International Conference
"Advanced Carbon Nanostructures"

Conference/School of Young Scientists

ADVANCED CARBON NANOSTRUCTURES AND METHODS OF THEIR DIAGNOSTIC

Abstracts of Lectures
&
Young Scientists Contributed Papers

July 3, 2013
St. Petersburg, Russia

Organizers

- **Ioffe Physical-Technical Institute**, St.Petersburg, Russia
- **National Research Center "Kurchatov Institute",** Moscow, Russia

Official Partners

- **Russian Foundation for Basic Research**
- **Fund for Infrastructure and Educational Programs**
- **Government of Saint-Petersburg**

Organizing Committee

Co-chairs of the Organizing Committee:

V.V.Afrosimov   Ioffe Physical Technical Institute, St.Petersburg

M.V.Kovalchuk   Russian Research Centre «Kurchatov Institute», Moscow

Members of the Organizing Committee

M.V.Baidakova   Ioffe Physical Technical Institute, St.Petersburg

S.G.Konnikov   Ioffe Physical Technical Institute, St.Petersburg

A.Ya. Vul'   Ioffe Physical Technical Institute, St.Petersburg

Local Organizing Committee

I.V. Vorobyova (Chair)   Ioffe Institute, St. Petersburg, Russia

Technical Group

D.B. Shustov   Web-site, Ioffe Institute, St. Petersburg, Russia

A.N. Trofimov   Ioffe Institute, St. Petersburg, Russia

K.N. Guliaeva   Ioffe Institute, St. Petersburg, Russia

in association with Agency for Science and Technology "Intellect"

The Third International School - Conference for Young Scientists "Advanced Carbon Nanostructures and Methods of their Diagnostics"

The third International School - Conference will be held on Wednesday **July 3**, **2013** in St Petersburg, Russia (in the frame of the Joint International Conference "Advanced Carbon Nanostructures").

The program of the School - Conference includes invited lectures, poster and oral sessions (short talks 1-2 minutes in Russian), where the reports of young scientists (up to 28 years old), devoted to the carbon nanostructures diagnostic techniques, will be presented. The participants of the School - Conference will be supplied by the tutorial materials in English.

Location and date

The Conference/School for Young Scientists will be held on July 3, 2013 in St Petersburg at the St Petersburg Academic University - Nanotechnology Research and Education Centre of the Russian Academy of Sciences (the Academic University) (8 Khlopina St) near the Ioffe Physical-Technical Institute (26 Polytechnicheskaya st).

Language

The conference official language is English except the event "Conference/School for young scientists" where lectures and short-form presentations of young scientists will be given in Russian. Work language on Poster Session 2 & School Poster Session is English.

Scientific Presentation

Reports of Young Scientists of One day Conference/School are to be presented on Poster boards on Wednesday, July 3, morning respectively.

A size of Poster board is 100×100 cm. On board will be pointed a number of Report.
The author is requested to be near the board during all time of Poster Session 2.
For further information please look at the Timetable and the list of papers.

Timetable

Wednesday July 3	9.00-10.50	Conference/School of Young Scientists (in Russian)
	10.50-11.10	*Coffee Break*
	11.10-13.00	Conference/School of Young Scientists (in Russian)
	13.00-15.00	*Lunch*
	15.00-17.10	Conference/School of Young Scientists (in Russian)
	17.10-17.30	*Coffee Break*
	17.30-19.00	**School poster session** & Poster session 2: **Fullerenes**

Scientific Program

July 3, Wednesday

Conference/School of Young Scientists (in Russian)

Advanced Carbon Nanostructures and Methods of Their Diagnostic

Chairmen: V.V. Afrosimov, M.V. Kovalchuk

9^{00}-9^{55} — Lecture 1
Alexander V. Eletskii, *National Research Center "Kurchatov Institute", Moscow, Russia*
Physical problems in CNT-based electron field emitters

9^{55}-10^{50} — Lecture 2
Levon B. Piotrovskiy, *Institute of experimental medicine NWB RAMS, Saint-Petersburg, Russia*
The biological potential of carbon nanostructures

10^{50}-11^{10} — *Coffee break*

11^{10}-12^{05} — Lecture 3
Evgeni Katz, *J. Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede Boqer, Israel*
Fullerenes, nanoclusters and nanotubes: forms and structures (from mathematics to physics, biology and architecture)

12^{05}-13^{00} — Lecture 4
Vladimir Yu. Osipov, *Ioffe Physical-Technical Institute RAS, Russia*
Nanographites: edge-localized states and their unconventional electronic properties

13^{00}-15^{00} — *Lunch*

15^{00}-15^{55} — Lecture 5
Evgeny D Eydelman, *Ioffe Physical Technical Institute RAS, Russia; St. Petersburg Academic University–Nanotechnology Research and Education Centre RAS, St. Petersburg State Chemical–Pharmaceutical Academy, St. Petersburg, Russia*
Thermoelectric effects in carbon nanostructures

15^{55}-16^{50} — Lecture 6
V.A. Bykov, *Research Institute of Physical Problems & NT-MDT Companies Group, Moscow, Russia*
Technologies of atomic force microscopy and scanning spectroscopy for carbon nanostructures investigations

16^{50}-17^{10} — **Short oral young scientist's presentations (1 minute)**

17^{10}-17^{30} — *Coffee break*

17^{30}-19^{00} — **School poster session** & Poster session 2: **Fullerenes**

CV of Invited Lecturers and Abstracts of Lectures

Alexander V. Eletskii

Dr. of Science (Physica), Professor, Major Researcher
National Research Center "Kurchatov Institute", Moscow,
Russia

Official address: National Research Center "Kurchatov Institute", Kurchatov Square, Moscow 123182, Russia
Phone: +7(499)196 99-78 (business)
Fax: +7(499) 196 98 40
Email: Eletskii@mail.ru

Date and place of birth: May 26 1943, Ekaterinburg reg., USSR

Education

1991   Moscow Institute for Physics and Technologies -Professor in Theoretical Physics

1977   Kurchatov Atomic Energy Institute
Dr. of Science Degree in Plasma Physics. Thesis: "Kinetic Processes in Gaseous Lasers", in Russian.

1970   Moscow Institute for Physics and Technologies
Ph D. Degree in Quantum Electronics. Thesis: "Some Problems in the Theory of Elementary Processes and Collisional Kinetics in Gaseous Lasers", in Russian.

1967   Moscow Power Engeneeering Institute, Dept. of Electronics M.S. Degree in Gaseous Electronics. Thesis: "The Theory of Gas Discharge Constriction", in Russian.

Career/Employment

2002-2008	KINTECH: Kinetic stimulations and calculations in gas discharge and electronic systems
2008-Present	KINTECH Lab Ltd: Kinetic stimulations and calculations in gas discharge and electronic systems
1971-Present	Kurchatov Atomic Energy Inst., Moscow. Major Researcher Gaseous lasers, Gas discharge phenomena, Collisional and kinetic phenomena in nonequilibrium gases and plasma, plasma chemistry, instabilities, carbon nanostructures.
1967-1971	Institute of Applied Physics, Moscow; Research Engineer High power gas lasers, Transport phenomena in gases and plasma

Specialization (*specify*)

(i)   main field – theoretical research in atomic physics and its applications in various scientific and technological fields

(ii)   other fields - plasma physics and gaseous lasers physics

(iii)   current research interest: theoretical research in carbon nanostrucres (fullerenes, carbon nanotubes, graphene)

Honours, Awards, Fellowships, Membership of Professional Societies, Conferences Committee

AWARDS: Kurchatov Prize in 1995 and 2011; Soros Professorship in 1998

Publications

- Number of papers in refereed journals: 215
- Number of communications to scientific meetings: more than 50
- Number of books or chapters in books: 6
-Citation index: 2400 (Elibrary)

Physical problems in CNT-based electron field emitters

Eletskii A.V.

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eletskii@mail.ru

High aspect ratio in combination with good electrical conductivity, high mechanical, chemical and thermal stability determine extraordinary electron field emission properties of carbon nanotubes (CNT's) and make them an appropriate element of cold field emission cathodes. Such cathodes provide quite high emission current at a relatively low applied voltage which makes prerequisites for development of low weight portable electron devices as lighting lamps, X-ray tubes etc. A special importance relates to the usage of CNT-based electron field emitters in telecommunication satellite systems for which weight limitations are of the most significance. A wide spread of devices containing CNT-based emitters is hindered by some physical effects limiting operation characteristics of such systems and determining the optimum regimes of their usage. The present report contains the detailed analysis of these effects and describes theoretical approaches to their exploration. There have been considered in detail such effects as statistical spread in parameters of individual CNTs and its influence on the current-voltage characteristics of a cathode, influence of the structure of the CNT's tip upon the field amplification factor, influence of the external and intrinsic electrical field onto the vertical orientation of CNTs comprising the emission array, phenomenon of electrostatic screening of nanotubes limiting the electrical field amplification factor, the thermal instability of the electron field emission that limits the emission current. Combined consideration of the above-listed physical mechanisms permits elaboration of the procedure of optimization of CNT-based cathode. Taking into account both screening effect and the thermal instability results in the optimum inter-tube distance in an array providing the maximum emission current density is determined by not only the height of nanotubes but also the range of operation current. The problem of lifetime of CNT-based electron field emission cathodes is treated in terms of sputtering of the CNT surface under the action of ion bombardment.

Levon Piotrovskiy

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Institute of Experimental Medicine, St. Petersburg, Russia

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Phone: +7 (812) 234-32-38,
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Date and place of birth: April 8, 1947, Leningrad, USSR

Education

Dr.Sci. Organic Chemistry and Pharmacology, 1994, Volgograd Medical Academy, Volgograd, Russia

Ph.D. Organic Chemistry, 1975, Leningrad Chemical-pharmaceutical Institute, St. Petersburg, Russia

Post-educated course in Organic Chemistry, 1970-73, Institute of Experimental Medicine AMS USSR, St. Petersburg, Russia

Leningrad State University (Russia), Chemical Department1965-1970

Career/Employment

2008-present,	Head of laboratory of drug design and nanotechology, Institute of experimental medicine NWB RAMS, St. Petersburg, Russia
1985-2008	Leading Researcher , IEM RAMS, St. Petersburg, Russia
1978-1985	Senior Researcher , IEM AMS USSR, St. Petersburg, Russia
1973-1978	Junior Researcher, IEM AMS USSR, St. Petersburg, Russia

Specialization (*specify*)

(i)   main field   drug design, structure-activity relationship
(ii)   other fields organic synthesis, mechanism of biological activity
(iii)   current research interest biological properties of fullerene C60 and other carbon nanostructures

Practical experience

Synthesis of heterocyclic compounds and peptides, QSAR studies of the ligands of neuronal glutamate receptors, UV-VIS, IR, NMR and other types of spectroscopy, preparation of water-soluble forms of fullerene C60, design of drug delivery systems based on fullerene C60.

Honours, Awards, Fellowships, Membership of Professional Societies, Conferences Committee

A.Oldenburgsky prize, 2010
Member of Russian Chemical Society
Member of Russian Academy of Natural Sciences
Pavlov medal of RANS

Publications
- Number of papers in refereed journals: more than 80
- Number of communications to scientific meetings: more than 120
- Number of books or chapters in books: 6

The biological potential of carbon nanostructures

Piotrovsky L.B.

Institute of Experimental Medicine NWB RAMS, Saint-Petersburg, Russia
levon-piotrovsky@yandex.ru

The unicity of carbon as the element is its ability to form a crowd of nanostructures. As for today we know fullerenes, endohedral fullerenes, single- and multiwalled carbon nanotubes, carbon nanohorns, grapheme, nanodiamonds etc. They can be divided into two groups - compounds, which can be characterized by molecules (fullerenes and endohedral fullerenes); and materials, which can be characterized by distribution of particles by size, mass etc. On the other hand they can be divided by hybridization state of carbon – sp^3 in nanodiamonds and sp^2 in all others. All these structures was more or less may be used in biology.There will by discussed the prospects of the use of different carbon nanostructures for improving the health of mankind, their opportunities and challenges. All carbon nanostructures are nanoparticles, and therefore all problems associated with the use of nanoparticles are related to them. There are the problems of standardization, toxicology etc. And despite some successes it is still long way before they can be used in medicine.

