Fundamental and Applied NanoElectroMagnetics

FANEM'12

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CONFERENCE PROCEEDINGS

May 22-25, 2012
Belarusian State University, Minsk, Belarus

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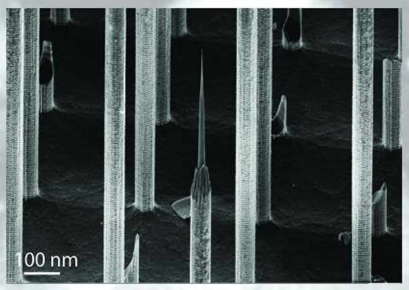

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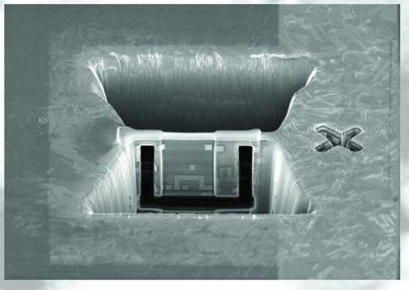

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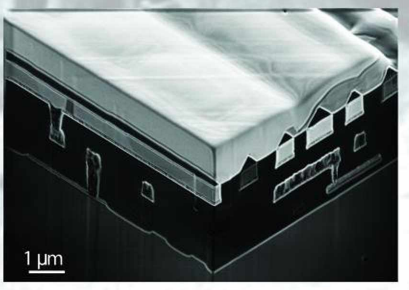

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General Session I

Surface Multiplasmonics

A. Lakhtakia
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The planar interface of a metal and a dielectric material can guide multiple surface-plasmon-polariton (SPP) waves—all of the same frequency, but different phase speed, attenuation rate, and spatial profiles of fields—provided that the dielectric material is periodically nonhomogeneous in the direction normal to the interface. Theoretical and experimental research during the last four years have validated this concept. Emerging applications of surface multiplasmonics include solar-energy harvesting as well as optical sensing of biological and chemical sensing.

NOTES

General Session II

Carbon Nanotubes and Graphene as Terahertz Emitters and Detectors

M. Portnoi, R. Hartmann, O. Kibis, M. Rosenau da Costa
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We propose and justify several schemes utilizing the unique electronic properties of different types of carbon nanotubes for a broad range of applications to terahertz (THz) optoelectronics, including THz generation by hot electrons in quasi-metallic nanotubes, frequency multiplication in chiral nanotubes, and tuneable THz radiation detection and optically-pumped THz emission in armchair nanotubes in a strong magnetic field. Another direction of our research is THz applications of graphene. As a gapless semiconductor with high carrier mobility, graphene represents an ideal material for detecting THz radiation. We calculate absorption rates in graphene focusing on the effect of momentum alignment (anisotropy of the distribution function) of photoexcited carriers created by linearly-polarized excitation. In conjunction with a strong angular dependence of the tunnelling probability for graphene p-n junctions, optical alignment of momenta raises the possibility of using graphene p-n junction structures in polarization-sensitive detectors.

NOTES

From nanophotonic devices to nanophotonic integrated circuits: advances and challenges in development of scalable simulation approaches

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Recent advances in nanophotonics allow integration of hundreds (and even thousands in few years) of photonic devices on a single chip. This rapid progress requires development of appropriate simulation tools that would facilitate design and verification of large-scale photonic integrated circuits. Importantly, the simulation techniques developed for modeling nanophotonic devices are badly scalable and become inefficient when applied to modeling large-scale circuits. The latter task requires development of new system-level simulation approaches. We show that fully passive photonic circuits can be efficiently modeled in the frequency domain using the S-matrix assembly technique. However, modeling of large-scale *active* photonic circuits presents a real challenge since the commonly used time-domain approach is not scalable. To address this problem, we have developed a new hybrid time-and-frequency-domain modeling (TFDM) approach. Here, we show scalability of this new approach, present our advances in its efficient implementation in the framework of the simulation tool VPIcomponentMaker Photonic Circuits, and discuss the remaining challenges.

NOTES

Elasticity at the nanoscopic scale

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Aside from new physics governed by quantum mechanics, some classical concepts may survive in the nanoworld. Elasticity is one of the fields of materials science that can reasonably be applied to nanostructures. Care should be taken, however, to stay with well-defined quantities. Not all the elastic constants keep on their meaning when transposed to the nanoscopic scale. For instance, Young modulus of about 5 TPa has been predicted for single-walled nanotube. The fact is that this modulus has no significance at the atomic level. Other elastic coefficients, by contrast, can be defined unambiguously at the atomic level and can be measured experimentally. The task is not easy, in general, which explains why available values, if any, may differ significantly from each other. Ab-initio calculations can be a substitute to experiment for providing the input data needed by classical mechanics. That is important because mechanical properties of nanostructures can be predicted from elasticity if and only if reliable data exist. It will be shown that the simple Kirchoff-Love theory of thin plates can be extrapolated top down by providing constitutive equations that remains well-defined for an atomic sheet. This approach will be illustrated for the case of graphene and nanotubes. A critical review on how to obtain the constitutive parameters will be proposed, which will permit to address interesting questions on the mechanical properties of these fascinating nanomaterails, among which: graphene sheet buckling, nanotube bending, structural instability of nanocarbons.

NOTES

Session «Quantum chemistry simulation»

Electron structure of pure and doped nanotubes calculated using linear augmented cylindrical wave method

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In the terms of muffin-tin and DFT theory, we developed a linear augmented cylindrical wave (LACW) method for electronic structure of the single- and double-wall nanotubes. We calculated the band structures of the nanotubes up to the chiral (100, 99) tubule. The electronic spectrum of nanotubes is governed by the electrons movement in interatomic space of cylindrical layers, by scattering on the atomic spheres, and tunneling between the layers. A model for electronic structure of nanotubes embedded in a crystal matrix is developed too. The LACW-Green function theory is elaborated for the nanotubes with point defects. A first-principles numerical method for calculation of the electronic structure of the point impurities in the single-walled carbon nanotubes nanotubes based on a Green's function technique is developed. The host nanotubes electron Green's function is calculated using a linear augmented cylindrical wave theory. The Green's function of the impurities is calculated in the terms of matrix Dyson equation. The impurities are described by the single-site perturbed muffin-tin potentials in otherwise perfect nanotubes with the rotational and helical symmetries. Due to the account of these symmetry properties, the method is developed applicable to any tubule including the chiral nanotubes with point defects independent of the number of atoms in translational unit cell of the host systems. Finally, a relativistic version of the LACW method is elaborated and applied to calculating the spin-orbit coupling effects in the armchair nanotubes. This study was performed in the frames of the Program “Researches and developments on priority directions of scientific-technological complex of Russia in 2007-2012”. It was supported by RFBR (11-03-00691).

NOTES

Simulation of Electromagnetic Properties in CNT and Graphene Based Nanostructures

Yu. Shunin, Yu. Zhukovskii, N. Burlutskaya, T. Lobanova-Shunina, V. Gopeyenko, S. Bellucci
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CNT and graphene nanostructures (e.g.,GNR) constitute the basis of high-speed nanoelectronics and nanosensors. Special attention is paid to fundamental properties of various CNT-Me, GNR-Me and CNT-graphene interconnects. The cluster approach based on the multiple scattering theory formalism as well as effective medium approximation can be used for nano-sized systems modeling including calculation of dispersion law, electronic density of states, conductivity,etc. The multiple scattering problems are solved for radial (quantum dots) and axial (nanowires,nanotubes) symmetry approaches. Technological interest to contacts of CNTs or GNRs with other conducting elements in a nanocircuit is a reason to estimate C-Me interconnect resistances depending on chirality effects in interconnects of single-wall and multi-wall CNTs, single-layer and multi-layer GNRs with the fitting metals for the predefined carbon system geometry. Simulations of electromagnetic properties of interconnects demand the calculations of interconnect impedances. Evaluation of interconnect capacitances and frequency properties (GHz&THz) have been performed. Temperature properties of CMT-Me and GNR-Me interconnects have been simulated too. Parametric calculations of CNT dc- and ac-conductivities for various chiralities (Kubo-Greenwood formula) provide important information for nanotechnology. The model of CNT growth with predefined chiralities in a magnetically managed CVD process using magnetically anisotropic FexPt1-x nanoparticles with various substitutional disorders has been developed. Special attention is paid to presence of dangling atomic bonds in interconnects that make them chemically, electrically and magnetically sensitive. Thus, interconnects can be considered as perspective nanosensor structures.

NOTES

Electronic and optical properties of silicon nanowires

D. Migas
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By means of first principles calculations the electronic and optical properties of -, -, - and -oriented silicon nanowires passivated by hydrogen have been investigated. Silicon nanowires with axes are found to possess the direct bend gap nature. In the case of - and -oriented silicon nanowires their band gap is characterized by quasidirect nature because the energy difference between the first direct and indirect transitions has turned out to be a few meV. Nevertheless, an expansion in the lattice parameter along the wire axis leads to the stabilization of the first direct transition. The indirect nature of the gap is revealed for silicon nanowires in growth orientation. Estimates of the dipole matrix elements of the first direct transition for - and -oriented silicon nanowires have shown sizable values if silicon dimmers are formed on {001} facets indicating these nanostructures to be a perspective material for manufacturing light emitting devices integrated in the common silicon technology.

NOTES

Electronic and magnetic structure of zigzag graphene nanoribbons: quantum chemical calculations

N. Poklonski, E. Kislyakov, S. Vyrko, O. Bubel', S. Ratkevich
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Zigzag graphene nanoribbons (zGNR) due to their unique and peculiar edge states are one of the most interesting graphene nanostructures from the fundamental point of view. They are promising also for applications [1]. Therefore, thorough quantitative information about their structure is needed. To gain this information we have performed quantum chemical calculations of zGNRs using well tested for carbon systems semiempirical molecular orbital PM3 method [2]. Our calculations have been done for one-dimensionally periodic infinite nanoribbons of different width using Born–von Karman boundary conditions. We have calculated antiferromagnetic (AFM) and ferromagnetic (FM) ground states of zGNRs. The AFM state of 4zGNR (consisting of four zigzag carbon chains) is found to be lower in energy by 0.3 eV/atom than FM state. These states differ in their geometrical structures considerably. Calculations of electron energy band structures of FM and AFM states of zGNR show that AFM state is a semiconductor with the band gap decreasing with the number N of carbon chains in NzGNR, while FM state is a semimetal. The conductivity of the FM state of zGNR is localized in edge states.

[1] Graphene and its fascinating attributes / Eds. S.K. Pati, T. Enoki, C.N.R. Rao (New Jersey: World Scientific, 2011) 270 p.
[2] J.J.P. Stewart. J. Comp. Chem., 10 (2), 209–264 (1989).

NOTES

Session «Electromagnetic shielding I (ISTC Workshop) »

Electrical Conductivity of Single-Wall Carbon Nanotubes Films

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We report results of experimental investigations of electrical conductivity of carbon nanotubes films fabricated from single-wall carbon nanotubes (SWCNTs) bundles comprising individual nanotubes of different length (in the range from 150-300 nm up to 2 μm).
The samples were prepared by spraying of the isopropanol-SWCNTs suspension or water-sodium dodecyl sulfate (SDS)-SWCNT suspension onto substrates with 4 parallel Pd electrodes with length of 5 mm and width of 5 μm. SWCNTs produced by arc-discharged method or by gas-phase catalysis (HiPCO process) with diameter of 1.2-1.5 nm were used as pristine nanotubes for preparation of homogeneous SWCNTs dispersions. The substrates were heated during spraying to rapidly evaporate at temperature 120 ^{0}C.
Temperature dependencies of the resistance R(T) and IV-characteristics were measured in the temperature range 2-300 K in close-cycled refrigerator Cryogenics in order to determine charge transport mechanisms in the samples. Carbon nanotubes films obtained from isopropanol-SWCNT suspension show negative temperature coefficient of resistance ($dR/dT<0$) in the whole investigated temperature range. A crossover between metallic ($dR/dT>0$) and non-metallic ($dR/dT<0$) temperature dependence of the resistance was observed for SWCNT films prepared from water-SDS-SWCNT suspension. Nonlinear IV- characteristics observed for all types of samples with nonlinearity rising as the temperature decreased.

