kappa_{ph.} + \kappa_c$. The first term dominates in orientational-ordered dielectric crystals, and the second term prevails in disordered ones. It`s similar to our previous representation of $\kappa(T)$ for the case of thermal conductivity of orientationally ordered crystals in the temperature range dominated by phonon-phonon scattering processes, as $\kappa = A/T+B$.

An approximation of the temperature dependence of the "coherences" contribution of the $\kappa(T)$ channel in the form of an Arrhenius-type exponential dependence is proposed: $\kappa_C = \kappa_0 \cdot \exp(-E/T)$, where κ_0 and E are parameters which characterize excitations which responsible for heat transfer process. Values of E for investigated clatrathe-type crystals are 5.3 K $\leq E \leq$ 100 K.

[1] R. Christian, M. Ikeda, G. Lientschnig, L. Prochaska, A. Prokofiev, P. Tomeš and S. Paschen, Physica status solidi (a) **213**(3), 784-801 (2016).

[2] U. Aydemir, C. Candolfi, A. Ormeci, Y. Oztan, M. Baitinger, N. Oeschler, and Y. Grin, Phys. Rev. B **84**(19), 195137 (2011).
[3] O. Andersson, and Y. Nakazawa, J. Phys. Chem. B, **119**(9), 3846-3853 (2015).
[4] M. Simoncelli, N. Marzari & F. Mauri, Nature Physics **15** (8), 809-813 (2019).

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Influence of MWCNTs additives on the thermal conductivity of HA-MWCNTs composite

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Abstract

The appearance of bone defects is one of the possible injuries that significantly influence the quality of human life. The use of biomaterials and implants created on their basis allows the replacement of damaged parts of the human bones and renovates people's potential to have an active life. The size and characteristics of implants depend on the mechanical properties of used biomaterials, including the modulus of elasticity, yield strength, and tensile strength. In addition, biomaterials should be biocompatible with bone tissue. Medical implants need further improvement due to the various problems with their mechanical, biological and thermal characteristics [1-2]. In particular, HA ceramics based on hydroxyapatite ($Ca_5(OH)(PO_4)_3$) have low mechanical characteristics in comparison with bone tissues. However, such ceramics have excellent biocompatibility, bioactivity, and osteoconductivity, which are advantages compared to other materials for implants [3].

The use of multi-walled carbon nanotubes MWCNTs as reinforcing additives allows for improving the mechanical characteristics of HA ceramics

Possible changes in the temperature dependence of the coefficient of thermal conductivity of the hydroxyapatite composite (HA-MWCNTs) with small amounts of MWCNTs additives (0.5 wt.%) were analyzed in comparison with the dependence of HA without additives. It was found that MWCNTs can contribute to the increase of the thermal conductivity coefficient. The magnitude of the effect of increasing thermal conductivity varies from relatively small values (about 1%) to a significant increase up to ~20 times that depending on the interaction at the HA-MWCNTs interface and the degree of homogeneity of the MWCNTs distribution in the HA matrix. It was found that long-term high-temperature annealing can lead to changes in the anisotropy, structure and properties of MWCNTs due to oxidation effects, which can influence the resulting composite properties.

[1]. Holzapfel, B. M., Reichert, J. C., Schantz, J.-T., Gbureck, U., Rackwitz, L., Nöth, U., Jakob F., Rudert M., Groll J., Hutmacher, D. W. (2013). How smart do biomaterials need to be? A translational science and clinical point of view. Advanced Drug Delivery Reviews, **65(4)**, 581–603. doi:10.1016/j.addr.2012.07.009

[2]. Kaur, M., & Singh, K. (2019). Review on titanium and titanium based alloys as biomaterials for orthopaedic applications. Materials Science and Engineering: C. doi:10.1016/j.msec.2019.04.064

[3]. SHEKHAWAT, Deepika, et al. Bioceramic composites for orthopaedic applications: A comprehensive review of mechanical, biological, and microstructural properties. Ceramics International, 2021, **47(3)**: 3013-3030

AUTHOR INDEX

A

Akutsu H. …14 **Amrit J.** …12 **Andersson O.** 20

B

Barabashko M.S. … 16, 27 **Bagatskii M.I**.… 16 **Bezkrovnyi O.** …27
Barabash Yu. M. … 23 **Basnukaeva R.M.** .27 **Baloh P**. … 17

D

Dovbeshko G.I. … 23 **Drozd M..** … 27 **Dolbin A.V**.. … 16, 27

F

Feher A. … 17

G

Grebelna Yu. V.. … 23 **Gorelov B.M.** … 24
Gevorkyan E. S.. … 25 **Gorb A.M.**. 24

H

Horbatenko Yu.V. … 26
Holomb R. 17

I

Ishii Y. 13 **Imajo S**. 14

K

Kawaguchi S. … 13 **Korolyuk O.A**. … 20, 26 **Kartel M. T.** … 23
Karachevtseva A.V. … 11 **Korotchenkov O.O**. … 24
Kislitsa M.V.. … 25 **Kohutych A.**. … 22
Konstantinov V.A. … 11 **Krivchikov A.I**. 11, 15,20,26

L

Liubachko V. … 22

M

Medintseva T.. … 12 **Mitsa O.** 17 **Morozovsky N. V.** 23
Mori T. … 13 **Mitsa V**. 17 **Morozova O.M**. 25
Murai N. … 13 **Matsumura Y**. … 14
Mori S. … 13 **Moratalla M**. 19

N

Nakazawa Y.. … 14 **Nambu Y..**. … 13
Nadtochiy A.B. 24 **Nemchenko K.**. … 12

O

Ohara K. … 13 **Orendáč M.** 17 **Oleaga A**. 22
Ohira-Kawamura S. 13 **Orendáčová A**. 17

P
Pogodin A.. … 22 **Polovina O.I..** … 24

R
Ramos M.A. 18, 19 **Rodríguez-López M**. … 19 **Rodríguez-Viejo J**. 19
Romantsova O.O. … 26

S
Sagan V.V. … 11 **Szewczyk D.** … 18, 19 **Sato N**. … 13
Sumarokov V.V. … 16 **Salazar A**.. … 22
Sementsov Yu.I.. … 23 **Shulga S.V.** 24

T
Tamarit J. Ll.. … 21 **Tkáč V.** 17 **Tarasenko R.** 17
Tkachenko M.V. 27

V
Vikhtinskaya T.. … 12 **Vysochanskii Yu**. 22

Y
Yamamoto A.. … 13 **Yamashita S**. 14

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