Eugene A. Katz

Ph.D., Professor
Ben-Gurion University of the Negev, Israel

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Date and place of birth: May 5, 1960, Penza, Russia

Short bio: E.A. Katz received a MSc in Semiconductor Materials Science (1982) and Ph.D. in solid state physics (1990) at Moscow Institute of Steel and Alloys. He is Professor of the Ben-Gurion University of the Negev. His research interests include photovoltaics based on non-traditional semiconductors (fullerenes, carbon nanotubes, conjugated polymers), photovoltaic characterization of concentrator solar cells and solar synthesis of nanomaterials. He has published more than 80 papers in peer-reviewed journals on these topics as well as popular scientific book "Фуллерены, углеродные нанотрубки и нанокластеры: Родословная форм и идей" ("Fullerenes, Carbon Nanotubes and Nanoclusters: Genealogy of Forms and Ideas") and a number of popular articles on history of science and fullerene-like structures in nanomaterials, living organisms and architecture.

Career/Employment

2013/present   Full Professor, Department of Solar Energy and Environmental Physics, J. Blaustein Institute for Desert Research, The Ben-Gurion University of the Negev;

1997/2013   Senior Researcher (different grades), Department of Solar Energy and Environmental Physics, J. Blaustein Institute for Desert Research, The Ben-Gurion University of the Negev;

2008   Visiting professor, French National (CNRS) Laboratory of Processes, Materials and Solar Energy (PROMES) and University of Perpignan, Odeillo/ Perpignan, France;

1995/1996   Visiting Scientist, The Ben-Gurion University of the Negev;

1993/1995 Senior Research Fellow, Physics Department, the State Institute of Rare Metals (ГИРЕДМЕТ), Moscow;

1982-1993 Research Fellow (different grades), Laboratory of Shaped Silicon Crystals, R&D Institute of Electro-thermal Equipment, Moscow.

Specialization (*specify*)

(i)   main field: solid state physics

(ii)   other fields: photovoltaics, carbon nanomaterials

(iii)   current research interests: photovoltaics based on non-traditional semiconductors (fullerenes, carbon nanotubes, conjugated polymers), photovoltaic characterization of concentrator solar cells and solar synthesis of nanomaterials.

Practical experience

Investigation of structure and electronic properties of nanostructured and organic semiconductor materials and thin films; photovoltaic characterization of solar cells of various types (including those operated under ultra-high concentration of sunlight)

Honours, Awards, Fellowships, Membership of Professional Societies, Conferences Committee

1999-present time: Member of Israeli Materials and Processes Society;

1999-present time: Member of Israeli Vacuum Society;

1997- 2002, 2005 - 2006: Member of the Materials Research Society;

1997-1998: Member of the Electrochemical Society;

2002 – Member of Advisory Committee of International Conference on Polycrystalline Semiconductors "POLYSE2000";

2003-2005: Member of the European Materials Research Society;

2005 - Ben-Gurion Foundation Judith and Abraham Pasternak prize;

2006: Organizing and Program Committee of the 25th Conference of Israeli Vacuum Society;

2006 - present time: Member of the Ilse-Katz Center for Nanoscale Science and Technology;

2009 - Member of Program Committee of the 8th Torunian Carbon Symposium "Fabrication, Modification and Investigations of Novel Forms of Carbon";

2009 - present time: European Society for Quantum Solar Energy Conversion;

2010: Co-chair of Symposium "Nanophotonics and Biophotonics" at the 14th International Conference "Laser Optics 2010", St.Petersburg, Russia, June 28 - July 02, 2010 ;

2010 – Member of Material Science Committee of Israel Science Foundation;

2010 - Member of Organizing Committee of the French-Israeli Workshop on Renewable Energy;

2010 – Certificate "Outstanding Immigrant Scientist" for "a significant contribution to promoting scientific research and development or social and economic growth in Israel over the last 20 years".

2012 - Co-organizer (co-chair) of symposium "Organic Photovoltaics" at the 38th IEEE Photovoltaic Specialists Conference (Austin, TX, USA).

2012 - Co-organizer (co-chair) of section "Nanophotonics and Biophotonics" at the XV International Conference "Laser Optics-2012" (St.Petersburg, Russia);

2012 – Member of Panel of experts for National Commission of Scientific and Technological Research in Chile (CONICYT).

Publications
- Number of papers in refereed journals: 82.
- Number of papers in Proceedings of scientific conferences: 76.
- Number of books or chapters in books: 4.
- Number of popular science papers and papers on history of science:25.

Fullerenes, nanoclusters and nanotubes: forms and structures (from mathematics to physics, biology and architecture)

Katz E.A.

Department of Solar Energy and Environmental Physics, J. Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede Boqer, Israel
keugene@bgu.ac.il

The discovery of C_{60}, a third variety of carbon, in addition to the more familiar diamond and graphite forms, has generated enormous interest in many areas of physics, chemistry and material science. Furthermore, it turns out that C_{60} is only the first of an entire class of closed-cage polyhedral molecules consisting of only carbon atoms - the fullerenes (C_{20}, C_{24}, C_{26}, … C_{60}, …C_{70}, … C_N, carbon nanotubes). This talk presents main principles for "design" of fullerene-like structures (based on symmetry considerations and Euler theorem on the relation between the numbers of faces, vertices and edges in polyhedra). We will discuss how Nature uses fullerene-like structures for minimization of energy and matter resources in molecules and nanoclusters, viruses and living organisms. Examples of achievement of such goals in architecture are also presented.

The discovery of fullerenes is a brilliant example of merging of different areas of science. We will discuss these distant (at first glance) scientific areas in the context of history of discoveries and the personalities of the discoverers [1] following James Clerk Maxwell's statement: "In Science, it is when we take some interest in the great discoverers and their lives that it becomes endurable, and only when we begin to trace the development of ideas that it becomes fascinating".

[1]   E. A. Katz, Fullerenes, Carbon Nanotubes and Nanoclusters: Genealogy of Forms and Ideas [in Russian] (Editorial URSS, Moscow, 2009, 2nd Edition). Е. А. Кац. Фуллерены, углеродные нанотрубки и нанокластеры: Родословная форм и идей (УРСС, Москва, 2009, 2ое издание).

Vladimir Osipov

Ph.D., Senior Scientist
Ioffe Physical-Technical Institute, St. Petersburg, Russia

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Email: osipov@mail.ioffe.ru

Vladimir Osipov was born in 1964 and received the degree of Electrical Engineer (Honors E.E.) in the field of "Optoelectronics and Optoelectronic Devices" in 1987 from Leningrad Electro-Technical Institute (LETI), Faculty of Electronics, Department of Optoelectronics. He joined the Ioffe Institute, Russia in 1987 as researcher and received his PhD on the speciality "Semiconductor and Dielectric Physics" in 1994 from Ioffe Physical-Technical Institute. He was appointed as senior scientist in 1999. He was a visiting Associate Professor (2002) and JSPS Fellow in Tokyo Institute of Technology (2004–2005). His research interests include magnetic, electron spin resonance and optical properties of edge-localized states in nanographites, defects in diamonds, and some issues of nonlinear optics. He is an expert in preparation of multishell nanographites and use the electron spin resonance technique for detecting π-electronic oxygen-sensitive edge-localized spin states of nanographene having unconventional electronic properties. Together with his international collaborator he first found the new unique X-band ESR signatures of NV- defect and multivacancy in diamonds in the half magnetic field region. Currently he is the head of Ioffe Institute team participating in the bilateral project under the Japan-Russia Research Cooperative Program and supported by Russian Fund for Basic Research and Japanese Society for Promotion of Science. He is the author of more than 65 papers in refereed journals and books.

Nanographites: edge-localized states and their unconventional electronic properties

Osipov V.Yu.

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Nanographenes and nanographites (NG) with open edges are the especial members in the nanocarbon family having unconventional electronic and magnetic properties. These properties are related with the existence of π- electronic edge-localized states giving a sharp peak in a density-of states between bonding (π-) and antibonding (π*-) bands. Both activated carbon fibers and multishell nanographites (MSNG) derived from nanodiamonds have the highest concentration of edge-localized spin states ($>5\text{-}10\times10^{18}$ g^{-1}). MSNG particles (mean size ~6 nm) consist of turbostratic graphitic blocks with in-plane crystalline size ~ 3.5 nm [1]. The specific surface area of MSNG is about ~450-500 m^2/g and defined by the surface of outermost graphitic shell having a lot of cracks, holes, split-off nanostrips and other cooperative defects. The edges of MSNG particles are terminated by atomic hydrogen, hydroxyl, carboxyl and carbonyl groups.

π-electronic edge-localized spins located on the outermost carbon atoms of zigzag chains are spin-polarized and can be considered as an entities with total magnetic moment depending upon the whole number of zigzag carbon atoms in the short chain. Usually the graphene edge of arbitrary shape consists of a number of zigzag chains having from ~3 to ~7 zigzags. Each outermost aromatic ring adjacent to the zigzag edge has the small magnetic moment which value does not exceed ~0.1-0.2 Bohr magnetons. At the same time the partial amount of electron density on a per edge carbon edge site is about ~0.14·e when the zigzag edge is terminated by atomic hydrogen. Few magnetic moments M_i localized on the different sides of one graphene sheet can interact antiferromagneticaly through mediation of magnetic interaction by conducting π- electrons. The resulting spin paramagnetism of MSNG particles is fairly described by contribution of spins S=$^1/_2$, where each MSNG particle has one or two spins ½ [2]. This fact is not trivial and need to be more elucidated from viewpoint of basic theory of spin-half paramagnetism. The in-plane orbital diamagnetic susceptibility of MSNG is ~ 4 times smaller than that for bulk graphite having the largest orbital susceptibility (χ = -22×10^{-6} emu/g) among all substances.

Zigzag and armchair edges of nanographites are also responsible for appearance of disorder-induced D-band (~1350 cm^{-1}) in the Raman spectrum of material. The band at ~1520 cm^{-1} (A-band) is related with 5- and 7- membered carbon rings clusters. Thus, the concentration of edges, defects and in-plane crystallite size of MSNG particles can be well controlled by Raman spectroscopy [3].

The edges of nanographites demonstrate unconventional chemical activity, therefore the nanographites may be used as catalysts of many technologically important chemical reactions. This is because the edges can easy accept or donate electrons from the molecules disposed near the edges and create intermediate exchange-coupled ion complexes with ions and ion-radicals of some molecules like O_2. Guest molecules physisorbed on the graphitic planes of NG particles can be used for probing the π- electronic system of nanographene sheets and their edges. Oxygen molecules in triplet state (S=1) are the most effective removable paramagnetic probes

for studying the paramagnetic properties of edge-localized spin states with extended wave function [4].

[1]   V.Yu. Osipov, T. Enoki, K. Takai, et al. *Carbon*, 2006; **44**(7): 1225-34.
[2]   V.Yu. Osipov, A.I. Shames, T. Enoki, et al. *Diam. Rel. Mater.* 2009; **18**(2-3): 220- 23.
[3]   V.Yu. Osipov, A.V. Baranov, V.A. Ermakov, et al. *Diam. Rel. Mater.* 2011; **20**(2): 205-09.
[4]   V.Yu. Osipov, A.I. Shames, T. Enoki, et al. *Diam. Rel. Mater.* 2010; **19**(5-6): 492- 95.