NOTES

Band structure of all-boron 2D metallic crystal as a prospective electromagnetic shielding material

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Due to the large neutron-capture cross-section of boron 10B isotope nucleus, the solid-state boron compounds and composites are good candidates for use as protection from neutron exposure. At the same time, materials with the high bulk concentration of B-atoms, e.g., nanotubular boron nitride BN, usually are non-metals and, therefore, not suitable for electromagnetic shielding purposes. However, the possibility of formation of all-boron layered structures (multi-layered planar sheets and multi-walled nanotubes) consisting of layers with metallic conductivity has been suggested. Intra-layer metallic conduction of layered boron opens an essentially new prospect for designing of materials which can combine the effective protection against neutron irradiation with the effective electromagnetic shielding. The evaluation of the efficiency of electromagnetic shielding provided by 2D boron crystals requires deep insight into their electronic structure. In this paper, a quasi-classical type theoretical method, developed in and successfully applied in calculations of the electronic structure of various BN modifications, is used to obtain electronic energy bands of an isolated B-sheet and map the corresponding Fermi-surface. These results may provide a proper theoretical basis for characterizing the properties of metallic layered nanosystems of elemental boron and assessing their potential for electromagnetic shielding.

NOTES

Session «Nanostructures synthesis and characterization I (ISTC Workshop)»

Direct chemical vapour deposition of semitransparent pyrolytic carbon film

T.Kaplas, Yu. Svirko
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Here we propose and demonstrate simple single step methane-based chemical vapour deposition (CVD) process in order to produce highly uniform, transparent, conducting pyrolytic carbon film. Methane is conventionally used in the CVD of nanocarbon materials. Its low reactivity at low temperature (500 °C-1000 °C) makes methane well-suited for various hot wall CVD experiments. Generally methane based CVD processes usually utilise catalysts, however at 1100 °C, the methane molecules start to decompose to CH2 and CH3 molecules more aggressively and eventually form C2- and C6-species, which lead to formation of graphitic nanocrystals. Since reactivity of different hydrocarbon species is related to the process temperature we used dynamic process temperature from 700 °C to 1100 °C in order to enhance the graphitic nanocrystal development. Moreover the employed hot wall CVD setup operates in static atmosphere i.e. there was no gas flow during the process. This prevented the replacement of CH2 and CH3 molecules with CH4. Samples were characterized by atomic force microscopy, Raman spectroscopy, optical transmission spectroscopy and conductivity measurements. The obtained results showed that pyrolytic carbon films manufactured using methane- and acetylene-based CVD technique have nearly the same properties. At the same time the manufactured films overperform those, synthesised using photoresist pyrolysis technique in terms of resistance/transmittance ratio. In conclusion, we have demonstrated synthesis of a high quality transparent pyrolytic carbon electrode. This proposed low cost technique does not need any pre- or post- processing of the sample and can be applied with the standard CVD setup.

NOTES

Peculiarities of carbon nanofibres obtained by PECVD

S. Fisenko, D.Takopulo
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Carbon nanofibers production has several features in industrial facilities. One of the most important features is the cost of nanofibre. The use of PECVD (plasma enhanced CVD) is one of promising ways in the development of industrial and semi-industrial facilities, which allows use gaseous methane as cheap and clean source of carbon [1].
Well known that plasmochemical pyrolysis creates soot nanoparticles (25-50 nm in diameter) in air-methane plasma flow. Influence of these soot nanoparticles on the performance of PECVD facility and nanofibre properties is discussed in the report. It was shown that the thermophoretic deposition of soot nanoparticles on metal surface drastically increase the probability of the formation of carbon clusters in supersaturated solid solution near the metal interfacial surface [2]. As a result of coalescence of carbon clusters nanofibre diameter nearly equals to the diameter of the primary soot nanoparticle d. For majority cases for PECVD the nanofibre growth runs at the base regime with carbon cap. It is worth to note that these nanofibres do not contain metal nanodroplets, which is important for electrodynamic parameters of nanofibres. To note that averaged value of nanofibres length/ diameter ratio is about 35.
For PECVD and all other CVD method it was discovered that highly porous carbon layer is formed on catalytic surface of the reactor. Thickness of this layer is about several tens of microns. For the first time the feedback between thickness of porous layer and temperature of the catalytic surface of the reactor is reported. The decreasing of surface temperature is the basic route of the formation of supersaturated solid carbon solution and, subsequently, the nucleation of carbon clusters [3]. This discovered feedback leads to the nanofibre growth at variable conditions. Manifestation of such unstable growth regime is curved shapes of carbon nanofibres.
Finally, it is shown this carbon layer inevitably leads to quasi-periodic mode of the facility operation and limits its productivity.
[1] S.A. Zhdanok, I.F. Buyakov, A.V. Krauklis, et al., On the conditions of formation of carbon nanostructures on the steel reactor surface from the products of hydrocarbon decomposition in low-temperature plasma. // J. Eng. Phys. Thermophys. 2009. 82, pp.
[2] D.A. Takopulo, S.P Fisenko. On formation of carbon clusters on a substrate in plasma pyrolysis of hydrocarbon gases //J. Eng. Phys. Thermophys. 2011. 84, pp. 1083-1086
[3] D.A. Takopulo, S.P Fisenko. Heat and mass transfer in hydrocarbon gas-porous layer-metall system and formation of supersaturated solid solutions of carbon // J. Eng. Phys. Thermophys. 2012. 85 (in press).

NOTES

Nanostructuring of Si-based alloy layers induced by fast recrystallization

P. Gaiduk, S. Prakopyeu, G. Ivlev
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In this talk, a short review of phase transitions, structural changes and segregation in Si-based alloy layers during fast melting and crystallization will be done. The samples of continuous layers of epitaxial, polycrystalline and amorphous SiGe alloys as well as nano-dotted layers of Ge or GeSn are used as initial structures. The structures were deposited by MBE, LPCVD, magnetron sputtering or prepared by ion-beam synthesis. The samples were then treated by pulsed laser beam (25-100 ns, 0.2-3.5 J/cm^2). Structural changes and optical properties of heterostuctures are studied by using electron microscopy, RBS/Channelling, photoluminescence, Raman spectrometry, time-resolution reflectivity, atomic force microscopy. The following subjects will be reviewed and discussed: - Fast crystallization of Si-based alloy layers and formation of cellular structures. We will concentrate on segregation of dopant to nanometer-scale cellular network; time-resolved reflectivity measurements of melting, crystallization and segregation; optical properties of segregated cellular SiGe/Si structures. - Pulsed laser modification of Ge and GeSn nanodots. Fast segregation is used for production of non-equilibrium compounds, e.g. metastable Ge1-xSnx dots with a tunable energy band gap. - Laser-induced melting and recrystallization of LPCVD grown polycrystalline Ge layers is used for modification of structural, optical and electronical properties of Ge layers for IR-photodetectors and solar cells due to suitable band-gap and high light absorption.

NOTES

Properties of systems with carbon nanotubes based on the swift heavy ion track technology

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Investigations of electronic elements with nanometric carbon-based materials are very prospective at present. These systems can have a number of functional advantages as being compared with traditional semiconductor systems. On this concern a development of methods of the carbon nanotubes (CNT) synthesis in nanopores created by the swift heavy ion tracks technology in SiO_2 on a silicon substrate is important. This method is connected with irradiation of SiO_2 thin layers by Au ions at energy of 350 MeV and fluence of ~ 1E9 cm–2, when latent ion tracks are formed there. Subsequent chemical etching leads to the formation in silicon oxide of conical nanopores with average diameter ~ 150 nm and density of ~ 1E8 cm–2, in which Ni clusters were deposited electrochemically. Investigations of CNTs growth processes in nanopores by the PCVD method has shown that structure and type of carbon-based systems depend on a degree of nanopores filling with Ni catalyst. In the case of a not complete filling (about 50%) of nanopores CNTs appeared, and at a complete filling of nanopores SiC wiskers growth have been observed. This fact was confirmed by Raman spectroscopy studies. Samples with CNTs have demonstrated a high efficiency of field emission, with the threshold less than 1 V/μm. A light emission of CNT array was found which showed high stability and homogeneity. Optimal values of interelectrode distance and applied voltage which provide a large light emission area were determined.

NOTES

Session «Nanostructures synthesis and characterization II (ISTC Workshop)»

SERS substrates on the base of semiconductor self-assembled quantum dots Ge-on-Si nanostrustures to characterize inorganic microcrystals

E. Klyachkovskaya [1], N.D.Strekal' [2], I.G.Motevich [2], S.V.Vaschenko[1], A.N.Harbachova[1], M.V.Bel'kov[1], S. Gaponenko[1], C.Dais [3], H.Sigg [3], T.Stoica [3], D.Grützmacher [4]

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Semiconductor self-assembled quantum dot Ge-on-Si structures were successfully employed as Surface-Enhanced Raman Scattering (SERS) substrates to characterize ultramarine blue inorganic art pigment. This nanostructures were grown by chemical vapor deposition (CVD) with using SiH_2Cl_2 and GeH_4 as reactive gases in an H2 atmosphere at ptot = 0.1 Torr. In the result of self-assembled process the germanium pyramids with a square base has been formed on the silicon surface. After vacuum deposition of Au on top of these structures, they allow to detect SERS spectra of ultramarine blue inorganic art pigment. The observed enhancement factors are different for different bands ranging from approximately one order of the magnitude for the principal bands to two orders of the magnitude for overtones and linear combinations of principal modes. Theoretical modeling predicts 10^10-fold enhancement in close vicinity of a silver spherical nanoparticle (0.24 nm) with rapid decay of enhancement factor to 1 in the range of approximately 50 nm. Experimental enhancement factor is treated as overall effect within the small portion of every microcrystal in the close vicinity of silver nanoparticle(s) and exceeds the value of 10^6. These results can be considered as importance extension of traditional surface enhanced molecular Raman spectroscopy towards bigger inorganic probes and purposefully used in cultural heritage examination.

NOTES

Magnetic properties of Gd-based nanocomposites prepared by laser assisted techniques

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Nanoscale compounds and alloys of gadolinium are promising materials for applications as therapeutic agents in drug delivery and as magnetic particles for the hyperthermia treatment due to the largest magnetocaloric effect known near the room temperature. In this paper magnetic properties of the binary Gd–Si and the ternary Gd5(Si1-xGex)4 nanosystems formed under various experimental conditions in the laser ablation and post-irradiated processes in liquid have been studied. The Nd:YAG laser (LOTIS TII, LS2134D), operating in a double-pulse mode at 1064 nm (energy 80 mJ/pulse, repetition rate 10 Hz, pulse duration 8 ns), was used for ablation. To obtain compound Gd-Si nanoparticles we used laser ablation of a combined target consisted of gadolinium and silicon plates tightly pressed to each other by polished surfaces. To obtain Gd (Si, Ge) nanoparticles we used laser irradiation processes in two different ways. First, the compound nanoparticles were synthesized by four step process which involved a sequential ablation of silicon, gadolinium and germanium targets followed by additional laser irradiation of the mixture of the formed colloids. Second, laser ablation of the relevant target consisted of Gd (Si Ge) alloy produced by thermal melting of stoichiometric mixture of the virgin components (powders) in an argon atmosphere in a water-cooled graphite oven was used. The magnetic properties of the formed nanoparticles were investigated in the temperature range 5.