Evgeny D. Eydelman

Ph.D., Professor, Senior Scientist
[1]Chemical-Pharmaceutical Academy, St. Petersburg, Russia
[2]Ioffe Physical-Technical Institute, St. Petersburg, Russia
[3]Academic University RAS

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Email: Evgeny.Eidelman@pharminnotech.com,
Eidelman@mail.ioffe.ru

Date and place of birth: July 10, 1945

Education

1968	M. S. In Physics Engineering Technical Univ. (Polytechnical Institute), St. Petersburg
1985	Ph. D. In Theoretical Physics, Technical Univ. (Polytechnical Institute); St. Petersburg
1986	M. S. in Mathematics, Pedagogical Univ.
1995	D. Sc. in Theoretical Physics, Ioffe PTI

Career/Employment

2011-date	develop the theory of aggregation in diamond nanoparnical suspensions
2009-date	develop the theory of Heat properties of metal – diamond nanopartical composites
2005-2012	develop the theory of optical and reological properties of diamond nanoparnical suspensions
2003-2011	develop the theory of Thermoelectric effect by ballistic phonon drag of electrons in carbon manostructures
2002-2010	developed the theory of Cold field emission Cathode based on carbon manostructures
2000-2005	investigated a description of the frontiers between the science and pseudoscience
1998-2002	formulated a Theory of Instability on GaAS surface at Helium temperatures in the microwave field
1997-date	develop a mathematical and physical description of resalts of experiments in biological and Chemical investigations of Pharmaceutical Substances
1996-2002	headed a reseach group that analyzed basic concepts of Conformation of Macromolecule
1995-1997	headed a reseach group that analyzed the role of Electrical field in the Mechanism of a Molten Zone formation under the Action of Laser Emission
1985-1995	developed a new aspect of Convection – Thermoelectrical Convection. Predicted some experiments, for example, the Penetration of alloying

	materials into the sample. For summery, see "Excitation of an electric instability by heating" Physics-Uspekhi, v. 38, N 11, 1995
1968-1995	developed a theory of Cosmological Expansion of the Universe. Predicted Rotation as result of Relativistic Expansion
1975-2002	elaborated a Theory of Convection in

1968-1995 developed a theory of Cosmological Expansion of the Universe. Predicted Rotation as result of Relativistic Expansion

1975-2002 elaborated a Theory of Convection in
 a) Liquid Dielectrics
 b) Liquid Helium
 c) Liquid Semiconductors
 d) Liquid Crystals
 e) Liquids with Compressibility
 f) Electron – Hole Gas

1968-1980 formulated theory of the Stellar Magnetic Field Generation

1970-date developed methods of Physics Education for Pupils, Student and Teachers.
Scientific Advisor of number of M. S., Ph. D. students.

Honours

Soros Professor 1997 and 1998

Professor of St.-Petersburg 2004

Publications

Over 120 article in major International Scientific Journals and 9 books.

Basic once

[5] E.D. Eydelman "Physics with elements of biophysics" Textbook 2013. C.512 (in Russian)

[6] A.P.Meilakhs, E.D.Eidelman. New Model of Heat Transport across the Metal-Insulator Interface by the Example of Boundaries in a Diamond-Metal Composite. *JETP Letters* 2013,v.97,N1, pp.38-40

[7] A.Ya.Vul', E.D.Eydelman, A.E.Aleksenskiy,. L.V.Sharonova, S.V.Konjakhin Absorption and scattering of light in nanodiamond hydrosols . *Diamond and Related Materials*,2011,v.20, Is.3, p.279-284.

[8] K.B.Reich, E.D.Eidelman. Effect of electron-phonon interaction on field emission from carbon nanostructures. *EuroPhys. Letters*, February 2009,v.85,47007-1-5.

[9] A.Ya Vul', E.D.Eydelman, M.Inakuma, E.Ōsawa. Correlation between viscosity and absorption of electromagnetic waves in an aqueous UNCD suspension. *Diamond and Related Materials*, 2007, v.16, Is.12, p.2023-2008.

[10] E.D.Eidelman, A.Ya Vul'. The strong thermoelectric effect in nanocarbon generated by the ballistic phonon drag of electrons. J.*Phys.: Condens. Matter*, 2007, vol.19, N26, pp. 266210-22.

[11] E.D.Eidelman. Conformational Properties of Macromolecules in Two-Phase Systems *Polymer Science*, 2000, ser. A, v. 42, N 4, p 405-411.

[12] E.D.Eidel'man. Thermoelectric Convection in a Liquid Layer in the presence of a Longitudinal Temperature Gradient. *JEPT*, 1996, v.38, p.490-494.

[13] E.D.Eidel'man.Excitation of an Electric Instability by Heating. *Physics-Uspechi*, 1995, v.38, N11, p.1068-1083.

[14] E.D.Eidel'man. Some aspects of Relativistic Motion that depends on the spatial variable *Theoretical and Mathematical Physics*, 1995, v.103, N1 (april), p.412-423.

[15]   E.D.Eidel'man. Calculation of the Relative Dimensions of a Region Heated by a Laser Beam *JEPT,* 1994, v.78, N2, p.157-158.

[16]   E.D.Eidel'man. Thermoelectric Convections in a. Horizontal Fluid Layer *JEPT,* 1993, v.77, N3(9), pp.428-434.

[17]   I.V.Ioffe, E.D.Eidel'man. Regarding the Theory of the Instability of a Metal Layer melted by a Light Beam. *Sov. Tech. Phys. Letters*, 1989, v.15, N 1, p.41-42.

[18]   I.V.Ioffe , B.I.Lembricov, E.D.Eidel'man. Anomalies convection gradient of temperature in Liquid Crystals. *Sov. Tech. Phys. Letters*, 1976, v.2, N 10, p.361-362.

[19]   A.D.Chernin, E.D.Eidel`man. Interaction between vortex and potential motions in relativistic hydrodynamics I *Astrophysics*, 1969,v.5,pp.337-338

Thermoelectric effects in carbon nanostructures

Eydelman E.D.

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The thermoelectric power [1] and thermoelectric figure of merit in carbon nanostructure consists of graphite-like (sp^2) and diamond-like (sp^3) regions have been investigated. Probability of electron collisions with quasi-ballistic phonons in sp^2 regions has been analyzed [2]. We have shown that the probability is not small. We have analyzed the influence of various factors on the process of electron-ballistic phonon drag effect (phonon drag effect). The thermoelectric power and thermoelectric figure of merit under conditions of ballistic transport were found to be substantially higher than those in the case of the drag by thermalized phonons or of electron diffusion. The thermoelectric figure of merit (ZT) in the case of a ballistic phonon contribution to the phonon drag of electrons should be in 50 times higher for chaotic phonons and 500 higher than that in the case of diffusion process. In that case the ZT should be record ($ZT \geq 2$-3).

In this presentation we investigate contribution of the phonon drag into thermoelectric current in grapheme also [3]. We studied the situation of the free standing graphene with the degenerate gas of carriers and took into account the interaction with intrinsic acoustic phonons. The contribution from phonon drag to the thermoelectric power depends on Fermi energy and phonon relaxation time and do not depends on temperature like diffusion contribution. The dependencies of these terms on the temperature and Fermi energy principally divers, which allow expecting that for low temperatures, high densities of carriers and the samples with high thermal conductivity the contribution of phonon drag, can become dominant.

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Expert in:
Physical chemistry of surfaces, ordered molecular films (LB-films, lyotropic liquid crystal films, self assembling systems)

Specialization
Scanning probe microscopy (STM, AFM, SNOM, ...)
Nanotechnology, nanoelectronics, molecular nanotechnology
MEMS for nanotechnology and scanning probe microscopy
Biosensors (creation of new types of biosensors)
Self assembling technology, LB – technology

Technologies of atomic force microscopy and scanning spectroscopy for carbon nanostructures investigations

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During last years the development of SPM technology was transformed to the side of specialization. The application field was increased very wide – from one side micro- and nanoelectronics with extra high-level the metrology requirements and up to material science, biology, ecology with requirements to the side of simplification in operation procedures, possibility of the materials and molecules recognitions.

Carbon materials, such as nanotubes, graphene, diamond are in the list of the most interested perspective materials as for nanoelectronics, MEMS and NEMS, composite materials.

Carbon materials are very for the high intensity of light action do them convenient objects for Raman spectroscopy investigations.
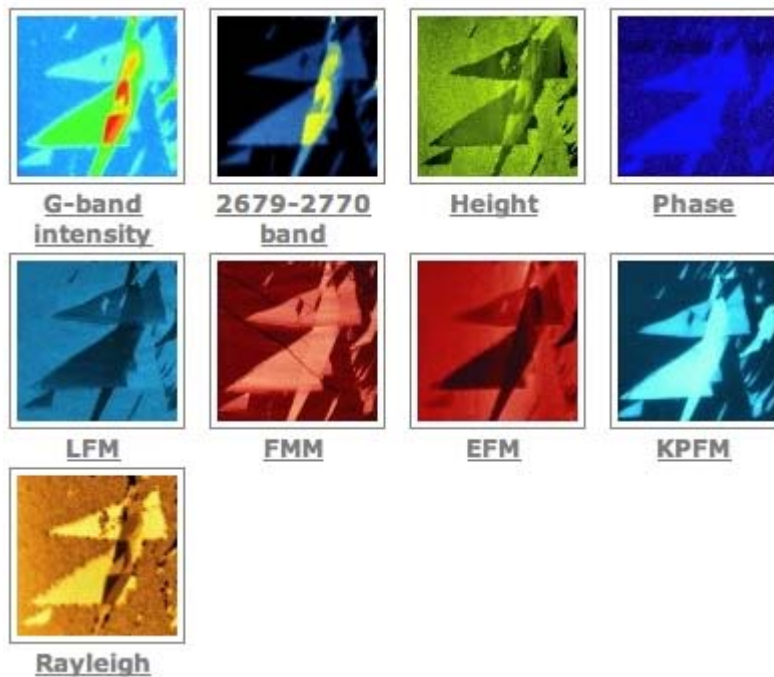
Fig. 1. Multimode AFM image of graphene on the gold substrate. Data courtesy: E. Kuznetsov, S. Timofeev, P. Dorozhkin, NT-MDT Co. (http://www.ntmdt.com/scan-gallery/scan/graphene-flakes-on-gold-substrate).

Scanning Probe Microscopy gives an opportunity to carry out studies of spatial, physical and chemical properties of objects with the typical dimensions of less than a few nanometers. Owing to its multifunctionality, availability and simplicity, Atomic-Force Microscope (AFM) has become one of the most prevailing "tools for nanotechnology" nowadays. NTEGRA platform has been designed as the special base for the constantly developing options of Scanning Probe Microscopy that combines them with various other modern research methods. Integration of SPM and confocal microscopy / luminescence / Raman scattering spectroscopy. Owing to the effect of

giant amplification of Raman scattering (TERS – Tip Enhances Raman Scattering) it allows carrying out spectroscopy studies and obtaining images with 50nm resolution.

Progress in micromechanics manufacturing resulted in significant increase of the cantilever yield rate (to practically 100%) with repeatability of resonant characteristics at 10% level, thus preconditioning implementation of the concept of multi-probe cartridges for AFM.
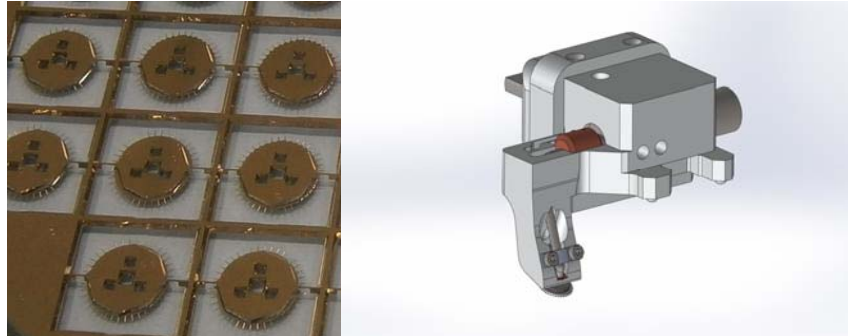
Fig. 2. Part of multi-probe cartridge and SPM head with multi-probe cartridge for scanning probe microscope NEXT.

A cartridge of this type is a multi-probe contour-type sensor with 38 cantilevers. A cantilever to operate is selected by a control program using optical feedback. The cantilevers can be either of the same type or "colored" with predefined coverings and rigidities. A cartridge can be exchanged manually through a simple procedure. The cartridges operate in dedicated measuring heads, which are designed for integration in the latest instruments by the Company (NEXT, OPEN, SOLVER-NANO, EDUCATOR-II).

Development of modes for scanning spectroscopy combined with SPM in the instruments NTEGRA-SPECTRA and SPECTRUM provides new options of confocal laser luminescence spectroscopy and Raman spectroscopy as well as higher reliability of detection for TERS and high-resolution magnetic resonance probe-optical spectroscopy. Probes with diamond nanocrystals containing N-V defects are capable to detect magnetic states as microscopic as single spins and so they are promising for studies of surface catalytic activity and for detection of free radicals, including applications in biology and medicine.

Young Scientists Contributed Papers

The low temperature heat capacity of the C_{60}-CH_4 solution

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The heat capacity (C) of the interstitial solution $(CH_4)_{0.39}(C_{60})_{0.61}$ prepared by introducing CH_4 molecules into the octahedral interstitial sites of the C_{60} lattice has been investigated in the temperature interval 1.2-120 K using an adiabatic calorimeter [1]. The contribution (ΔC_{CH4})of the CH_4 molecules to the heat capacity (C) of the solution has been separated. It is shown that in the region T=10-35 K the heat capacity ΔC_{CH4} is described adequately by the sum ($\Delta C_{calc}=C_{tr}+C_{lib}+C_{tunn}$) of the contributions made by translational and rotational vibrations as well as by the tunnel rotation of the CH_4 molecules. C_{tr} and C_{lib} were calculated within the Einstein model. It is assumed that the discrepancy between $\Delta C_{CH4}(T)$ and ($\Delta C_{calc}(T)$ at $T = 40 -90$ K is due to the effect produced on the rotational motion of the CH_4 molecules by the change in the rotational motion of the C_{60} molecules in the course of the formation of an orientational glass. Above 90 K the character of the rotational motion of the CH_4 molecules changes from libration vibrations to hindered rotation. The contribution of tunnel rotation $C_{tunn}(T)$ of the CH_4 molecules to the heat capacity $\Delta C_{CH4}(T)$ is dominant below 6 K. The effect of the nuclear spin conversion of the CH_4 molecules upon the heat capacity $C_{tunn}(T)$ has been revealed. The feature observed in the dependence $\Delta C_{CH4}(T)$ near T=9 K may be an exhibition of a first-order phase transition in the orientational glass of the CH_4-C60 solution [2].

The contributions of the CH_4 and CD_4 molecules to the heat capacities of the $(CH_4)_{0.39}(C_{60})_{0.61}$ and $(CD_4)_{0.397}(C_{60})_{0.603}$[3], respectively, have been compared. The highest isotopic effect was observed in the region T<6 K where the contributions of the tunnel rotation $C_{tunn}(T)$ of the CH_4 and CD_4 molecules to the heat capacity ΔC_{CH4} and ΔC_{CD4} are dominant.

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Processing and characterization of epoxy nanocomposites modified by multi-wall carbon nanotube Graphistrength® C S1-25

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Carbon nanotubes have the potential to realize electrically conductive polymer nanocomposites with improved or retaining physical mechanical performance [1].

Structure and properties of nanocomposites based on bisphenol-A epoxy resin (ED-20), anhydride hardener system and master batch Graphistrength® C S1-25 are investigated. Master batch contained 25% by weight multi-wall carbon nanotubes (MWCNTs). To prepare compositions master batch was diluted many times with epoxy resin at 80°C. The MWCNTs were dispersed in uncured matrix by sonification and the stirring process in high speed mixer (2000 rpm) at room temperature for 30 min. Nanotubes weight fraction in prepared formulations were varied in the range 0.1 to 1.3%. Prepared formulations were cast in mettle moulds to produce cured bulk nanocomposites at 140°C for 120 min/

Electrical and thermal properties of nanocomposites were studied. Volume electrical resistivity measurements were taken by the standard technique. Thermal properties were performed by differencial scanning calorimetry (DSC). Structure of MWCNTs in master batch and in diluted state was determined by wide angle X-ray scattering method (see figure below).
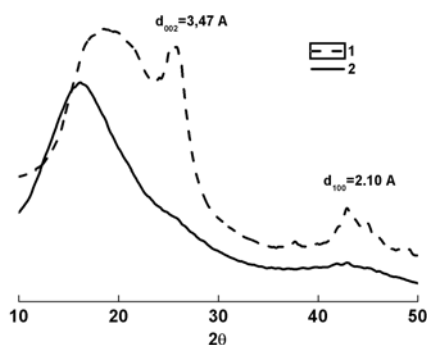
Fig. 1. Wide angle X-ray scattering patterns of the Graphistrength® C S1-25 (1) and the epoxy compound containing 1.3% by weight CNTs (2).

It is seen on the figure that both peaks in the range of $2\theta = 27$ and $43°$ due to MWCNTs are present in the composite containing 1.3 w% CNTs. Peak in the range of $43°$ corresponding to d_{100}-spacing of 2.10 Å representative of crystalline structure of the graphite (cell constant along graphite layer). Peak in the range of $27°$ ($d_{002} = 3.47$ Å) is characteristic of turbostrate structure in carbon fiber and seems to relate with distance between coaxial tubes in MWCNTs.

It is shown that MWCNTs in the range 0.1 to 1.3 w% does not strongly influence the glass transition temperature (T_g) of epoxy nanocomposites. The maximum rise of T_g is about 2°C.

Nanocomposites containing more than 0.2% by weight MWCNTs become electrically conductive. The bulk percolation threshold under optimal aggregation conditions is about 0.18% by weight MWCNT. An attempt was made to evaluate the aspect ratio of carbon nanotubes under study.

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Field electron emission from carbon films fabricated by magnetron sputtering

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Nanodispersed carbon films demonstrate high efficiency if field electron emission: currents produced by such objects are typically a few times greater than for the case of three-dimensional structures [1]. Many authors reported on dependency of between quantities of sp^2 и sp^3 carbon phases in nanodipersed films and substrate temperature maintained during film deposition [2]. There is little doubt that the sp^2/sp^3 ratio affects field-emission properties of a film. Therefore we performed direct experimental study of correlation between film growth temperature and its field emission activity.

Carbon films with normalized thickness of tens through hundreds of nanometers were deposited at silicon substrates by magnetron sputtering. Substrate temperature during the film growth process was maintained at a value from the range 200..800°C. An atomic force microscope (Pacific Nanotechnologies Inc., model NanoDST[tm]) was used to obtain surface morphology images (Fig.1) for films deposited at different temperatures from the indicated range.
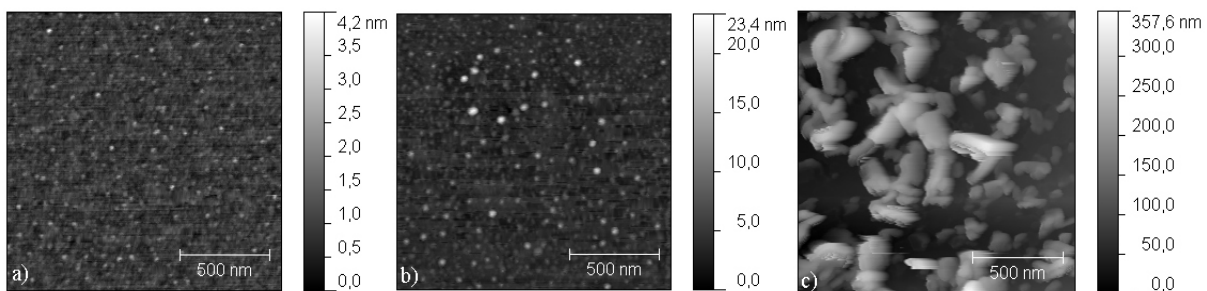
Fig.1. Surface morphology images for films deposited at: (a) 400°C ; (b) 700°C; (c) 780°C.

The performed experiments demonstrated that only film prepared at 700..770°C reveal field emission activity. A series of samples was fabricated with deposition temperature values covering this range with the step of 10°C. Their surface was investigated with the atomic force microscope, and emission threshold field values were determined as a characteristic of emission activity.

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Ab initio study of atomic structure and surface states of graphene covered MnO polar (111) surfaces

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Magnetism in graphene is of great technological interest due to potential applications in spintronic devices [1]. In the present work we perform an extensive first-principles calculations of graphene/MnO(111) interfaces using projector-augmented wave (PAW) method [2] within DFT framework.

Both manganese an oxygen terminated surfaces covered by a single-layer graphene are considered. It is shown that for oxygen terminated surface graphene forms chemical bonds with the substrate, while for Mn-terminated surface no bonding was found. Formation of the bonds breaks the planar atomic structure of graphene that results in emergence of the ripples. Equilibrium distance between substrate surface and graphene changed from 2.5 to 3.9 Å due to different terminations.

We demonstrate the occurrence of local magnetic ordering in graphene depending on the antiferromagnetic ordering of the substrate and chemical bonding with surface atoms. It is also shown that band structure of the interface near the Fermi level is strongly depends on the spin direction. In particular we predict the mobility of majority-spin electrons by an order of magnitude higher than that of minority-spin.
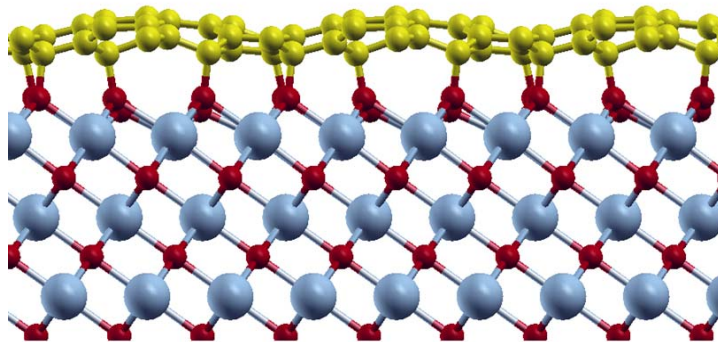
Fig. 1. Fragment of the completely relaxed interface graphene/MnO(111). Here the substrate terminated by oxygen is used.

For several interfaces and spin projections the values of charge carriers effective mass were estimated from analysis of the dispersion law.

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Biosensors based on composites of aligned carbon nanotubes and RNA

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Biosensors are the devices converting the chemical information into an analytical signal, in which the recognition system has a biochemical nature and uses reactions involving the individual biomolecules or biological supramolecular structures. In this work we present results of the development of biosensor based on array of aligned carbon nanotubes and modified RNA molecules and the study of electrochemical activity of the biosensor.

Aligned carbon nanotubes were grown over silicon substrates by chemical vapor deposition (CVD) method from 2% solution of ferrocene in toluene at 700° C. The attachment of oligonucleotides or their pyrene derivatives PyrpA(pA)$_9$ on the surface of nanotubes was carried out by the formation of noncovalent complexes from aqueous solutions at room temperature. Pyrene derivatives of oligoribonucleotides were obtained following the procedure [1]. In the case of unmodified oligoribonucleotides noncovalent interactions with the nanotube is due to stacking interactions of heterocyclic bases with the surface of the nanotube.