NOTES

Poster session I

Rabi chain based terahertz nanoantennas

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The new type of terahertz nanoantennas is proposed. It is based on the Rabi-waves predicted in the earlier work of the authors [G.Ya.Slepyan et all, Phys.Rev.B81, 085115, (2010)] and corresponds to the wave of quantum transitions propagating in the assembly of coupled quantum dots (QDs) excited by the light wave traveling along the antenna. The terahertz component of emission is stimulated by the tunnel current induced on the Rabi frequency by the motion of quantum transitions over the QD-system. Three concrete examples of nanoantennas have been considered: single wire, single ring, 2D-array. The ordinary antenna characteristics (radiation patterns, etc.) are calculated. As a result, it was shown that emitting characteristics of such antennas are electrically tunable via the varying of intensity and phase velocity of the light wave. The antennas have been considered are promising for a lot of practical applications in nanoelectronics and nanophotonics due to the ability of electrical antenna scanning.

NOTES

Quantum Chemical Simulation of The Structure of The Endohedral Backminsterfullerene Derivatives

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Metallofullerene cluster can be presented as a super-atom that possess an electropositive metal nucleus and an electronegative fullerene case. These clusters have a good perspective for application as molecular conductors, magnetics and ferroelectrics. The most important areas of the cluster practical application are NMR tomography and radio-medicine, particularly, a novel kind of the beam therapy and medical nano-robot creation. This binary technology was designed for a selective attack to a tumor. It uses agents that are tropic to the tumor containing specific nuclides (10B, 113Cd, 157Gd etc.). The nuclide ingests neutrons and emits secondary radiation resulting in the tumor cells death. Fullerene based nanocluster derivatives and their analogs can be used for the selective shipping of the nuclides of interest to tissues and organs affected.
Neutron capture therapy action targets a tumor by selective reagent concentrating as opposed to neutron or proton therapy where beam targets organs affected, which can be resulted in radiation sickness. Neutron capture technology excludes this damage because of neutron radiation dose does not exceed the normal tissue tolerance, but is enough to kill the tumor. Realization of this technology needs a seek of 10B-rich boron-containing or 157Gd-rich gadolinium-containing agents that have to concentrate in tumors with contents of more than 20 mkg/g tumor for 10B and 5.5 mkg/g tumor for 157Gd. 157Gd has the largest capture section of thermal neutrons (44000 barn) including 113Cd (25000 barn) and 10B (750 barn). One of the perspective way for selective shipping of boron-, cadmium-, gadolinium- and other element-organic compounds as well as 6Li2H to affected tissues and organs can be the use of carborane, backminsterfullerene, carbon nanotube and their analogue based nanocluster derivatives.

NOTES

$C_{60}(FeCp_2)_2$ based composition material for the potential medical application

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Fullerene-based molecular solids have been attracting continuous interest due to their unique electronic, magnetic, and biological properties. The medical application of fullerene and the derivatives was studied in the work [1] where the authors concluded that there is a possibility to apply these compounds as the anticancer drug, the antibacterial agent, the antiviral agent. Ferrocene derivatives in particular ferrocenium salts demonstrated antitumor activity [2, 3]. In this work we synthesized composition material based on the nanoporuos Al_2O_3 and the $C60(FeCp_2)_2$ uniform particles. The influence of the pore diameter on the fulleride particle size was discussed.

Single crystalline nanosize specimens of $C_{60}(FeCp_2)_2$ were grown from the solution of a stoichiometric mixture of C_{60} and ferrocene in benzene by slow evaporation at 300 K on the nanoporuos Al2O3 substrate. $C_{60}(FeCp_2)_2$ crystallization occurs inside nanopores as well as on the substrate surface. Inside nanopore crystallization takes place mainly on the bottom. The crystal sizes correspond basically to the pore diameter and vary between 20 and 50 nm.

So we can conclude that the $C_{60}(FeCp_2)_2$ based composition material with quite uniform distribution of the fulleride particle size can be formed by crystallization from the benzene solution on the nanoporous substrate.

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NOTES

Two level system dynamics modelling near real nano- and microstructures

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In this report we discuss the Green function's approach to the problem of two level system interaction with real nano- and microstructures. The method is based on description of the electromagnetic environment by mean of Green functions of Maxwell equations with subsequent applying collective operator technique and algebraic solution of obtained motion equations for two level system. The main advantage of the proposed method is that it does not involve any approximation or assumptions on Green function spectrum. As the examples of proposed approach applications we consider two level atom evolution in the two and three dimensional photonic crystals and near the metallic nanoantenas. The Green function's were calculated by FDTD method for dielectric systems, by semi-analytical approach for metallic nanoantenas and by FEM technique for complex metallic nanoobjects.

NOTES

Self Amplified Spontaneous Emission in carbon nanotubes and graphene

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Electromagnetic wave slowing down is one of the remarkable properties of carbon nanotubes [1]. This effect leads to possibility of Cherenkov synchronism between electron beams and electromagnetic wave [2]. Collective radiation generation based on this mechanism in nanotubes and graphene is analyzed. The initiation of generation from quantum fluctuation that leads to the random microbunching of electron beam is considered and compared with input seed generation mechanism.

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NOTES

Electron band structure of carbon nanotubes intercalated cupper

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Preparation of the carbon nanotubes offers strong possibilities of manufacturing the nanowires with intriguing mechanical, electronic, and magnetic properties. The inner cavity of these tubules can be filled with a variety of substances including the transition metals. We are now being confronted with a problem of predicting properties of nanotubes intercalated with transition metals. Here, we present a linear augmented cylindrical wave (LACW) method and its application to band structure of the tubes doped with copper. The band structures and densities of states are calculated. It is shown that in the vicinity of Fermi level, the branches of the carbon and metal subsystems are intersected, which point to their considerable interaction and joint participation in conductivity. In the pure carbon armchair tube, the Fermi level is known to be located in dip of electron density of states. Intercalation of the transition metal fills this dip, which results in a growth of electron density of states in the Fermi level and consequently in a considerable increase in conductivity of the armchair carbon nanotubes. A metallization of the zigzag tubules due to the cupper intercalation is demonstrated too.

NOTES

Functionalized SNOM-probes with nanodiamond crystals hosting nitrogen-vacancy color-centers

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The optical resolution of existing scanning near-field optical microscopes (SNOM), based on the use of aperture SNOM-probes, made of sharpened metallized fiber with a hole at the apex of the cone, is essentially limited by the size of the aperture. In order to improve the optical resolution of SNOM and, therefore, to overcome this restriction it was proposed to use point-like light sources. Additional practical requirements for such light sources are simplicity of their creation, the ability of stable operation at room temperature, possibility of single-photon emission. Color-centers in diamond, in particular nitrogen-vacancy (NV) centers, appear to match all of the above mentioned requirements. We performed the attachment of nanodiamond nanocrystal with nitrogen-vacancy color-centers at the vertex of an optical probe. Spectrophotometric measurements and normalized second order time-intensity correlation functions of the functionalized optical probe measured with Hanbury Brown and Twiss scheme giving evidence for NV-center presence. The work can be of great importance in various fields of nanotechnology, where a high optical resolution is required: in medical biophysics, plasmonics, quantum cryptography.

NOTES

Influence of electromagnetic radiation on an array of carbon nanotubes in the presence of electric nanosecond impulses

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For an array of carbon nanotubes (CN) the dependence of nonlinear current density on width of forward front of amplitude of an alternating (high-frequency) field is investigated for various values of constant (or non-stationary) fields. It is shown that in the case of metal "zigzag"-like CN the current density does not depend on CN radius. The dependence of reinforced microwave radiation in two- millimeter range on longitudinal coordinate is received. The problem of generation of submillimeter radiation is investigated under influence of two-frequency carbon-dioxide laser radiation (CO2-laser) on the system of parallel oriented CN in the presence of constant (or non-stationary) fields. The dependence of amplitude of submillimeter radiation has beating behavior. The possibility of the use of freely oriented in space parallel each other CN is shown.

NOTES

Cluster Embedding Method for Quantum-Chemical Simulation of Nanodevices

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Applicability of cluster embedding method with non-orthogonal wave functions for theoretical study of processes in nanodevices is studied. Processes in nanodevices are treated in the frameworks of time-dependent DFT. We demonstrate that our cluster embedding method is compatible with DFT Kohn-Sham method and quantum transport theory based on time-dependent DFT. We conclude that approach for electric current calculation developed for orthogonal wave functions may be applied for non-orthogonal wave functions if we transform initial equations assuming that overlaps are small and we may neglect contributions of highest powers of overlaps.

NOTES

Hardware-software system for studying the properties of magnetic shields and electrical products based on film and composite nanostructures

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The problems of development and use of hardware and software system, and methodological support for research the characteristics of the magnetic shields and electrical products based on film and composite nanostructures are discussed. Apparatus and methods for measuring the magnetic field distribution in free space and near the products made from magnetic materials are considered. Hardware and software package is designed that provides: -automatic scanning of the examined area, -measurement of magnetometering probe displacement, -measurement of the three components of the magnetic field and its module, -setting of external magnetic fields with permanent magnets, solenoids and Helmholtz coils, -magnetization and demagnetization of the samples, -acquisition and processing of output signals from the photomultiplier tubes that are protected by magnetic shields in order to determine the parameters of the most efficient technologies and designs of screening, -presentation of measurement results on a computer screen in the form of tables and graphs. With the use of hardware and software system measurements of magnetic fields inside the cylindrical magnetic shields were carried out , close to their internal and external surfaces when exposed to DC, AC and pulsed magnetic fields. A comparison of the efficiencies of multilayer thin-film and conventional magnetic shields used for the screening of photomultiplier tubes and electronic components of onboard spectrometer is provided. The results of studies of magnetic fields of permanent magnets, magnetic circuits, metal sheet and bar products, products based on nanoscale granular and multilayer structures, single-layer magnetic shields and shields based on multilayer thin-film nanostructures are presented.

NOTES

Numerical analysis of the electrical conduction in carbon nanostructures

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The problem of the single molecule conductance measurement and calculation attracts much attention due to its possible use in the molecular electronics. Another promising line of research is connected with consideration of carbon nanostructures, in particular graphene and nanotubes, as possible elements of nanoelectronic devices. Here, we present the results of modeling of the conduction in systems including fullerenes. Among other members of the carbon nanostructures family, the fullerenes have advantages of relatively low cost and suitability for mass production and manipulation. The size of the fullerenes and their spacing in the fullerite crystal are appropriate to form quantum dots possessing specific physical properties that may be useful for many applications. The systems consisting of the single fullerene molecule or a simple-cubic lattice of the fullerite placed between two metal electrodes has been considered. The electric current as a function of the bias voltage was calculated using the Landauer formula, connecting the charge transport with the transmission of electrons. To obtain the transmission matrix components the supplementary problem of the electron scattering by the model potential had been solved. The transmission probability as a function of the electron energy and the electric current as a function of the bias voltage have been calculated. Our simulation has shown that the current – voltage characteristics of systems including fullerenes have negative-conductance regions that makes it possible to use them as active elements of nanoelectronic devices (particularly, generators of the RF-radiation).

NOTES

Non-plasmonic hyperthermia: prerequisites for realization and materials

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Nanoparticles of biologically compatible alloys with intensive electron-electron scattering are considered as potential substitutes for gold nanoparticles and silica-gold nanoshells in the photothermal cancer therapy. In this approach, it is proposed to heat the nanoparticles at the expense of the Joule heat generation, rather than due to plasmon excitation. Correspondingly, it is suggested that the resonance absorption of the laser radiation should be achieved due to specificity of the electron structure of the nanoparticle material, namely due to an enhanced electron density of states at the Fermi energy and also within the energy range 1.3 to 1.9 eV, i.e., in the transparency window of the biological tissues, above it. Estimations show that application of nanoparticles of the alloys with intensive electron-electron scattering can improve an efficiency of the laser radiation energy-to-heat conversion. In this case, the nanoparticles need not to have neither special cores nor the rice grain-like shape. The manufacture of the uniform spherical coreless nanoparticles is simpler and lower in cost. It seems likely that in the non-plasmonic hyperthermia, besides the gold alloys, the other biologically compatible metals and alloys can be applied (for example, tantalum and its alloys, and also the NiTi alloy).