Measurement of electrochemical properties of the electrodes was performed by cyclic voltammetry with linear potential sweep in a three-electrode cell with an Ag/AgCl reference electrode. Solutions of (pU)$_{12}$ and (pC)$_8$ oligonucleotides, which were complementary or non-complementary to RNA molecules deposited on the nanotubes, was used as an electrolyte. The cacodylate buffer was used as a reference. The kinetic changes of electrochemical properties of the composites were determined based on the cyclic voltammograms plotted using the data obtained.

Modification of RNA by pyrene (***Pyr***) allowed avoiding the biomolecule displacement from the nanotubes surface upon its hybridization with a complementary oligonucleotide. In this case, voltammograms obtained are different from the voltammograms for the first type of biosensor. The curves exhibited peaks at 270 mV (charge) and 610 mV (discharge) corresponding to the complementary duplex forming between (pA)$_{10}$ and (pU)$_{12}$. In experiments with non-complementary oligonucleotides the peaks were not observed. Also interaction between nanotubes/PyrpA(pA)$_9$ composite and (pU)$_{12}$ resulted in significant increase of the electrode capacitance. In the case of use of PyrpA(pA)$_9$ the form of cyclic voltammogram was close to the square indicating the high activity of the material.

Thus, it is shown that composites of aligned carbon nanotubes and modified RNA can be used as material for biochemical sensors due to their ability to record formation of RNA duplexes on the surface of the nanotube using electrochemical methods.

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Importance of detonation nanodiamonds post-synthetic processing

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Synthesis conditions, methods of detonation nanodiamonds (DND) allocation and post-synthetic processing impact on surface properties. We can regulate the surface properties of DND particles by changing technology of blasting, processing or DND drying.

In this work we have investigated how post-synthetic DND drying influences colloidal and chemical properties. Three DND samples, synthesized by blasting in the water environment were used for this research. But different ways of drying them have been used, namely, drying by evaporation, convection drying, flash drying.

A comparative studying of extent oxidation of the particles' surface of the DND depending on type of drying has been carried out according to the Chugayev-Tserevitinov's method. Besides, additional drying has been held in two ways: vacuum and sublimation drying. After carrying out these works, also, extent oxidation of the particles surface of the DND has been investigated and comparative results have been obtained (Fig. 1).
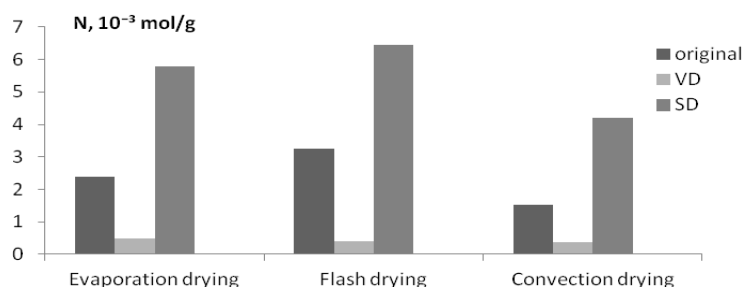
Fig. 1. Number of hydroxyl groups (10^{-3} mol/g), depending on a method of post-synthetic and additional drying

In the picture 1, we can see, that flash drying gives the biggest oxidation extent of the surface, and convection drying – the smallest. Picture 1 data shows that vacuum drying (VD) sharply reduces a hydroxyl group's concentration on the DND surface. However, sublimation drying (SD) leads to some growth of these groups. This growth of hydroxyl groups is explained, probably, by increasing of BET surface area, because of a DND units' disaggregation, stabilized by hydrogen communications. So, convection drying provides formation of the densest particles DND units.

During the research, also, the time dependence of carrying out the reaction of extent oxidation of a surface of the DND from a way of drying has been studied. Packing density of the DND units has been estimated by data of the kinetic analysis of this method.

Structures of the DND suspensions in polar and unpolar environments have been estimated by the method of dynamic light scattering. The analysis of these experiments has allowed to estimate parameters of curves polydispersion of the DND units, and also estimate indirectly the hydrophobic-hydrophilic balance of the DND units' surface, drained in the different ways.

By the results of the work, the conclusion has been made that a different choice of post-synthetic drying technology is a perspective way of receiving the DND with in advance set colloidal and chemical characteristics, for example, such as particles dispersion of the DND, their specific surface, a oxidation extent of surface.

Electron field emission features of carbon nanostructured cathode

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It is well known that at present there has been an increased interest in field electron emission of carbon nanostructured cathode . First of all it is caused efficiency low voltage emission of carbon fibers.

The field emission properties have been examined in the vacuum diode system by applying voltage between the emitter (cathode) and a flat anode. The cathode was make from carbon fiber by diameter d = 7μm and height h= 7 mm and have emitting end surface. The emitting surface consists of nanosized fibrils. The pressure of residual gas P= 10^{-5}–10^{-7} Torr.

Experimental studies have shown that the carbon cathode with the above characteristics performs mechanical vibrations in the field electron emission process [1].

Researches of field electron emission together with cathode mechanical vibrations process in a vacuum diode conducted. Diode system consists of a carbon cathode and a flat anode. Cathode - anode distance was 1 mm. The researches were conducted under various current limit through an external circuit. Limiting resistances R_1 = 1 Mom and R_2 = 10 MOm was used. Operating voltage of the diode was U_{AC} = 0.70 - 1.25 kV.

Researches process showeded a significant influence of limiting resistance on the field electron emission.

When R_1 = 1 Mom, the voltage drop across the resistor R_1 is U_{R1} = 20 V at the maximum emission current I = 20 μA. U_{AC} redistribution between the diode and R_1 has little influence on the emission mode.

The use of restrictive resistance R_2 = 10 Mom leads to a fundamental changes in the emission mode and mechanical vibrations mode. The current reaches I = 10 μA in the range of operating voltages U_{AC}. In this case, the voltage drop across R_2 is U_{R1} = 50 - 100 V. Such redistribution U_{AC} has a significant impact the emission characteristics and the process of cathode mechanical vibrations. In case of R_2 current may differ from current in case of R_1 by 25 – 50 % in the voltage range U_{AC} = 1.05 - 1.25 kV. Simultaneously decreases the amplitude of the mechanical vibrations.

Current growth slowed relative to current voltage characteristic at R_1 in this voltage range. This is probably due to a growth of the voltage drop at limiting resistance with increasing current. Indeed, in the range of U_{AC} = 1.05 - 1.25 kV current has a value I = 5 - 10 μA, which determines the voltage drop U_{R2} = 50 - 100 V on R_2. The dependence I (U_{AC}) shows that when the U_{R2} = 50 - 100 V current can change by 25-50%, i.e. has a significant influence on the emission process.

Thus, the field electron emission researches of nanostructured carbon fiber showed that on the collaborative process of emission and cathode mechanical vibrations have a significant influence the limit current conditions in the external circuit.

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The filling of single-walled carbon nanotube channels is a method of directional modification of their electronic properties

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In the absence of synthetic protocols for the preparation of single-walled carbon nanotubes (SWCNTs) with a specified diameter and structure, the control of the electronic properties can be achieved through the controllable formation of defects, chemical modification of tubular external surface (e.g. decoration or coating) or filling of the SWCNT channels with appropriate substances. An internal channel of carbon nanotubes has been shown to serve as a template for the growth of one-dimensional crystals of metal halides, chalcogenides and other substances. It should be noted that despite the large number of reports on the development of synthetic procedures, theoretical and experimental studies of the atomic and electronic structure of such nanostructures, direct information on the electronic structure is still lacking in many cases.

The aims of our study were the filling of single-walled carbon nanotubes with inner diameter of 1.4 nm with metals (Ag, Cu), metal halides ($MHal_2$, where M=Fe, Co, Ni and Hal=Cl, Br, I) and metal chalcogenides (SnX, Bi_2X_3 and GaX, where X=S, Se, Te) and the investigation of influence of these substances on the electronic properties of SWCNTs. The obtained nanocomposites were investigated by high-resolution transmission electron microscopy, Raman spectroscopy, optical spectroscopy, X-ray absorption spectroscopy and X-ray photoelectron spectroscopy (XPS).

The X-ray photoemission and Raman spectroscopy data show no noticeable interaction between the 1D SnX, Bi_2X_3 and GaX crystals and the SWCNTs, except for a minor influence of the intercalated crystals on metallic SWCNTs. This suggests that these nanocomposites are well-suited model systems to study the physics of non-interacting 1D-crystals. It was found that metals and metal halides influence the electronic properties of nanotubes in the opposite way. According to the XPS measurements, the insertion of metals results in an increase of the SWCNTs Fermi level and the charge transfer from metal nanoparticles to carbon nanotubes (donor doping of SWCNTs). At the same time, in the nanocomposites on basis of carbon nanotubes filled with metal halides there are a decrease of the SWCNTs Fermi level and the charge transfer from nanotube walls to 1D nanocrystals (acceptor doping of SWCNTs). Thus, the filling of the SWCNT cavities with proper substances allows performing a direct modification of nanotube electronic properties..

The electron-phonon matrix element in the Dirac point of graphene

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Electron-phonon interaction can affect transport properties of extremely pure graphene and consequently its investigation is important for creating the electronic devices based on graphene layers. The conductance and the valence bands in graphene are well described within the tight-binding model. Finding the phonon dispersion of graphene employs here the harmonic crystal approximation [1]. Finally the deformation potential approximation [2] was used here to treat the changes in electronic structure of the crystal after variation of bond lengths caused by phonon.
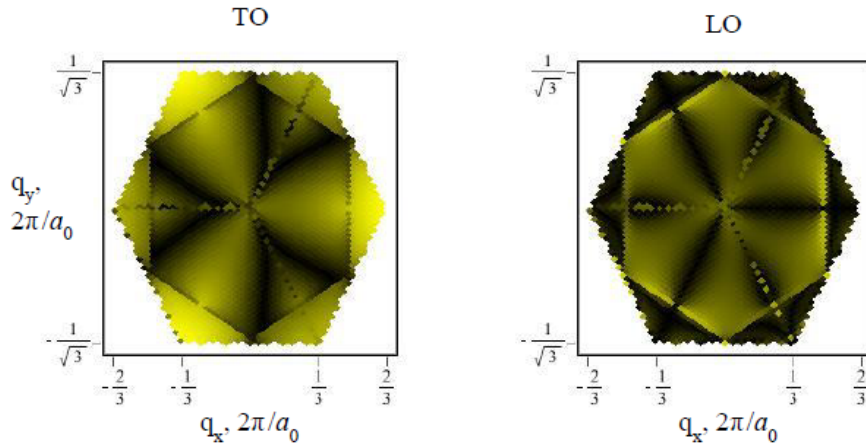
The electron-phonon matrix element for optical modes. Lighter areas correspond to larger absolute value of M_{e-ph}.

High anisotropy of the electron-phonon matrix element can be directly seen from figure. Patterns obey D_{3h} symmetry, which is strictly necessary for the K point. Generally the directions in Brillouin zone and segments of hexagonal Brilloiun zone with high and low values of the electron-phonon matrix element match to ones from [3]. So for the TO phonon mode the singularities around K points and low values near unequivalent K' points are similar. However in [3] authors predict zero absolute value of matrix element for TO mode in the center of Brillouin zone, and it differs from results above.

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Investigation of low-aspect-ratio carbonic field-emission nanostructures

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Numerous experimental investigations performed in the recent decade demonstrated the capability of diverse nanocarbonic structures to yield electron field-emission current in moderate electric field (~1 V/μm or less). Up to date, the best results have been obtained with carbon nanotube arrays. Their high emission efficiency is explained by concentration of the applied field at small areas (tips). Though, the high field strength at these spots results in relatively fast degradation of emitters. Hence, structures with "smoother" surface morphology providing lower field enhancement at surface elements may have even better prospects for practical applications.

The main objective of the presented work consisted in experimental verification of the hypothesis that conductive nanoparticles electrically insulated from the rest of the emitter can serve as active emission sites [1]. When external field is applied, a potential difference appears across the junction between such particle and the substrate, which eventually results in tunnel current through the junction. The electrons injected in the particle have energies above the thermodynamically equilibrium value. Characteristic time thermalization of "hot" electrons in nanocrystallites is very high, which increases probability of their emission into vacuum and thus determines enhanced efficiency of the emitter.

We experimentally investigated emission properties (*I-V* curves, area distributions of emission current) of nanostructured carbon films fabricated by methods of chemical deposition and magnetron sputtering. Sample surface morphology was characterized using AFM and SEM methods before and after the emission tests. Structure of the films was studied by x-ray diffractometry. Some of the samples initially including a fraction of amorphous sp^3 carbon were subject to *in-situ* thermal treatment in the course of the emission tests. This treatment led to graphitization of amorphous carbon and, for some of tested structures, to consecutive transformation of emission properties in accordance with the proposed model of facilitated electron emission [1].

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Forming of monolayer graphene oxide films on silicon substrate

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Graphene is planar monolayer of carbon atoms, densely packed in the hexagonal lattice. Along with the linear carriers dispersion law graphene possesses the number of unique electrical, optical, mechanical properties. This makes the opportunity to regard this material as the promising base for future electronics.

Existing methods do not allow preparation large sized uniform monolayer graphene films. The film is mosaic structure and size of disoriented fragments relative to each other is not large. We have suggested a technique for preparation monolayer graphene films from graphene oxide aqueous suspension. The natural graphite was oxidized by modified Hummer's method [1]. As a result the water suspension of the graphene oxide particles was obtained. Then the graphene oxide was deposited on silicon substrates using method, similar to Langmuir-Blodgett's one [2]. Finally in order to obtain the graphene films the samples were treated by annealing in a hydrogen atmosphere.

The samples were studied by TEM, SEM, AFM techniques. The results have demonstrated low imperfection of films and their monolayer structure [3]. The fragment size forming graphene film attains 50 μm.

Resistance of the reduced films was measured using pressed contacts. Minimum distance between contacts was 5 μm. The film resistance after reducing comprised $7 \cdot 10^4$ Ω/sq and corresponding conductivity was $1.5 \cdot 10^3$ S/m at film thickness of 0.5 nm.

Presented results demonstrate that our method allows preparing good quality monolayer graphene films with large size of uniform fragments.

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Heat Transport across the metal-nanodiamond interface

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Under investigation is new model for heat transport at metal-nanodiamond interface. Two coupled semi-infinite one dimensional chains are considered. β_j, β, determining the interactions between the atoms inside the materials and at the boundary, masses of the atoms m_j and the interatomic distances as a_j are the chain parameters; $j = 1, 2$ specify the materials. A plane wave with the given frequency ω is incident on the boundary from one side. Then there are two possible cases. If the frequency of the incident wave is less than both maximum possible frequencies of the infinite chains, then there would be a transmitted and reflected waves with the same frequency. The problem of finding the amplitudes of the transmitted and reflected waves taking into account the conditions at the interface between two materials is completely solved in [1].

If the frequency of the wave incident from the diamond on the metal is higher than the maximum frequency of the eigenmodes of the metal, situation changes [2]. It is physically clear that the forced oscillations with the frequency of the incident wave should arise near the boundary of the second chain. Indeed, in this case exponentially decaying modes arises, with dispersion relation

$$\omega = \omega \cosh\left(\frac{qa}{2}\right) \,,$$
(1)

where ω_m is maximum possible frequency in metal.
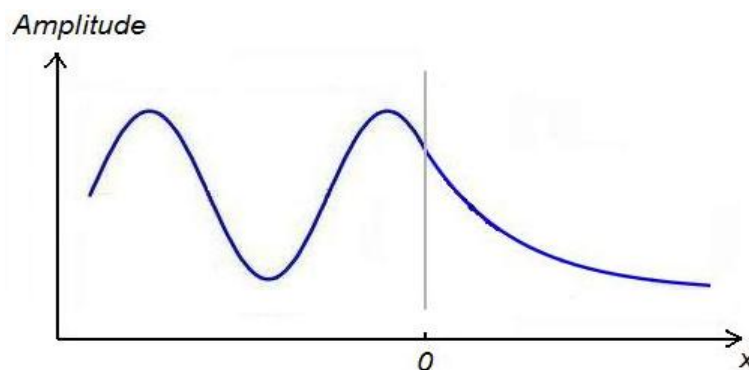
Result of the propagation of oscillations along two different coupled semi-infinite one dimensional chains (axis *x*) at an oscillation frequency in the insulator (on the left) higher than the maximum possible oscillation frequency in the metal (on the right). The interface (*x*=0) is denoted by a vertical line. It is seen that the highfrequency oscillations penetrate into the metal but decay there.

It is obvious that the high frequency oscillations of the metal crystal lattice arise owing to the penetration of the oscillations from the diamond into the metal. The energy of these oscillations is transmitted to the electron gas. Thus, the energy is transferred from the diamond to the metal.

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Influence of the edge and substrate effects of zigzag graphene nanoribbons on atomic and electronic structures of the 8-ZGNR/h-BN(0001) interface

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The influence of the edge and substrate effects of zigzag graphene nanoribbons on atomic and electronic structures of the 8-ZGNR/h-BN(0001) interface are presented, suitable as a component of spintronics devices using the density functional theory (DFT).

To study the atomic structure of the 8-ZGNR/h-BN(0001) interface, relaxation of graphene nanoribbon and one upper boron nitride atomic plane of the plate was performed. Two lower layers of the h-BN(0001) substrate were "frozen". Relaxation was carried out until the sum total of all forces in the system was reduced below 0,001 eV/Å. We established equilibrium parameter values for the lattices, atomic positions of the nanoribbon and the upper layer of boron nitride, and the length of the d_1 bond between the nanoribbon and substrate atomic layers. Equilibrium bond length for 8-ZGNR and h-BN(0001) substrate was $d_1 = 0.339$ nm.

Layout of the zones corresponding to 8-ZGNR to a large extent remains unchanged in the 8-ZGNR-AF/h-BN(0001) system, in particular, location and the shape of σ-bands and π-bands responsible for conductivity. However, some changes in 8-ZGNR states under the substrate influence are observed in the immediate vicinity of the Fermi level. For the spin up electron subsystem, the main contribution in the energy gap opening is made by the effect of the GNR edge. Moreover, the value of the Δ_1 parameter localized in the Dirac point area ($k = 2\pi/3$) practically does not change, while the value of the Δ_2 parameter localized in the ($k = \pi$) area even decreases by 0.05 eV. The cause of this situation in the spin up electron subsystem is unclear. At least it is essential that in the ($k = 2\pi/3$) Dirac point having practical significance the h-BN(0001) substrate practically does not alter the energy gap width.

DFT calculation of the energy gap properties for different spins helped differentiate the contributions of the effects of the nanoribbon edge and substrate in the energy gap opening in the 8-ZGNR-AF/h-BN(0001) interface with antiferromagnetic ordering. For the spin up electron subsystem, the main contribution in the energy gap opening is made by the effect of the ZGNR edge. In the spin down electron subsystem, the h-BN(0001) substrate contribution in the E_g value is approximately 6% of the contribution made by the 8-ZGNR edge effect.

Effect of BaTiO$_3$ modification by shungite carbon deposition on the dielectric properties of polymer based composites containing modified BatiO$_3$ as a filler

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Hybrid organo-inorganic composites are promising materials for protective dielectric layers in displays, electroluminescent panels, capacitors and other electronic devices due to unique combination of flexibility and adhesion intrinsic to a polymer binder and excellent dielectric properties of such inorganic fillers as barium titanate. These composites are also advantageous in respect of the possibility to control their properties in a wide range by the variation of the ratio between the components and modification of their compatibility. In our previous studies [1, 2] composites based on cyan-ethyl ester of poly(vinyl alcohol) (CEPVA) as a binder with one of the highest permittivity values among the polymers ($k\sim19$) and barium titanate HPBT-1B produced by Fuji Titanium Co. (Japan) as a filler with an extremely high $k \sim 4400$ were synthesized. However, k values of these composites were below 150 since the electric properties of such materials follow the inverse proportionality relating to k values of the individual components acting as consecutively connected elements in the electric circuit unless they are chemically bound. A specific functionalization of the filler surface by a sol-gel deposition of Nb$_2$O$_5$ [1] and SiO$_2$ [2] resulted in the increase of k value for the composite up to 200-250 due to the formation of a highly developed surface containing functional groups (FG) capable of interaction with acidic hydroxyls in CEPVA.

In this study the surface of the same barium titanate was modified by shungite carbon (ShC) nanoclusters deposited from a stable aqueous dispersion according to the procedure described in [3]. An average size of clusters determined by DLS was 53.6±25.0 nm. The modified BaTiO$_3$ samples in the earlier optimized amount 40 vol.% were mixed with CEPVA solution. The composites were deposited onto aluminum supports as 80-130 μm layers and dried. The obtained data show that the deposition of ShC nanoclusters under optimal conditions (ShC concentration ca. 0.6 mg/L, ratio ShC:BaTiO$_3$ ca. 0.64 mg/g) provides a drastic increase in the dielectric permittivity of the composites up to $k\sim2350$ in combination with a significant growth of $tg\delta$ value. The observed increase in these performances was found to correlate with the growth of the total content of Brensted neutral (pK$_a$ ~7) and basic (pK$_a$ ~13) centers (hydroxyl groups) on the modified filler surface. The formation of these groups can be determined by the distortion of bridging oxygen bonds followed by hydroxylation and presence of hydroxyls intrinsic to ShC itself. These data are in the complete agreement with the earlier obtained results [1, 2] indicating that these types of surface centers are responsible for interfacial interactions in the composites. Furthermore, the addition of ShC can impart the material with a certain conductivity thus also contributing to the observed increase of the dielectric parameters.

Generally, the considered approach is promising for the development of hybrid composites with adjustable electric performances useful in various technical applications.

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ZnS:Cu phosphors modified by shungite nanocarbon deposition

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Phosphors based on AIIBVI compounds are widely used in various electronic devices such as displays, electroluminescent panels, etc. One of the important requirements for the extended and efficient application of these materials is the possibility to control their emission spectra, brightness and stability due to specific doping and modification in addition to the incorporation of conventional activators and additives.

In this study a commercial ZnS:Cu based electroluminescent phosphor (produced by NPF Luminofor Co., Stavropol, Russia) was modified by the deposition of shungite carbon (ShC) nanoclusters from stable aqueous dispersions according to the procedure described in [1]. An average size of clusters determined by DLS was 53.6 ± 25.0 nm and the ratio ShC:phosphor was varied in the range 0.8–1.3 mg/g.

The obtained samples were characterized by measuring their electroluminescence (EL) intensity at voltage 180 V and frequency 400 Hz and study of their surface properties by the adsorption of a series of acid-base indicators with various pK_a values.

EL intensity of the modified phosphors measured was found to grow in the range 400-470 nm with the increase of the deposited ShC amount. The achieved EL enhancement clearly correlates with changes in the surface functionality of the material, i.e. with the decrease in the content of Brensted acidic centers with pK_a 2.5 and increase in the content of centers with a stronger Brensted acidity (pK_a 2.1). These two types of surface centers represented by Cu_xSH groups according to [2] are featured with an inverse linear correlation between their contents with the coefficient – 0.99. The observed effect is probably determined by the redistribution of electron density in the surface layer and certain changes in the energy of electronic levels corresponding to dopant centers.

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Infrared absorption studies of chemically modified nanodiamonds of dynamic synthesis

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Nanodiamonds with mean size ranging from ~5 nm to ~100 nm obtained by detonation (DND) and dynamic (DyND) syntheses are the most interesting objects among other developed nanomaterials. The reason for such an interest originates from unique properties of the DND surface to be chemically modified and functionalized by various atomic groups. The use of DND and DyND suppose to be very promising for applications in plastics and biopolymers reinforcement, enhancement of their wear-resistant properties by nanodiamond fillers.