NOTES

A simple way for the passive THz imaging

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Progress in terahertz (THz) optics and commercial availability of the infrared thermal imaging cameras with thermal sensitivities of 12 to 45 milliKelvins allow putting forward a simple way for the passive imaging the objects-sources of the THz radiation. In the framework of this approach, the THz objective forms the image of the object on the two-dimensional THz radiation-to-heat converter. The converter represents a matrix of the material transparent in the THz wavelength range, with a lot of embedded 9 nm nickel nanoparticles isolated from each other. The nanoparticles being heated by the THz radiation, convert the THz energy to heat. And the two-dimensional pattern being formed by heated nanoparticles in the converter is visualized by the infrared thermal imaging camera. In accordance with the number of pixels and thermal sensitivity of the specific commercial uncooled infrared camera, it is estimated the number of nickel nanoparticles per the element-object of the converter corresponding to the pixel-image.

NOTES

Isomeric transition of C10 molecule from star to ring conformations

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Studying the possible path of fullerene formation [1] in arc discharge plasma we have predicted a new metastable star-shaped isomer of the C10 molecule which along with the ring-shaped isomer plays the key role in formation of the C20 fullerene.

There is an open question on the possibility of radiative transition from star to ring conformations of the C10 molecule. To get an answer to this question we have performed quantum chemical calculations on the C10 molecule using the semiempirical molecular orbital PM3 method [2] and the ab-initio plane-wave pseudopotential method (PWscf program of ESPRESSO package [3]). Our calculations show that C10 transition conserves the D5h symmetry of the isomers. Note that conformation transition have been observed for molecules (e.g. the barrier for inversion of the ammonia molecule is 0.2 eV [4]).

By using the PM3 method we have calculated reaction coordinate of the star to ring transition. The corresponding energies for PM3 obtained atomic configurations was calculated also by using PWscf. The ring isomer was found to be lower in energy by 9.39 eV (PM3) and by 12.52 eV (PWscf) than the star isomer. Barrier for transition from the metastable star state to the ring state is 8.41 eV (PM3) and 1.70 eV (PWscf). Energies of E1' type vibrations of the star and ring isomers calculated by the PM3 method are 0.24 eV and 0.08 eV, respectively.

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NOTES

Dynamical diffraction theory of waves in photonic crystals built from anisotropically scattering elements

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The process of refraction and diffraction of waves in natural and artificial crystals built from anisotropically scattering elements is considered. As an example, the refraction of electromagnetic waves in two-dimensional photonic crystal formed from parallel metallic threads is studied in details. The expression for the effective scattering amplitude of the wave by a thread (in the crystal) is found for the case when the scattering by a single thread is anisotropic. It is shown that, unlike the case of a wave with polarization parallel to the threads, the refractive index for waves with orthogonal polarization can be greater than 1; this leads to the possibility of Cherenkov radiation in such a crystal. A system of equations describing the dynamical diffraction of waves in photonic crystals is obtained. The properties of parametric ("quasi-Cherenkov") radiation of charged particles in photonic crystals are considered. Since to describe the process of the scattering the most general approach is used, the obtained results are valid for a wide range of problems, not limited by considering only electromagnetic waves, or only specific type of crystals. In particular, they may be useful when studying diffraction of cold neutrons in artificial crystals.

NOTES

Plasmon-enhanced luminescence of fluorescein-labeled biomolecules on top of silver nanostructures

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Plasmonic enhancement of luminescence in nanostructures has big application potential but many proposed nanostructures are expensive and based on complicated procedures. The real-life implementation needs cheap, easy to synthesis, durable and reproducible plasmonic nanotechnology. We proposed a simple method of plasmonic nanostructures formation using silver colloidal films and polyelectrolyte layers as a dielectric spacer. Bovine serum albumin molecules labeled by fluorescein isothiocyanate were used as model biological targets. Silver sols with different nanoparticle sizes were synthesized by AgNO3 reduction using sodium citrate. To develop a dielectric spacer between a silver film and biomolecules, the substrate surface was covered by alternate polyelectrolyte layers, followed by aqueous solution of labeled molecules. Luminescence excitation was performed by LED (460 nm). Plasmonic effects on biomolecules luminescence for different silver nanoparticle sizes, excitation light polarization, and molecule-silver spacing were examined. The enhancement factor exhibited smooth dependence upon polyelectrolyte spacer thickness with maximum for 5 layers. For unpolarized excitation the highest enhancement factor was 7 for 50-90 nm silver nanoparticles. The maximal 9-fold enhancement was observed for p-polarized excitation. Experimental results are in good agreement with performed theoretical calculations taking into account local intensity enhancement, radiative and nonradiative rates modification, light polarization, molecule position and its dipole moment orientation.

NOTES

Size and temperature dependence of the surface plasmon resonance in silver nanoparticles

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The dependences of the surface plasmon energy were studied for silver nanoparticles in the size range 11–30 nm and in the temperature interval 293–650 K. The energy of SPR in silver nanoparticles embedded in silica glass host matrix depends on the size and the temperature of the nanoparticles. Our experiments exhibit the nonlinear red shift of the SPR as the size of the nanoparticles decreases. The increase of the surface scattering rate of the free electrons causes the red shift of the SPR energy as the particle size decreases. As the temperature of the sample increases, the SPR red shifts. The volume thermal expansion of the nanoparticles leads to red shift of the SPR. As the temperature of the particle increases, the volume of the nanoparticle increases and the density of the free electrons decreases. The lower electron density leads to the lower plasma frequency of the electrons and subsequently to the red shift of the SPR. The red shift of SPR with the increase of temperature is linear for large (25 nm and 30 nm) silver nanoparticles and becomes nonlinear (superlinear) for smaller nanoparticles (17 nm, 11 nm). The nonlinearity of the dependence of SPR energy on temperature becomes stronger for smaller nanoparticles (17 nm, 11 nm). These two effects can be rationalized by the dependence of the coefficient of the volume thermal expansion on the size and temperature of the nanoparticles, The coefficient of the volume thermal expansion increases when the nanoparticle size decreases and with the increase of the temperature of the nanoparticle.

NOTES

Modelling of a magnetic resonance in nanoparticles array

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Nanoparticles, possessing magnetic properties, represent appreciable interest for medicine. In our research we address to the solution of the following problems: development of the model, which describes magnetic field interaction with the magnetic nanoparticles array; and modeling of the magnetic resonance in the nanoparticles array. As a result of our calculations we have received 3D magnetization distributions, total energies and magnetic resonance spectra of separate nanoparticle and nanoparticles ensemble interacted by magnetodipole mechanism. It is established that separate nanoparticle in alternating and constant magnetic fields demonstrates the paramagnetic resonance appearing due to enhancement of magnetization oscillation. Characteristic reflexes of paramagnetic resonance for one nanoparticle in two directions are determined, as well as magnetization change along the direction of constant field. It is revealed that in system of interacting nanoparticles of variable and constant magnetic fields the dynamics of magnetization is characterized by the random process with the elements of stochastic resonance. It is shown that in the system of interacting nanoparticles with the characteristic size of 2 nm the ferromagnetic resonance (FMR) appearing at concentration of order 5e18 cm-3 upon the concentration decreases down to 5e16 cm-3 FMR is transformed into the paramagnetic resonance, characteristic for the noninteracting particles system.

NOTES

Design of high-pass multiband multilayer filter for Raman

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Nanoplasmonic structures offer enormous enhancement of Raman scattering rate for molecules adsorbed on a nanotextured metal surface. This phenomenon principally can lead to development of palmtop Raman testers for certain practical applications. In such devices multiband haigh-pass filters are desirable with narrow transmission bands adapted for certain combination of laser wavelength and probe molecules. The potential applications include e.g. medical diagnostics. In this contribution we report on design of three-band high-pass multilayer filters aimed at oral cancer diagnostics. The filters сотефшт 24 and 27 layers and have transmission peaks at 661, 680 and 706 inverse cm adapted for a He-Ne 632 nm laser source. The peak transmission is 1 in every band whereas the background transmision between bands is no more than 0.1. Practical implementation is feasible with commercially available dielectric materials and vacuum deposition technique.

NOTES

Luminescence properties of biological molecules infiltrated in synthetic opal

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Photonic crystals (PC) are of great interest in device applications for optics, optoelectronics, sensors due to their potential in control of light emission and propagation. Forbidden and stop zones for light propagation are one of the characteristic features of PC that drastically affects the optical properties of PC as well as molecules inserted in the PC cavities. We have studied the opals infiltrated by DNA (deoxyribonucleic acid), poly-A (polyadenylic acid) and Glycine [1, 2]. Nanodispersive silica globules (with particles size near 240 nm in diameter) were synthesized by the method of Stober. PC was obtained by conventional sedimentation. For registration of spectra of luminescence and visualisation of biological molecules we applied LS-55 Fluorescence Spectrometer (PerkinElmer) and.confocal microscopy LCM 510 (Carl Zeiss, Germany) microscope. Enhancement of luminescence of DNA infiltrated in opal seems to be connected with coincidence the energy levels in DNA and SiO_2, transition and/or conversion energy. Visualization of biological molecules on the surface PC is probably due the same fact. Acknowledgment: we thank Ukrainian-Russian project and STCU #5525 for financial support.

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NOTES

Anomalous retroreflection from strongly absorbing nanoporous semiconductors

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Pronounced retroreflection behavior is reported for a fishnet nanoporous strongly absorbing semiconductor material. Retroreflection features a half–cone about 0.35 rad along with diffusive specular reflection for all angles of incidence. Retroreflection is apparent by the naked eye with daylight illumination and exhibits no selectivity with respect to wavelength and polarization of incident light featuring minor depolarization of retroreflected light. The reflectance in the backward direction measures 12% with respect to a white scattering etalon. The phenomenon can be classified neither as coherent backscattering nor as Anderson localization of light. The primary model includes light scattering from strongly absorptive and refractive superwavelength clusters existing within the porous fishnet structure. A reasonable qualitative explanation is based on the fact that strict retroreflection obeys shorter paths inside absorbing medium, whereas all alternative paths will lead to stronger absorption of light.

NOTES

Comparative electrooptical response from zero-, one, and two-dimensional CdSe nanocrystals

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We synthesized by colloidal chemistry way the quantum confined CdSe nanocrystals of different dimensionality: 0D (quantum dots), 1D (nanorods), 2D (platelets). CdSe nanocrystals have been introduced into the polymeric films sandwiched between two transparent conductive electrodes. The room temperature electrooptical effects were studied in form of differential absorption spectra of nanocrystals versus the applied electric field. We observed an order of magnitude larger electrooptical response from CdSe platelets, as compared to quantum dots, while, CdSe nanorods show a little effect. The mechanisms for dimensionality-dependent electrooptical effect in semiconductor nanocrystals, as well as possible practical applications are discussed in the presentation.

NOTES

Main properties of effective dimensional reduction for relativistic Dirac particles

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We consider an example of an effective dimensional reduction for a Dirac particle in a curved spacetime and use it for investigation of general properties of Dirac particles in effective two-dimensional spaces. The reduction is just effective because the particle remains in the three-dimensional space while one of its dimensions is compactified. This is assumed to be a model for the generic low-dimensional structures. We perform the Foldy-Wouthuysen transformation of the covariant Dirac equation for three spatial dimensions and determine general properties of momentum and spin dynamics at the above reduction. We use the specific metric admitting such a reduction. We derive the corresponding relativistic Foldy-Wouthuysen Hamiltonian and equations of motion. We formulate general conditions and find general properties of the effective dimensional reduction. We find the quantum mechanical and semiclassical equations of spin motion. For a particle in a curved spacetime, the axis of spin quantization coincides with the axis corresponding to the compactified dimension. However, the direction of this axis can be changed by an additional electromagnetic interaction. For this case, the semiclassical and classical limits are studied. The work is supported by the Belarusian Republican Foundation for Fundamental Research (Grant No. Ф10Д-001).

NOTES

Numerical simulation of surface plasmons in Si/SiGe layers with incorporated nanoholes and metallic nanoparticles

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In this talk, a short review of numerical methods of multilayer plasmonic structure analysis will be done. The study is motivated by possible improvement of solar cell efficiency by using plasmonic nano-structures. Recently this subject has been recognized as one of most promising for further development of solar cells due to consequent reduction of the thickness and increasing of the absorption of photovoltaic devices. A lot of attention has been lately devoted to 'on-surface' plasmonic structures, while the structures with incorporated nanoparticles and nanoholes are fewer investigated. The following results will be presented and discussed: - Optical properties of gold and silver nanoparticles are simulated as a function of particle size and dielectric constant of medium (Si, Ge, SiGe, colloids). Numerical calculation data is compared with experimental results of structural and optical investigation. - Simulation of surface plasmon excitation in Si and SiGe layers with incorporated nanoholes and metallic nanoparticles and their complexes.

NOTES

Synthesis and physicochemical properties of composites on the based iron- and cobaltcontaining nanoparticles and polymers for electromagnetic shielding

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The thermal decomposition of iron and cobalt formate was employed for the creation of the nanocomposite that represents iron- and cobalt-containing nanoparticles stabilized in the high-pressure polyethylene matrix. Concentration of nanoparticles was variation from 10 to 40 wt. percent. The structures of resulting nanomaterials were studied using the transmission electron microscopy, X-ray diffraction, NMR, EXAFS, Mossbauer spectroscopy, ESR. The concentration dependences of the electrophysical properties of the synthesized nanomaterials were analyzed. Magnetic properties of nanocomposites in polyethylene matrix have been investigated. It was shown that the material has higher saturation magnetization values per atom than in a bulk state. The reflection and attenuation factors for the 30 GHz waveguide containing composite samples were measured. It was shown that such materials could be used in devices which effectively for electromagnetic shielding.

NOTES

Enhanced light-matter interaction in plasmonic nanostructures

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A general consideration of nanoplasmonic enhancement of light–matter interaction is proposed in terms of incident field concentration and photon density of states concentration providing a rationale for huge enhancement factors for Raman scattering and noticeable enhancement factors for luminescence. The proposed model sheds light on the so-called “hot spots” as such places on a nanotextured metal surface or near metal nanobodies where simultaneous spatial redistribution of electromagnetic field occurs both at the frequency of the incident primary radiation at the frequency of secondary radiation. Experimental performance of enhanced secondary emission for atomic, molecular systems, semiconductor quantum dots and inorganic microcrystals using multilayer and spatially organized metal-dielectric nanostructures is discussed in detail.

NOTES

Luminescent nanodiamonds of divers origin

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For the last decade an interest to the luminescent nanodiamond has multiply increased. This is explained by promising results on use of luminescent NDs as a source of a single-photon emission for quantum information technologies and, alternatively, as a bright light source applicable for biolableling. The brightest color centers used for a production of the luminescent nanodiamond are nitrogen-vacancy (NV) and silicon-vacancy (SiV) centers.

We studied the color center photoluminescence in CVD, detonation and meteoritic nanodiamonds (ND). It was demonstrated that the luminescent SiV centers are efficiently produced and are thermodynamically stable in 3-5-nm diamond crystallites produced by CVD technique. Representative classes of NDs produced by detonation shock wave conversion of diferent carbon precursor materials have been systematically investigated. There was shown that (i) ND particles larger than 30 nm may contain in situ produced optically active NV centers, (ii) in ND produced from explosives, NV centers are detected only in ND produced by wet synthesis, (iii) NDs synthesized from a mixture of graphite/hexogen have the largest concentration of NV centers among all studied NDs. Recently, SiV luminescence was found in meteoritic nanodiamond particles with a mean size of 1.5-2 nm. This finding opens the door to non-perturbative fluorescent probes as markers in microscopy and sensing, and provides a remarkable fingerprint for identification of nanodiamonds in astrophysical environment.

This study was supported by the Ministry of Education and Science of the Russian Federation, State contract no. П925, the RFBR grant no. 11-02-01432, the grant of RAN program no. 24, the grant of President of the Russian Federation НШ-3076.2012.2.

NOTES

Expanding possibilities for investigating of chemical composition with m-XRF spectrometer M4 TORNADO from Bruker. AXS

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OPTEC LLC, Ukraine

m-XRF spectrometer M4 TORNADO is a new standard in non-destructive elemental analysis. The use of the modern X-ray tubes and polycapillary X-ray optics provides generating high fluorescence intensities even of smallest sample areas. The X-ray optics allow to focus tube radiation from a large solid angle and concentrate it on spots down to 25 μm for Mo-K radiation, provide maximum intensity in spot. The M4 TORNADO is equipped with XFlash® silicon drift detector (SDD) technology (active detector area is 10 mm^2, the energy resolution down135 eV). High-precision optical system and the software provides obtaining qualitative and quantitative analysis in seconds, "on the fly". Analysis of any type samples (metals, alloys, powders, liquids including in homogeneous and irregular shaped specimens) is based on standard models and standard less calculation. These functional features allow to recommend M4 TORNADO spectrometer for applications in various fields of science, manufacturing, training: metallurgy, machine-building and instrument-making industries, geology, nanotechnology, etc.

NOTES

General Session IV

Colloidal Nanocrystal Architectures for Nanophotonics

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Nowadays assembly approaches are recognized as being the main working tool of bottom up chemical nanotechnology. The assembly of strongly emitting semiconductor nanocrystals can be performed on flat, porous and spherical surfaces and thus are very important for thin-film technologies, doping of mesoporous materials, modification of pre-patterned substrates, the creation of microshells and cavities, etc. Self-assembly approaches or the use of removable templates make possible the formation of nanowires, nanosheets or nanoporous 3D ordered materials created solely from the assembled nanoparticles. Hierarchical assembling and assembling of nanocrystals with other organic or inorganic entities opens up the possibility to achieve composites with literally unlimited functionalities. The understanding and governing of charge and energy transfer processes between the components of the composites are the key points in their efficient utilization as building blocks in novel types of LEDs, photovoltaic and photonic devices and various optical sensors.

NOTES

Resonant energy transfer in the complexes of semiconductor nanocrystals and organic dye molecules

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Forster resonant energy transfer (FRET) within the luminescent donor-acceptor complexes is a powerful tool for biomedical fluorescent detection platforms, optical sensors. Luminescent semiconductor colloidal nanocrystals or quantum dots are ideal candidates for FRET donors due to very broad spectral range of optical absorption and narrow photoluminescence bands, whose spectral position can be easily tuned either by size or chemical composition of quantum dots. Additionally, the shape of semiconductor nanocrystals can be varied from spherical (quantum dots) to elongated (nanorods), nanowires, tetrapods. Based on the experimental results, here we discuss how to construct the efficient FRET complexes with luminescent CdSe nanocrystals, how the shape of CdSe nanocrystals may affect on the FRET efficiency in the nanocrystal-dye complexes, how to control with FRET the radiative and non-radiative pathways in double band-emitting ZnSe quantum dots doped with Mn ions.

NOTES

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Magic-number nanocrystals by chemical methods and their potential applications

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The high-end nanotechnology that essentially depends on excellent nano-chemistry, has prompted chemists to undertake new challenges, not only in synthesis but in tailoring desired optical properties for useful applications in electronics and optical devices. In recent years, Quantum dots have greatly influenced the fate of photonic devices and of late, their potential as sensitizers for replacing organic dyes in dye-sensitized solar cells and their conjugation with bio-molecules for bio-solar cells has attracted many researchers. Enhanced experimental skills of chemists are now playing major role in isolation of thermodynamically stable pre-mature 'early-stage' elongated nano-particles which upon isolation are termed as 'Magic-number nano-crystals'. Because of their not-so-perfect crystal structure these magic-number NCs differ with QDs in their optical properties e.g. a doublet absorption and broad emission wavelength in compare to single narrow absorption and emission of QDs. The optical properties can be tuned either for magic-size NCs alone or a combination of with QDs and or can be converted to ofthat of pure QDs in case of CdSe. These high-end nano-crystals thus become potential candidate for white LEDs. QDs synthesis via organometallic reactions are often preferred but warrants special efforts. Alkeno-1,2,3-selenadiazoles are excellent Se-provider reasonably greener synthesis of magic-sized NCs as well as of regular metal selenides that includes CdSe. The high-end products/particles can be isolated with ease directly or via formation of molecular cluster of [Cd(C12H18Se2Br2)]. This lecture will deal with the chemical aspects of high quality nano-crystals.

NOTES

Studies of Complex Materials with Hot Neutrons

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Studies of high-energy atomic, molecular and magnetic dynamics in condensed matter are being performed at ILL on the hot-neutron spectrometer called IN1. This instrument comprises two different secondary spectrometer options which can be alternatively connected to the unique single crystal monochromator with three reflecting faces supplying monochromatic neutron beams in the broad energy range (10 - 1000 meV). Flexibility in the choice of the experimental conditions combined with convenience of the changes permit a wide range for the optimisation on resolution/intensity. The classical-scheme three-axis spectrometer IN1-TAS is used for measurements of dispersion curves of elementary excitations in single crystals and liquid or amorphous samples. This secondary spectrometer is now equipped with a new double-focussing copper crystal analyser. The new secondary spectrometer IN1-LAGRANGE (LArge GRaphite ANalyser for Genuine Excitations) commissioned few months ago opens new perspectives for studies of phonon density of states on polycrystalline samples. Particular emphasis is given to a possibility of high-resolution measurements of extremely small samples (containing down to 0.1 mg of Hydrogen). Examples are given of the experiments performed on both spectrometers which include magnetic moment dynamics in magnets, atomic dynamics in liquids with the high-resolution Brillouin scattering setup, proton dynamics in complex molecular compounds.

NOTES

Electromagnetic shielding efficiency in Ka-band: carbon foam versus epoxy resin nanocomposites

P. Kuzhir, A. Paddubskaya, A. Pliushch, S. Maksimenko, A. Celzard, V. Fierro, G. Amaral-Labat, A. Pizzi, J. Macutkevic, G. Valusis, M. Ivanov, J. Banys, L. Coderoni, F. Micciulla, I. Sacco, S. Bellucci

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We report on the comparative study of the effectiveness of electromagnetic (EM) shielding in Ka-band provided by epoxy resin filled with nanostructured carbon additives in relatively small concentrations (0.25-2 wt.%) and micro-structural porous carbon solids (carbon foams) of different bulk densities, from 0.042 to 0.150 g/cm3. Microwave probing of carbon foams shows that transmission of 2 millimeter thick layer strongly decreases with the decrease of pore size up to the level of 0.6% due to significant rise of the reflectance ability. The series of pre-percolative and close-to-percolation threshold nanocarbon based samples were prepared using Epoxy resin, an own curing agent A1 (modified TEPA) and different types of functional filler: artificial and natural graphite, thermally exfoliated graphite, thick graphene, carbon blacks having different surface areas, activated carbon of different granulometries, and carbon nanotubes (both single- and multi-walled). We found that 2 mm thick epoxy resin nanocomposites in some cases (1.5-2 wt.% content of thermally exfoliated graphite, thick graphene and carbon nanotubes) demonstrate pretty high EM attenuation of 26-37 GHz signal on the level of -18 □ -22 dB. To conclude, both carbon foam and epoxy resin loaded with nano-sized carbon inclusions could lead to fabrication of effective EM coating, thin and light, to be used for EM protection.