The surface of as-prepared DND/ DyND particles is terminated by various functional groups that are covalently bound to the surface and form "dense" molecular shell around the nanoparticle. Among these groups are carboxyl, carbonyl, hydroxyl and anhydride ones, as well as the surface C-H groups. This set of oxygen containing groups appears on the surface of the DND particle during its manufacturing process at the stage of the removal of non-diamond sp^2-component from the detonation soot or the graphitic material treated by shock-wave loading. The removal process is carried out by the treatment of the detonation soot with strong acids in autoclave at T > 220 ^{o}C or by treatment with other oxidizing agents (oxidation and gasification in air at ~430 ^{o}C). Due to oxidizing reactions the surface is partially terminated by carboxyl and carbonyl groups.

In this research the analysis of surface functional groups in DND/DyND samples of various industrial suppliers was done by infrared (IR) absorption spectroscopy method and is presented here in dependence of the main method of their chemical treatment – oxidation, fluorination and gasification of surface groups during subsequent heat treatment, and its main size.

Several DND samples (mean size 5 nm) synthesized and chemically purified in nitric acid by FGUP "SCTB "Technolog" (Russia) and one DND manufactured in PlasmaChem GmbH (Germany) and thereafter fluorinated at T = 350 ^{o}C and T = 500 ^{o}C were investigated. DyND samples (Super Syndia SSX) of different mean size manufactured by L.M. Van Moppes & Sons SA (Switzerland) with the use of shock-wave loading of graphite target were specially purified by us in strong acids in autoclave and also investigated.

We found that fluorination strongly affects on the state of the diamond surface. Strong absorption bands related with surface fluorocarbon species appear at 1244 and 1340 cm^{-1}. The band at 1340 cm^{-1} is especially strong and looks as a featured δ-peak. Nevertheless, the essential absorption in the range 1050-1200 cm^{-1} related with C-O and C-O-C groups still exists in the spectra of fluorinated DND. It means that remaining amount of C-O and C-O-C bonds still exists on the DND surface or inside the DND aggregates even after the fluorination. The intensity of strong absorption band at ~1100 cm^{-1} found in the spectra of polycrystalline DyND particles of different sizes depends upon the particle volume, and not upon its surface, as it is the case for absorption bands of hydroxyl (~1630 cm^{-1}) and carbonyl groups (~1810 cm^{-1}). It probably means that the band at ~1100 cm^{-1} is a specific signature of C-O and C-O-C bonds hardly cemented the diamond grains in a large polycrystalline DyND particles of different median size ranging from ~25 nm to ~100 nm. Thus, the ratio of intensities of absorption bands at ~1100 cm^{-1} and ~1730-1810 cm^{-1} in nanodiamonds passed through the oxidative treatment may be very good independent criterium for evaluation the actual size of hardly-cemented (by covalent bonds) aggregates in DyND powders. This criterium might be also extrapolated down to the lowest mean sizes of ~ 5-10 nm where this ratio achieves the minimal value.

H-SWCNT: X-ray absorption spectroscopy and semiempirical calculations

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In this work, high-resolution near edge X-ray absorption fine structure spectroscopy (NEXAFS) technique was used to elucidate the nature of chemical bonding between carbon and hydrogen atoms on the surface and inside hydrogenated single-walled carbon nanotubes (H-SWCNTs). High-resolution measurements of the C 1s absorption spectra for pristine and hydrogenated single-walled carbon nanotubes (SWCNTs) with hydrogen concentration 5.335 wt.% were conducted. Experimental NEXAFS spectra of pristine and hydrogenated nanotubes were recorded at the C K-edge and measurements were performed at the Russian-German beamline at the BESSY II (Berlin, Germany).

The experimental spectrum of H-SWCNT in comparison with those of SWCNT shows a drastic decrease in intensity of the π-band maximum and an appearance of new structures. They result from the C1s electron transitions to vacant C2p-derived states of a new phase, which forms in SWCNTs owing to hydrogenation. The C1*s* absorption spectra point to formation of covalent chemical bonding between the hydrogen and carbon atoms in H-SWCNTs.

In order to get detailed understanding of the origin of the chemical bond between C and H atoms in H-SWNTs, semiempirical calculations were carried out using the MOPAC2009 code with PM6 parameterization. Models of C-H chemical bonds where H atoms are connected to the SWCNT outer surface were investigated. Fig. 2 shows the model structure of C-H chemical bonds that is a result of geometry optimization. In the case when hydrogen was located on the nanotube surface, formation of a tetrahedral structure with C-H bonds was observed.
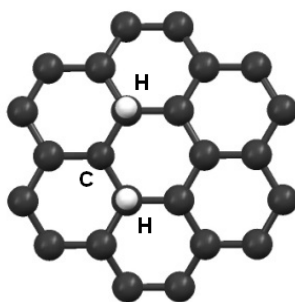
Fig. 1. The model structure of H-SWNTs used for calculations.

It was found out that SWCNT hydrogenation is accompanied by chemical binding of hydrogen and carbon atoms on the tube side walls. Hydrogen atoms do not substitute carbon atoms in graphene layers of SWCNTs but they join perpendicularly to them due to covalent mixing between C 2pz and H 1s states. The coordination of carbon atoms changes from sp2-triangular to sp3-tetrahedral.

Would it be possible to control a synthesis process of detonation diamonds?

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Detonation synthesis nanodiamonds (DND) pertain a class of nanomaterials fabrication, modification, and application of which attract the attention of scientists and engineers from different countries. This area of science and technology is at the boundary of solid-state physics and chemistry.

The detonation synthesis can be presented as a multiple process of reduction-oxidation reactions. In the conditions of oxygen deficiency the product of synthesis represents mechanically non divided mixture of the intermediate products which form in course of free atoms interaction, radicals in their fast reactions with initial reagents and among each other.

From literature it is known [1] that processes of chain burning can be effectively regulated by input of oxidation process regulators into a system. Essentially, it gives the opportunity to affect both structure of detonation synthesis products, and superficial properties of components.

In this work we investigate how environment containing the detonation synthesis influences colloidal and chemical properties. For this research the DND, synthesized by blasting in the water environment with modifying additives of various acceptors produced by SCTB «Technolog», were used.

Five samples, received in different options of detonation synthesis, have been studied.

A comparative studying of extent oxidation of a particles surface of the DND depending on features of blasting has been out according to the Chugayev-Tserevitinov's method. From the analysis of kinetics data of this method packing density of the DNDs units has been estimated. The specific surface of studied samples of the DND depending on acceptor number of a modifying additive have been estimated by the method of low-temperature desorption of nitrogen.

Structures of the DND suspensions in polar and unpolar environments have been estimated by the method of dynamic light scattering. The analysis of these experiments has allowed to estimate parameters of the DND units' polydispersion curves, and also estimate indirectly to hydrophobic-hydrophilic balance of the DND units' surface, synthesized in the various environments.

By the results of the work, the conclusion has been made that the water environment modification of the detonation synthesis by substances with the expressed acceptor ability is a perspective way of receiving the DND with in advance set colloidal and chemical characteristics, for example, such as particles dispersion of the DND, their specific surface, a oxidation extent of surface.

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The features of applicability of dynamic light scattering method for the size analysis of carbon nanoparticles in sols

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Dynamic Light Scattering (DLS) is one of the most widely used methods for integrated analysis of the colloidal particle sizes ranging from few micrometers to few nanometers. A wide range of materials exist as molecules or particles that can be characterised by DLS. However, the unstability problem underlying in mathematical apparatus naturally limits the range of applicability of DLS.

This paper presents the results of study of the detonation nanodiamond (DND) hydrosols by DLS undertaken to identify the range of applicability of this method realized in the Malvern Zetasizer ZS 3600. The choice of particles is determined by the possibility of obtaining DND sols with narrow size distribution in the range of 5 nm. Moreover, the polarization effects that arise in the interaction of light with metallic particles, absent in the case of DND particles. This is a great advantage of applying of nanodiamond sols as calibration standards with particle sizes less than 50 nm.

It was found that the solution of unstable problem underlying the mathematical treatment of autocorrelation function of scattered light intensity strongly depends on the signal accumulation time. In addition, the shadowing of signal from small particles by signal from larger particles observed under certain conditions of concentrations of particles with different sizes in the hydrosol. When the signal difference overrides the dynamic range of the detector, the signal from small particles is comparable with the noise level. We have estimated the threshold concentration ratio of particles with different sizes in the hydrosol, by which the full shadowing of signal from small particles by signal from larger particles happens.

Highly tritium labeled detonation nanodiamond

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Detonation nanodiamond (ND) attracts ever-increasing interest due to their unique physical and chemical properties: the size of primary particles is 5 nm, an advanced specific surface more than 300 m^2/g, high adsorption ability, presence of superficial functional groups and biocompatibility. These properties allow to use it not only in various areas of a science and technics, but also in biology and medicine. Since recently ND are suggested to be perspective carriers in drug delivery system, with consequent challenge for quantitative determination of ND in biological samples (organs, tissues and biological fluids). The most convenient method providing maximum sensitivity appears to be the introduction of various radioisotopes onto ND: ^{125}I, ^{99}Tc, ^{188}Re and especially ^3H. Tritium (^3H) can be used as one of the perspective ND radiolabeling agent due to long half-value period (12,33 years), relatively cheap and low energy beta decay. Therefore it can be useful for extended period of time without special safety precautions and suitable for biological applications. Tritium thermal activation technique appears to be a most suitable method for radiolabeling of carbon nanoparticles. Tritium introduction on ND depends on the presence of numerous surface groups containing hydrogen which may be interchanged with tritium. Therefore ND with maximal content of C-H groups and minimal content of labile hydrogen is the most appropriate candidate for high-performance tritium labeling.

In the present study tritium was first proposed for ND radioactive labeling and subsequent visualization in biomedical applications. For this purpose, unique device for synthesis of tritium-substituted compounds enabling tritium thermal activation technique (TTAT) was used. Method for improving effective tritium introduction on the surface of ND was developed. To purify tritium labeled detonation nanodiamond (^3H-ND) from labile tritium (–OH, –COOH, etc.) and possible tritium impurities the ND water suspension was kept for several days. Then solids were precipitated by centrifugation and supernatant was picked out following by the addition of new portion of solvent. The specific radioactivity of ^3H-ND was 34 GBq/g.

The increased content of C–H surface groups after hydrogenation in gaseous hydrogen (H_2, 800°C, 5 h) provides specific radioactivity equal to 90 GBq/g, while initial values of radioactivity of ND and reconstructed ND were similar.

Preliminary dispersion of hydrated ND (with aggregate size less than 50-100 nm) enabled considerable enhance (in 29 times – from 90 to 2600 GBq/g) of tritium label content and thus yield highly ^3H-ND.

Keeping ^3H-ND in solution for one year did not affect changes in specific radioactivity, with the exception of tritium decayed (5%) over that period. This confirms the formation of hydrolysis-resistant stable C–^3H covalent bond.

ND with radioactive ^3H-label can be effectively used in biopharmaceutical research, studies on pharmacokinetic, biodistribution and any other types of biological experiments.