NOTES

Broadband dielectric spectroscopy of carbon nanotubes composites

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The dielectric properties of composites with carbon nanotubes (CNT) are widely studied, due to their attractive applications and interesting fundamental physics. High dielectric permittivity and electric conductivity are reported for polymer composites with carbon nanotubes embedded in concentrations close and above the percolation threshold. However, there is a lack of a deep understanding of relations between microscopic CNT parameters (such as, dielectric poliarizability, matrix microstructure chain length and degree of polymeratation, etc) and dielectric properties of fabricated composites as a whole. In this contribution the effects of processing conditions and CNT oxidation treatment on dielectric properties of multiwall carbon nanotube/PMMA composites has been discussed. We present the dielectric properties of polymethyl methacrylate (PMMA) composite filled with multi-walled carbon nanotubes (MWCNT) with different average diameter in wide frequency (20 Hz – 1 MHz) and temperature range (300 – 400 K). CNT with narrow outher diameter distribution and known number of inner shells were produced via reaction of ethylene decomposition at 650-700 ^{0}C in standard CVD setup using Fe-Co catalysts. Two types of CNT were investigated, named FCA and FCM series, with average outer diameter ~ 9 nm and 12-14 nm respectively. The wall number has been estimated for thin nanotubes as 3-7, for the thick ones as 8-15 walls. The composites were produced via coagulation precipitation technique and in-situ polymerization of MMA. The temperature dependence of complex dielectric permittivity at different frequencies is mainly caused by β relaxation for all investigated samples. The mean relaxation time decreases on cooling according to Arrhenius law.

NOTES

Effect of nitrogen doping on the polarizability of carbon nanotubes

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Anisotropic polarization properties of carbon nanotubes (CNTs) are important for development of chemical sensors, electromechanical systems, antennas, detectors and sources of electromagnetic radiation in terahertz region, and shielding composite materials. These properties can be modified by inserting nitrogen atoms in the CNT walls in the results of decomposition of nitrogen-containing precursor. The content as well as the chemical state of incorporating nitrogen is dependent on the synthetic conditions. The nitrogen concentration in single-walled CNTs (SWCNTs) is limited to ~ 1at.% while it may exceed ~3-5 at.% in multi-walled CNTs (MWCNTs). Here we use density functional theory (DFT) for calculation of the substitutional energy for nitrogen atoms in CNT and the static polarizability of models. It is found that static polarizability is sensitive to the position of nitrogen atoms in CNT wall. The thermodynamically most preferable configuration, when the nitrogen atoms occupy the sites in pentagonal rings near the closed CNT tip, provides the largest gain in polarizability especially for the longitudinal component. Formation of such rings in graphitic network promotes closing of nanotube that could explain bamboo-like structure of nitrogen-doped MWCNTs. Assembly of conical graphitic segments containing nitrogen near the cone tip should give much higher longitudinal polarizability of nitrogen-doped MWCNTs as compared with the undoped counterparts or nitrogen-doped SWCNTs. High anisotropy of polarizability response expected for nitrogen-doped MWCNTs would open their utilization for development of electromagnetic protecting materials.

NOTES

Simulation of Electromechanical Pproperties of Ordered Carbon Nanotube Arrays

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Carbon nanotube arrays are shown to have interesting mechanical resonant properties which manifest themselves in electromechanical phenomena such as excitation of resonant vibrations of nanotubes in electromagnetic fields due to the action of ponderomotive forces. Hierarchical simulation approach to the modeling of such arrays is necessary including quantum mechanical, molecular-dynamical and continual description levels. Elastic properties of carbon nanotubes can be calculated by molecular dynamics simulations and then be used for continual modeling of nanotube arrays electromechanical behaviour by multiphysics methods. This program was realized for electromagnetic fields of radio and UHF regions both for individual nanotubes and arrays. Possible applications of resonant behaviour of the arrays are discussed.

NOTES

Session «Optical & electromagnetic properties of nanostructures II»

Photo- and Electroluminescence CdS/CNT Hybrids

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Simple and effective methods for synthesis of the hybrid material from the CdS nanoparticles (NP) on carbon nanotubes (CNTs) are proposed. CNT arrays were grown on silicon substrates using aerosol assistant chemical vapor deposition (CVD) method. The size and the shape of the CdS NP formed on CNT were found to depend on the temperature of water or other organic solutions. Method for deposition of CdS nanoparticles based on Langmuir–Blodgett technology was developed. Electron microscopy study revealed a direct contact between CdS nanoparticles and CNT surface. X-ray photoelectron spectroscopy examination of the CdS/CNT hybrid material detected surface oxidation of the grown nanoparticles. The synthesis methods allow preserving alignment of CNTs in the array and uniform decorating the CNTs with CdS nanoparticles or deposition only on nanotubes tips. Formation of the continuous CdS/CNT interface indicates that nucleation and growth of the NP take place directly on the nanotube surface. Electroluminescent properties of synthesized materials were studied on a set-up elaborated for measurement of field electron emission characteristics. To observe electroluminescence from CdS NP deposited on the CNT cathode, surface the phosphor screen was replaced by transparent glass coated with ITO. Image luminance of individual radiation centers is more homogenous than that observed on the phosphor screen. Furthermore, the radiation centers can have different spectrum, which is independent on the applied voltage. Photo luminescent bands were measured for samples with nanoparticles deposited on Si substrate and on CNT. Decrease of luminescence □ ~ 470 nm for CdS/CNT hybrids was detected and associated with Forster resonance energy transfer.

NOTES

Forming electronic waveguides from graphene grain boundaries

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Using wave packed dynamics based simulation [1,2] we investigated in atomic resolution the spreading of electronic wave packets on the graphene surface containing various configurations of grain boundaries (GBs). Our recent experiments [3] and simulations [4] show that in the regions in which an accumulation of graphene structural defects is found—like in GBs in CVD graphene—the charge-spreading phenomena are dramatically altered. Hence it is potentially possible to build all-carbon nanoelectronic circuits based on GB networks, or purposefully damagedregions on a graphene surface. In this paper we simulate the behavior of a few such nanoelectronic “building blocks”, namely a waveguide (made of two parallel GB-s) and a beam splitter (formed as Y junction of GBs). We study the “robustness” of the phenomena, e.g. the dependence on the structure and symmetry of the GB and on the electron energy.

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Graphene quantum dots: structures, properties, electronic and optic applications

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This report is review of experimental data of formation graphane, oxide and fluoride graphene nanostructures with graphene nanopeaces, their electronic and optics properties, and computer modeling of of main similar nanostructures prepared by special ways. We consider next main structures and methods of their preparations: 1) H (or F) covered graphene and begrapnene nanostructures; 2) semiconductor superlattices of periodically changed graphane/or fluoride graphene and graphene paths (or graphane peaces divided semiconductor grapnene peaces); 3) arrays of individual GQDs on graphane matrix, and GQDs formed on graphene nanoribbons. We consider also modeling of forming process of GQDs from C60 transforming discovered recently in 2011 experiments. Modeling of mechanisms of formation, electronic and optic properties of considered structures will be discussed.

NOTES

Electrical and magnetotransport in vertically oriented magnetically functionalized carbon nanotubes arrays

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Due to the possibility to utilize the unique physical properties like ballistic electrical transport, Luttinger liquid behavior, high thermal conductance and etc., carbon nanotubes (CNT) still attract much attention from the scientific community. On another hand the use of transition metals (Fe, Co, Ni) as the catalyst for CNT growth opens the perspective to synthesize materials where manifest both exclusive CNT properties and nanomagnetic phenomena. In this work we report studies on the electrical and magneto- transport in vertically oriented magnetically functionalized carbon nanotubes arrays. The arrays were synthesized by pyrolysis of ferrocene /xylene solution. For all samples studied in our work the conductance is increasing with temperature rising in whole temperature range (LHe - room temperature). The magnetotransport measurements performed in the magnetic field range -8 ... 8 T show negative magnetoresistance. The absolute value of magnetoresistance is increasing with temperature rising. The nature of negative magnetoresitance is explained in terms of weak localization. The contribution of iron nanoparticlas into the arrays transport properties is also discussed.

NOTES

Session «Perspectives of biomedical applications»

Surface enhanced spectroscopy in science and medicine

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The enhancement of optical process by a factor 102..106 near rough surface of metal (Au, Ag, Cu, etc.) is known already for thirty years, for both optical transitions in adsorbed molecules (Raman scattering (RS) of light, luminescence, infra red (IR) absorption and the processes which do not depend on the presence of molecules on the metal surface (for example, second harmonics generation). The explanation of the effect is not simple and includes several mechanisms, such as: i) the increase of the electromagnetic field near rough metal surface or island metal films, ii) the increase of the dipole transition moment of the adsorbed molecules, etc. The energy is transferred from photon to local plasmon oscillations. The energy from plasmon vibrations is transferred to the adsorbed molecules, which causes increased molecular absorbance. The enhancement of infrared (IR) absorption by rough metallic surface is named as SEIRA (surface enhanced infra red absorption) and enhancement of RS is named as SERS (Surface enhanced Raman Scattering). Here we demonstrate and discussed different applications of SEIRA, SERS, enhanced fluorescent spectroscopy and imaging in nanotechnology, medicine, biology [1] as well new non-metallic substrates for it. We thank for financial assistance Project STCU 5525 (2012-2013), Ukrainian- German project № M366 (2011-2012). 1. G. Dovbeshko, O. Fesenko, O. Gnatyuk, Ya. Shtogun, L. Woods, S. Bertarione, A. Damin, D. Scarano, Adriano Zecchina, Nucleic acid interaction and interfaces with single-walled carbon nanotubes, “Carbon Nanotubes”, 2010, Ed. By Jose Mauricio Marulanda, In-Tech., 2010. pp.697-719.

NOTES

Localized plasmon resonance in composite materials containing single-wall carbon nanotubes: theory and experiments

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The origin of the broad THz conductivity peak (TCP) of thin single-wall carbon nanotube (SWNT) film is currently under debate. As was shown elsewhere [Slepyan, et al., Phys. Rev. B 81, 205423 (2010)], the main contribution to TCP formation at room temperature comes from the finite-length effect in SWNTs. We have now experimentally demonstrated the dependence of the TCP frequency on the SWNT length. A passive acid-cutting approach was developed to obtain SWNTs with different length distributions and weak sidewall degradation. Thin SWNTs films with different average SWNT lengths were prepared on silicon substrates. The far-infrared spectra of prepared samples demonstrate the TCP blue shift with decrease of SWNT length. The experimental results are well described by the theory of localized plasmon resonance in SWNTs.

NOTES

Ag nanoparticles induce stress reactions in higher plants

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Silver nanoparticles (Ag NPs) are the world's most widely used nanomaterial that has a number of applications in nanophotonics. Despite their positive aspects, Ag NPs accumulate in the soil and have become an important environmental contaminant. Some data show that Ag NPs inhibit growth of higher plants which are the most prevalent form of life on the Earth. Here, we have explored cellular mechanisms of Ag-NP-induced phytotocixity using model plant Arabidopsis thaliana. We have found that manufactured Ag NPs (40 nm; 0.05-10 g l 1) can decrease the rate of root elongation and leaf expansion and activate key plant stress reactions, such as transient Ca2+ elevation and production of reactive oxygen species (ROS). Ag NPs also inhibited photosynthetic efficiency, and their presence in media led to accumulation of very high Ag levels in plants. NPs had much more pronounced effect than bulk. Using electron paramagnetic resonance spectroscopy, we have demonstrated that Ag NPs probably interact with L-ascorbic acid promoting ROS imbalance. Overall, out data have shown for the first time that Ag NPs induce stress reactions in plant cells and shed the light on potential environmental issues arising from the use of metal nanoparticles.

NOTES

Comparative analysis of the effect of enhancement of IR signals of biomolecules adsorbed on single wall carbon nanotubes and graphene nano plates

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It is known an effect of surface enhanced infrared absorption (SEIRA) of molecules near rough metal surface by a factor 10-200. However, this effect could be registered for molecules adsorbed on non-metallic surface, namely carbon surfaces, semiconductors, etc. The aim of the present report is comparative analysis the effect of enhancement of thymine adsorbed on single wall carbon nanotubes (SWCNT) and graphene nano plates and single layer graphene oxide. We studied thymine (Sigma-Aldrich), SWCNT (Moscow Institute of Physics), graphene nano plates and single layer graphene oxide (USA). The samples of thymine and thymine/graphene and thymine/oxide graphene complexes were prepared. All samples were mixed by ultrasonic mixer for 30 min. FTIR spectra have been registered with IFS-66 Bruker instrument in the 400–5000 cm-1 region. We got enhancement factor of about 2-6 for thymine adsorbed on SWCNT. The spectra of thymine/SWCNT shows that maximum factor of enhancement equalled to 6 for bands, which is corresponding to the C-H, C-OH and C-N. The maximum enhancement factors for thymine absorbed on the graphene plate and graphene oxide are 2 and 5 for band 1754 cm-1 (C2=O vibrations). Thus, we can assumed that the factor of enhancement of thymine adsorbed on the graphene plates is less than enhancement factor of thymine adsorbed on the SWCNT. Mechanism of enhancement of thymine molecules adsorbed on nanostructured carbon substrates, seems to have chemical and electromagnetic nature. The last mechanism could be connected with excitation of plasmon vibrations in carbon layers in IR region and discussed here. We thank for financial assistance Project STCU 5525 (2012-2013), Ukrainian- German project № M366 (2011-2012), Russian-Ukrainian Project (2012-2013).

NOTES

Session «Electromagnetics & Plasmonics»

Electrodynamics of Multiwall Carbon Nanotubes with Intershell Tunneling

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Carbon nanotubes (CNTs) (e.g.,[1]) can be used as possible alternative to metals like copper andaluminum to fabricate interconnects and antennas. The typical diameter of SWCNTs is about 1 nm and, depending on its chirality's, can be either metallic or semiconductor. On the other hand MWCNTs have diameters in a wide range of a few to hundreds of nanometers and are composed of both metallic and semiconducting CNT shells. The electromagnetic behavior of MWCNTs, in the low frequency regime where only intraband transitions are allowed, depend on the number of effective conducting channels of each shell [2], the electron tunneling between adjacent shells [3] and the electromagnetic interaction between shells and environment. In [4] a transmission line model has been proposed to account for the intershell tunneling on the propagation of electric signals. The intershell tunneling qualitatively change the form of the standard transmission line equations through the tunneling inductance and capacitance operators, which have to be added to the kinetic and magnetic inductance matrices and to the quantum and electrical capacitance matrices. The tunneling inductance operator is responsible of a strong spatial dispersion and coupling between the lines.
Since in [4] the effects of the tunneling transverse currents have been disregarded the transmission line model is only valid in the frequency range from microwave up to terahertz. In this paper we remove this limitation by accounting for the effects of the tunneling transverse currents and obtain a model that is valid from dc up to terahertz frequencies. The description of the tunneling ransverse currents is carried on the basis of the density matrix formalism and Liouville equation [3].

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NOTES

Plasmon polariton slowing down in graphene structures

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Dispersion of plasmon polariton in few layer graphene is derived and analyzed. It is shown that dispersion properties and electromagnetic wave slowing down in graphene considerably depend on the electron band which conduction electron occupied. The electron tunneling effect between graphene layers is considerable obstacle for strong wave slowing down. There are electron bands in vicinity of graphene Dirac point K with the states which concentrated mainly on dedicated layers. If the level of graphene doping corresponds to occupation of such zones by conduction electron then tunneling effect is suppressed. This gives possibility to strong wave slowing down and Cherenkov synchronism of plasmon polariton with nonrelativistic electron beam.

NOTES

Pulling nanoparticles by a non-diffractive light beam

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Pulling radiation pressure force recently revealed is discussed. In contrast to the ordinary optical manipulation based on the gradient-field forces we push forward the idea of dragging nanoparticles with the single gradientless (non-difracting) electromagnetic beam, e.g., Bessel beam. Except the strong non-paraxial nature of the beam there are no more heavy limitations on the parameters of the beam or material parameters of a nano-sized bead. Thus, pulling and pushing as result of dominating forward and backward scattering, respectively, is the advanced technique in optical manipulation.

NOTES

Angle-dependent excitation of surface plasmon polaritons in gold nanowires in alumina

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Extinction spectra of parallel gold nanowires (diameter – 28 nm, length – 9 mkm) in porous alumina were studied in spectral range of 360 – 1200 nm. The spectra were measured at various angles of incidence theta of exciting light beam. Here, theta is the angle between the propagation direction of exciting beam and the axis of nanowire. The extinction spectra contain two bands. First, T-band is caused by the excitation of the transversal oscillations of the free electrons, i.e. longitudinal surface plasmon (SP) mode in Au nanowire. Second, L-band is caused by longitudinal surface plasmon modes of nanowire. The spectral position of L-band changes non-monotonically with theta: it red shifts at the increase of theta from 0 to 30 degrees and blue shifts at the increase of theta from 30 to 70 degrees. The bandwidth changes with change of theta non-monotonically as well: it has maximum at theta = 30 degrees, and has smaller values at lower and higher incidence angles. The longitudinal surface plasmon modes in long metallic nanowires have the character of surface plasmon polaritons (SPP) propagating along the axis of nanowire. SPPs are reflected from the ends of the nanowire, and the standing SPP waves arise. Thus, the nanowire acts as optical resonator. The theoretical calculations show that theta = 30 degress is the angle at which the most efficient excitation of the longitudinal SPP occurs. At this condition the axial SPPs are excited that propagate along the nanowire axis. This mode has lowest energy and damping. At other angles of incidence the non-axial SPP modes are excited that propagate angle-wise to wire axis. Non-axial modes have the higher energies and damping that explains the observed dependencies of L-band characteristics on theta.

NOTES

General session V

Towards Single Photon Sources at Room Temperatures for Quantum Cryptography Application

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Single quantum dots (QDs) are promising candidates for the realization of electrically triggered sources of single photons or entangled photon pairs for application in quantum cryptography. Devices based on III-N QDs are operable at much higher temperatures than their arsenide counterparts, and provide the possibility to tune the emission wave length over a wide range. In this presentation, we study the fundamental processes of photon emission by excitonic complexes confined in single III-N QDs using InGaN/GaN and GaN/AlN QDs as examples. Furthermore, a comparison with corresponding results in InGaAs QDs will be given. Experimental results from single-QD spectroscopy are evaluated as well as theoretical results obtained by eight-band k.p theory.

NOTES

Solid-state based room temperature terahertz imaging systems

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Conventional way to realize room temperature terahertz (THz) imaging is based on usage optoelectronic approach when femtosecond lasers are used to generate-detect radiation via coherent scheme [1]. Such set-ups are rather bulky, hence, for practical aims, one need to have compact room temperature operating THz imaging systems which is free of optical laboratory environment and precise alignment issues. In a given lecture, we discuss several principles can be applied to realise such THz imaging systems based on solid-state devices. Our focus will be given to electronic multiplier sources [2], quantum-cascade lasers [3] and plasmonic nanometric field effect transistors [4]. We consider room temperature THz sensors – plasmonic nanometric field effect transistors, too, and bow-tie diodes [5] with special emphasis on spectroscopic THz imaging applications [6]. Particular attention will be given to illustrate bow-tie diodes' heterodyne detection scheme and its advantages in the context of operation frequency range, sensitivity and noise-equivalent power.

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NOTES

General session VI

38

Nonlocal analysis of natural and artificial materials using a transport formulation

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Natural materials (plasma and semiconductors) and artificial wire materials exhibiting spatial dispersion are considered using a transport model. The connection between drift-diffusion and electron transport in natural materials is highlighted, and then applied to various forms of wire media, such as a carbon nanotube effective medium, leading to the definition of effective conductivity and diffusion parameters that characterize the material. It is shown that the effective material parameters lead to a Debye length that provides a quantitative measure of the strength of spatial dispersion for wire media. Further, it is shown that Pekar's additional boundary condition applies in many instances to natural materials as well as artificial wire media, and can be derived from elementary electromagnetics. Examples for simple structures will be presented illustrating the presented theory. Time permitting, the analysis of the nonlinear and spatially-dispersive response of a semiconductor or plasma to large-amplitude time-harmonic electromagnetic fields will be discussed.

NOTES

Concept of photonic density of states in nanoelectromagnetics: theory and applications

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Concept of photonic density of states in nanoelectromagnetics: theory and applications During the last years the concept of photonic density of states (DOS) has attracted much attention as a basis building block for modern nanooptics and nanophotonics. The field started with the prediction of the spontaneous emission rate enhancement in microcavities (Parcell effect,1946). Various systems used for photonic DOS tuning are discussed, including microcavities, photonic crystals, graphene ribbons, nanoantennas based on carbon nanotubes and plasmon guiding nanowires. This lecture provides a common theoretical frame for electrodynamics of this structures, describes basis numerical techniques for photonic DOS calculation and their different applications. The two types of physical processes which are most important for nanophotonics are discussed in terms of photonic DOS: spontaneous decay of the excited quantum state and thermal light emission. This lecture concludes with an outlook on the future of photonic DOS concept applications to the theory of noise properties of nanoscale circuit elements, interconnectors and nanoantennas.

NOTES

Nonlinear optical phenomena in planar microcavities

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A semiconductor microcavity is a photonic structure designed to enhance the light-matter interaction. The cavity photons are confined between two mirrors and resonantly interact with the excitonic transition of a 2-dimensional semiconductor quantum well. In strong coupling regime the normal modes of the system are cavity polaritons that are half-light, half-matter quasiparticles. Being composite objects, polaritons inherit the properties of both cavity photons and excitons. The presence of the photonic component results in extremely small effective mass of cavity polaritons (10-4- 10-5 of free electron mass), while excitonic component leads to the efficient polariton-polariton interactions. This makes cavity polaritons a unique laboratory for study of the nonlinear optical phenomena at low pumping powers. In the talk we plan to give an overview of the polariton physics and in this context discuss the nonlinear effects, including bistability, multistability and pattern formation.

NOTES

General session VII

Single NV Centers in Nanostructured Diamond for Quantum Informatics and Quantum Magnetometry

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Individual nitrogen-vacancy (NV) color centers coupled to proximal 13C isotopic atoms in nano-structured diamond are now considered as one of the most perspective candidates for practical implementation of hardware for quantum information (QI) processing such as room-temperature processor for quantum computer, single-photon emitter for quantum cryptography, quantum memory, quantum repeater etc. Moreover, surface-functionalized nanodiamonds hosting single NV centers can be used as nano-sized sensor for detection of weak magnetic fields providing the capability to probe biologically relevant spins in living cells with unprecedented spatial resolution. All these promising applications require a precise characterization and complete understanding of properties of single NV centers in nano-structured diamond.
In the report we are going to present a review of our results on DFT simulation of structural, electronic and spin properties of NV center in bulk and nano-structured diamond as well as on interpretation of a wide range of experimental data on single NV centers or on their complexes with nearby 13C nuclear spins. Kramers degenerated spin systems comprising electron spin of a single NV center and odd number of nearby 13C nuclear spins in nano-sized diamond are studied and their application as a probe for local magnetometry is discussed. As well, control of single NV emission in nano-structured diamond like photonic crystal is studied and perspectives to implement various diamond-based QI applications are discussed.

NOTES

QED in 5 nm diamond ball with floating electron

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Cavity quantum electrodynamics (QED) has novel effective application with nitrogen-vacancy (NV) centers in diamond nanocrystals. A few theoretical models of QED diamond balls have been analyzed. Taking into account good defined properties of diamond quantum dot and Purcell effect we estimated the Purcell factor of 5 nm diamond ball for several external fields and special boundary conditions. Using the exact analytic solution in the semiclassical Jaynes-Cummings model without the rotating-wave approximation we describe QED cavity with diamond lattice in different states, i.e. before and after quantum chaos. The comparisons these solutions with chaotic Rabi vacuum oscillations in cavity QED allow to estimate quantitative characteristics of interaction into realistic model of nanodiamond. We discuss a few approaches to problem of self-consistency of volume 3D and surface 2D wave functions of 5 nm diamond ball, e.g. introduction of collective excitations or quasiparticles, strongly modified plasmon-matter interaction, floating electrons as anti-quasiparticle, possibility of semi-periodic spherical Bloch function etc. The theoretical models were applied to explain of (1) recent experimental realization of a cavity QED system in which NV centers in diamond nanocrystals are coupled to a whispering gallery mode in a nanosphere, (2) the Josephson junctions of superconductive diamond after boron doping and (3) the superlattice of 5 nm diamond balls (with & without NV centers) with floating electron.