Small-angle scattering from detonation nanodiamonds as polydisperse particles with diffusive surface

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Highly dispersed systems especially those developed for the practical use often contain heterogeneous (multicomponent) and polydisperse nanoparticles, as well as their aggregates. When such systems are investigated by means of small-angle X-ray (SAXS) and neutron (SANS) scattering, an important question is the influence of particle polydispersity on the determination of the structural parameters of such systems. In this work we consider a specific kind of polydisperse inhomogeneous particles whose structure, on the one hand, allows significant simplifications of the general contrast variation approach in the small-angle scattering, and, on the other hand, makes it possible to analyze the scattering in the same manner as for polydisperse homogeneous particles [1]. The non-homogeneity of these particles is determined by their interface defined as the 'diffusive surface'. It is close to the concept introduced by Schmidt [2] of the diffusive interface between two homogeneous phases to explain the experimentally observed deviations of the scattering from the Porod law towards lower values of the power-law exponent (< -4) at large *q*-values. Such kind of non-Porod scattering behavior is observed for detonation nanodiamond (DND) particles in liquid dispersions and can be related with the intrinsic inhomogeneous structure of the particles because of graphitic states of carbon at their surface. At the same time, the particles are rather polydisperse, since the scattering curves from DND are well smeared. So, the aim of this work is to consider the two indicated aspects (structural non-homogeneity and polydispersity) in analysis of small-angle scattering from DND. The actual case of small 'diffusivity' of the surface is considered, which makes it possible to deduce relatively simple expressions for the scattering invariants. The possibilities of the proposed approach are then discussed basing on the model scattering curves and experimental SANS curves obtained previously for the liquid DND dispersions [3].

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Study of cluster reorganization in C_{60}/NMP/H_2O solutions by dynamic light scattering

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To date the fullerene clusterization in solutions is an intrigue problem of colloidal chemistry [1-4]. The work presents the analysis of the dynamic light scattering (DLS) data for the cluster solutions of fullerene C_{60} in N-methylpyrrolidone (NMP) and its mixtures with water. This study confirms that the clusters in C_{60}/NMP develop within one month with the gradual increase in their size up to the level of several hundreds nanometers. In addition to the previously reported data it is found that starting from at least two weeks after the preparation of the initial C_{60}/NMP solution the addition of water (volume fraction above 40% in the mixture) results in rather strong effect of the cluster reorganization related with the partial cluster dissolution and is well observed by DLS. The fullerene clusters themselves detected at this stage by DLS in the initial solutions are significantly smaller in size as compared to the clusters in one month old solutions C_{60}/NMP. So, it can be concluded that the modified C_{60}-NMP complexes which provide the dissolution of C_{60} in the mixture are formed already after two weeks in C_{60}/NMP including non-aggregated C_{60} molecules. Since the cluster growth continues, this means that the peripheral parts of the clusters are composed of the modified C_{60}-NMP complexes which are dissolved on adding water, which testifies the previous conclusions [3]. Based on the cluster size distribution functions obtained by DLS the curves expected in small-angle neutron scattering (SANS) experiments are calculated and compared with the available experimental data. The problem whether it is possible to catch the moment when the formation of the modified C_{60}-NMP complexes in C_{60}/NMP is completed during the period less than two weeks after the solution preparation by the combined DLS and SANS analysis is discussed.

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Structure and optical properties of fullerene C_{60} complex with dipyridinated iron(II) phthalocyanine $[Fe(II)Pc(C_5H_5N)_2] \cdot C_{60} \cdot 4C_6H_4Cl_2$

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Complexes of fullerenes with metallomacroheterocycles attract much attention due to promising photophysical properties. Up to now mainly fullerene complexes with substituted metal-free and metal-containing porphyrins have been obtained and structurally characterized. These are octaethyl- (OEP), tetraphenylporphyrinates (TPP) [1,2]. In this work we obtained first example of molecular solid containing neutral fullerenes and phthalocyanines. The crystals of molecular complex of fullerene C_{60}: $[Fe(II)Pc(C_5H_5N)_2] \cdot C_{60} \cdot 4C_6H_4Cl_2$ (**1**) with bisaxially coordinated Fe(II)Pc has been synthesized by slow diffusion of hexane into the *o*-dichlorobenzene solution containing $Fe(II)Pc(C_5H_5N)_2$ and C_{60}.
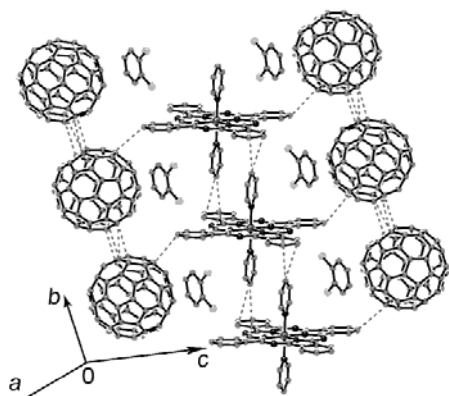
Fig. 1. Crystal structure of **1**: view on the chains formed by the C_{60} molecules and the $Fe(II)Pc(C_5H_5N)_2$ units.

Crystal structure of **1** involves columns formed by the C_{60} molecules and the $Fe(II)Pc \cdot (C_5H_5N)_2$ units arranged along the *b* axis. (Fig. 1). C_{60} molecules are formed closely packed linear columns with multiple van der Waals (wdW) C…C contacts between fullerenes (Fig. 1). Free space in the packing of $Fe(II)Pc(C_5H_5N)_2$ and C_{60} is occupied by solvent $C_6H_4Cl_2$ molecules. Totally each $Fe(II)Pc(C_5H_5N)_2$ unit forms vdW contacts with four C_{60} molecules. Two of four molecules are located near two adjacent phenylene substituents of Fe(II)Pc and form short vdW C…C(C_{60}) and H…C(C_{60}) contacts with the phthalocyanine plane in the 3.31-3.34 and 2.77-2.87 Å range. Two other fullerenes form only one H…C(C_{60}) contact with phthalocyanine (Fig. 1). Several shortened H…C(C_{60}) and Cl…C(C_{60}) contacts are also formed between fullerenes and pyridine and solvent $C_6H_4Cl_2$ molecules (are not shown in Fig.1)

The absence of absorption in the NIR-range at about 1100 nm indicates neutral state of fullerene C_{60} in **1** in accordance with the IR-spectral data.

Complex **1** is EPR silent at room temperature indicating the absence of ionic $[Fe(III)Pc^+] \cdot (C_5H_5N)_2$ and $C_{60}^{\cdot-}$ species which should form if charge transfer from $Fe(II)Pc(C_5H_5N)_2$ to C_{60} was realized in the sample. It is known that neutral $Fe(II)Pc(C_5H_5N)_2$ is diamagnetic ($S = 0$) and EPR silent.

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Anomalous absorption of ultra-thin pyrolytic carbon films

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The electromagnetic shielding is of great importance for many applications and, especially, for satellite and airplane communication systems, in which thickness and weight of shielding coatings is a critical issue. It has been demonstrated that the anomalous absorption take place in the ultra-thin metal films which thickness is much smaller than the skin depth [1,2]. Similar effect was demonstrated in the recent experiments with pyrolytic carbon (PyC) films [3]. PyC films can be grown directly on both dielectric and metallic substrates opening a new route towards fabrication of ultralight and nanometrically thin electromagnetic interference (EMI) protective coatings with enhanced shielding effectiveness.

In this work, we present the numerical simulation of microwave absorption of PyC in K_a-band and describe experimental results on the absorption spectrum of the PyC film placed in rectangular waveguide [3] supporting the $TE_{1,0}$ mode. The studied film is in several hundred times thinner the skin depth in the K_a-band.

The theoretical analysis was performed for the 25-nm thick PyC film deposited on 0.5 mm thick silica substrate. The boundary conditions for the amplitudes of the counter-propagated $TE_{1,0}$ modes in such system can be presented in the following form [4]:

$$
\begin{aligned}
&b_0^+ + b_0^- = b_1^+ + b_1^- \\
&K_0\left(b_0^+ - b_0^-\right) = K_1\left(b_1^+ - b_1^-\right) \\
&b_1^+ \exp\left(iK_1 l_1\right) + b_1^- \exp\left(-iK_1 l_1\right) = b_2^+ + b_2^- \\
&K_1\left[b_1^+ \exp\left(iK_1 l_1\right) - b_1^- \exp\left(-iK_1 l_1\right)\right] = K_2\left(b_2^+ - b_2^-\right) \\
&b_2^+ \exp\left(iK_2 l_2\right) + b_2^- \exp\left(-iK_2 l_2\right) = b_3^+ \\
&K_2\left[b_2^+ \exp\left(iK_2 l_2\right) - b_2^- \exp\left(-iK_2 l_2\right)\right] = K_0 b_3^+ .
\end{aligned}
\tag{1}
$$

Here l_1 is the thickness of substrate, l_2 is the thickness of PyC film, subscript i = 0, 1, 2, 3 label vacuum, substrate, PyC film and vacuum, respectively, $K_i = \sqrt{k^2 \varepsilon_i - (\pi/a)^2}$ is wave number in the i-th medium, a=7.2 mm is the rectangular waveguide width. Solution of system (1) allows us to obtain reflectivity $R = \left|b_0^- / b_0^+\right|^2$, transitivity $T = \left|b_3^+ / b_0^+\right|^2$ and absorptivity $A = 1 - R - T$ of the PyC film on the silica substrate.

The simulations were performed in the frequency range 26 – 37 GHz. Both the experimental and numerical results give the similar value of absorption coefficient ~ 30 %.

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Photoelectron spectroscopy with angular and spin (SARPES) resolution for the study of systems based on graphene

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Photoelectron spectroscopy with angular and spin resolution gives information on the spin and electronic structure of the system. Method is based on the analysis of the energy distribution of photoelectrons, emitted at different angles relative to the normal of the surface, considering spin direction of the photoelectron. Experimental equipment for (SARPES) includes: monochromatic light source, electron energy analyzer, Mott detector and electronics for data processing. After excitation of the photoelectrons from the sample and transmission of the energy analyzer, where is going a selection of the emission angle and the kinetic energy, photoelectrons enter the Mott detector, where is going a separation of the spin direction of the photoelectrons (spin-up and spin-down). The principle operation of the Mott detector is based on scattering in the photoelectron the nuclei of metal with a high atomic number (usually, as a metal high atomic number in the Mott detector used a gold foil) in depending on the direction of spin. The scattered photoelectron is carried out using the four channels in pairs along and across the plane of gold foil. The basic characteristic of the scattering of the photoelectron have is the asymmetry. This asymmetry used to determine the polarization of the electrons in this methodology. It can be defined as follows:

$$A = \frac{N_L + N_R}{N_L - N_R} \tag{1}$$

where, N_L, N_R registered number of scattered photoelectrons to the left and right channels relative to the plane of the gold foil. Then determined by the spin polarization of photoelectrons:

$$P = \frac{A}{S} \tag{2}$$

where S - Sherman function. Sherman function describes two important characteristics: the asymmetry of the scattering of a polarized beam and the magnitude of the polarization that occurs in the scattering of polarized beam. The values of the Sherman function in the range from -1 to 1. Considering for the spin polarization (P) and total measured intensity ($I_t = N_L + N_R$) can be obtaining the photoelectron spectra of the spin-resolution [1]:

$$\begin{cases} I_{up} = \frac{(1+P)I_t}{2} \\ I_{down} = \frac{(1-P)I_t}{2} \end{cases} \tag{3}$$

Typically, the valence band states of graphene are characterized by the negligible value of the spin splitting [2]. However, the results of our investigations show that the intercalation of Au underneath a graphene monolayer leads to the anomalously large effects of induced spin-orbit splitting of the π-states of graphene [3].

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Fund for Infrastructure and Educational Programs

The Fund for Infrastructure and Educational Programs was founded during the reorganization of the Russian Corporation of Nanotechnologies. Its purpose is to create infrastructure for innovation in the nanoindustry, including realizing projects and programs in education and infrastructure building that RUSNANO had previously begun. The Fund for Infrastructure and Educational Programs primarily focuses its work in these areas:

- Formation of manufacturing infrastructure
- Development of human resource potential for the sector
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- Refinements in metrology
- Popularization of nanotechnology and nano-enabled products

The highest governing body of the fund is its Supervisory Council, which is chaired by Dmitry Livanov, the Minister of Education and Science of the Russian Federation. In accordance with the charter of the fund, the Council determines priorities for its activities, establishes its strategies, and sets its budget.

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