NOTES

Multiphoton Resonant Excitation of Fermi-Dirac Sea in Graphene at the Interaction with Strong Laser Fields

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In the present work the microscopic theory of a graphene interaction with strong mid-infrared laser fields of arbitrary polarization is developed. We consider multiphoton interaction regime* to find out the nonlinear behavior of Fermi-Dirac sea in graphene and corresponding nonlinear optical response of the system. The evolutionary equation for a graphene single-particle density matrix in the field of moderately intense laser fields on the base of the second quantized formalism is formulated. The analytical solution for time-dependent density matrix in the given field of a laser radiation with arbitrary polarization is obtained. Rabi oscillations of the particle-hole states in graphene at multiphoton laser-excitation depending on the time, momentum, field polarization, and photons number are considered and analyzed on the base of numerical simulations as well. The obtained results demonstrate well expressed Rabi oscillations corresponding to multiphoton excitation of the system that can be observed by laser fields of moderate intensities and for the picosecond time scales, which is of special interest for a picosecond time-resolved photoemission spectroscopy. We also consider the particle-hole annihilation from the field induced coherent superposition states that will cause intense coherent radiation of harmonics of the applied wave-field. We consider the possibility of generation of odd as well as even harmonics of fundamental frequency strictly depending on the laser field polarization and initial state of graphene quasiparticles. This work was supported by State Committee of Science (SCS) of Republic of Armenia, Project No. 11RB-006. * H.K. Avetissian, A.K. Avetissian, G.F. Mkrtchian, and Kh.V. Sedrakian, arXiv:1112.2905v1, submitted to Phys. Rev. B.

NOTES

General session VIII

Atomistic simulations of defect containing tubular nanostructures

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Contemporary quantum-chemical simulations are becoming more and more capable to predict physical, chemical, and even mechanical properties of many interesting materials. However, very little has been reported on computer simulations of defective nanostructures, mainly because the lack of periodicity makes their study both very time-consuming computationally and costly. We demonstrate the advantage of first principles methods, which can exploit periodic rototranslation symmetry for efficient calculations on defect-containing nanotubes. Using density functional theory (DFT) realized either within the LCAO method or the formalism of linear augmented cylindrical waves, we calculate the equilibrium geometry and energetics of a Ni filament inside carbon nanotubes (CNTs), and single atom substitutions inside the wall of boron nitride nanotubes (BNNTs). As for CNTs, we consider monoatomic chains of nickel atoms encapsulated into CNTs of (n,0) and (n,n) chiralities with varied n indices. Our calculations show that CNTs with Ni filament exhibit metallic behavior, even if the pristine nanotube is semiconducting. Thus, we predict that the encapsulation of a Ni filament inside CNTs is a way for the reliable realization of stable conductive quasi-one-dimensional hybrid nanostructures. In BNNTs with (5,5) and (9,0) chiralities we consider P, As, Sb substitutions for the host N atom while In, Ga and Al substitute the host boron. The band gap of the BNNTs is virtually closed, due to the effect imposed by Sb, while the introduction of the In, Ga or Al atom in the BNNT results in a minor increase of its band gap. The obtained results can help to understand better the optical and photoelectron spectroscopy experiments, and the measured electrical properties of the doped BNNTs.

NOTES

Reflectance properties of nanocarbons: nanodiamond (ND), sp2/sp3 composites, onion-like carbon and multiwalled carbon nanotubes

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Carbon nanomaterials are the promising candidates for potential broadband limiting applications and design of extremely low reflectance coatings, particularly in the infrared, visible and UV spectral regions. The reflectance properties of nanocarbons are important for the design of absorbing paints, low reflectance coatings, sensors etc. We have performed the comparative study of diffuse reflectance of nanodiamond (ND), sp2/sp3 composites, onion-like carbon (OLC) and multiwalled carbon nanotubes (MWNTs) in infrared, visible and UV regions. The diffuse reflectance spectra of these materials are analyzed taking into account the size and defectiveness of graphene sheets which are the main building blocks of sp2-carbon based nanocarbons. We have controlled defectiveness of all nanocarbons with the uniform set of physical methods, namely HR TEM, Raman spectroscopy, temperature dependence conductivity and magnetoresistance measurements. The diffuse reflectance of carbon nanomaterials depends mainly on the electronic configuration, defect concentration, size of graphene-like ordered fragments and agglomerates of nanoparticles along with their morphology.

NOTES

Poster session II

42

Insight into multishell carbon nanostructure electrostatic response

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Diversity of carbon nanostructures determines variety of technological usage of carbon-based materials. Polymer composites providing effective absorption of electromagnetic radiation are the most perspective field of applications of multishell carbon nanostructures, such as carbon nanotubes and onion-like carbons. However, in spite of abundance of theoretical and experimental investigation of electromagnetic properties of mentioned above materials, today there is no clear understanding of the role of inner layers and screening effect in multishell carbon nanostructures. Here we present investigation of electrostatic response of multishell carbon onions, including experimental measurements of low-frequency characteristics of composites with onion-like carbons and calculations of static polarizability of two- and three-layer carbon onions using different approaches. Our theoretical data revealed that static polarizability of mutlishell fullerene structures depends on both calculation method (DFT or semiempirical) and basis set. On the example of the models Ar@C60 and C60@C240 we demonstrated that the screening coefficient correlates with strength of non-covalent interlayer interactions. Approximation of low-frequency dielectric permittivity of onion-like carbon-based composites by the Maxwell-Garnett model using screened random phase approximation polarizability of isolated fullerenes demonstrates the key role of inner layers in electrostatic response of carbon nanostructures.

NOTES

Electromagnetic properties of thermoplastic polymer composites containing carbon nanoparticles in frequency range 10 MHz - 1.5 Thz

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Design of carbon-loaded composited with tailorable electromagnetic properties is of crucial importance in the field of aviation and space research, novel electronics, etc. Carbon nanoparticles (CN), such as multiwall carbon nanotubes (MWNTs) and onion-like carbon (OLC) are promising material due to their lightness and superior mechanical, electrical and optic properties. Incorporation of CN in polymer matrix leads to significant improvement properties of composites – mechanical strength, electrical conductivity, fracture toughness, electromagnetic shielding properties, non-linear optic properties. Development of light-weight EM-active composites would allow to solve certain problems of electromagnetic compatibility and shielding of electronic devices. We present the results of research structural and electromagnetic properties of thermoplastic polymer composites filled CN with different structure, mean diameter, morphology and surface chemistry. Polymethylmethacrylate, polystyrene, polyethylene and polypropylene were chosen as matrices. Investigation of various composites with different physical-chemical properties (structure, surface tension, etc.) allows revealing significant differences in properties of composites containing same filler and produced by similar way. Electromagnetic properties of nanocarbon-loaded composites were investigated in ultra-wide range of frequencies (10 MHz-1.5 THz). Main regularities of electromagnetic response properties of composites depending on their structure, matrix and filler type and morphology were obtained. Investigated materials show high interaction with electromagnetic radiation depending on their structural and morphological properties allowing development of tailorable materials for wide variety of applications.

NOTES

Anisotropic properties of MWCNT/polystyrene composite films in terahertz region

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Anisotropic properties of composite materials based on carbon nanotubes (CNT) and polystyrene were investigated in terahertz region. Particularly it was measured electromagnetic response (transmission and reflection spectra) of composite for two different polarizations of the electric field relative to preferential direction of composite. This direction was formed during samples preparation process by using repeated forge rolling. Dispersion function of CNTs was theoretically modelled, and dielectric permittivity was calculated. Anisotropy of dielectric response of composite indicated that the forge rolling resulted predominant orientation of CNTs in polymer matrix.

NOTES

BC3 nanotubes: elelctronic and structural properties

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Recently, classes of tubules, originating from hexagonal compounds, i.e. BN and BC2N have been proposed [1]. Total energy calculations imply that the hexagonal compound sheets are as likely to form tubules as the graphite sheets [2,3]. Indeed, tubule forms of the hexagonal compounds of B, C, N have been observed experimentally in an arc-discharge setup [2]. Using chemical analysis, it has been determined, that part of the samples has an atomic composition of B:C≈ 1:3. In this paper we present the results of theoretical research into the properties of boron-carbon nanotubes BCn, n=3 of hexagonal type within the framework of an ionic-built covalent-cyclic cluster model and an appropriately modified MNDO quantum chemical scheme and density-functional theory. We studied the mechanism of BC3 nanotubes formation by rolling qusiplanar hexagonal BC3 layer. We used two structural modifications of BC3 tubes in which boron and carbon atoms occupy different positions, the so-called BC3 tubes of A or B types. We defined the optimal geometry of these structures and also their band structure. Analysis of the strain energies showed that the existence of tubule forms of BC3 is energetically favorable. The tubes of small diameter obtained by twisting a monolayer of boron are likely to be narrow-gap semiconductors.
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NOTES

Influence of metal superlattice to boron nanotube

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In this paper we present the results of theoretical research into the properties of boron nanotubes (BNTs) of hexagonal type within the framework of an ionic-built covalent-cyclic cluster model and an appropriately modified MNDO quantum chemical scheme. We studied the mechanism of sorption of Li, K and Na atoms on the external surface of single-walled boron arm-chair nanotubes. We defined the optimal geometry of the sorption complexes and obtained the values of the sorption energies. After these operations we considered the possibility of multiple regular adsorption of alkaline metal atoms on a BNT surface. We modeled the formation of superlattice from metal atoms above nanotube surface. Analysis of the band structure suggests that the band gap is insensitive to adsorption process. The electron density is located near boron atoms of the surface of the tube. The results suggest that the formation of metal-phase composites based on boron nanotubes is possible, which is promising for nano-based technology.

NOTES

Heat resistant phosphate materials containing pure and nitrogen- and boron-doped carbon nanotubes: effectiveness of electromagnetic interference shielding in microwave

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We report on the comparative study of the effectiveness of electromagnetic (EM) interference shielding in microwave range (26-37 GHz) provided by pure, as well as boron and nitrogen doped multi-walled carbon nanotubes (CNTs) dispersed in heat resistant phosphate ceramics. The series of pre-percolative and close-to-percolation threshold samples made in five different concentrations (0.25, 0.5, 1, 1.5 and 2 wt.%) were fabricated on the basis of thermal stable phosphates, consisting of aluminium-phosphate binder and filler containing corundum (Al_2O_3) and aluminium nitride. SEM and differential thermal analysis of obtained materials have been carried out. The inhibition effect of phosphate binder on the oxidation process of CNTs has been established. The experimental data collected in microwave frequency range demonstrate the prospects for utilizing of phosphate adhesive compositions for the preparation of heat-resistant electromagnetic coating both on the basis of pure CNTs and B- and N-doped CNTs, in favor of pure ones. This conclusion was supported by DC analysis showing high DC conductivity of fabricated composites at room temperatures, when filler concentration is not less than 1 wt.%.

NOTES

Investigation of the interaction of carbon nanotubes and the most commonly used polymers

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Every day we need more and better materials. All new types of materials press oneself into our lives, in our everyday life. Nanotubes - a unique material, they are considered an ideal reinforcing material, including, for polymeric materials. Carbon nanotubes in polymer matrices have a great influence on the electrical conductivity, viscosity, shear and other transport properties, as the hybrid nano-sized fillers and additives. We carried out a theoretical study of the interaction of nanotubes with a few monomer units most common polymers. Mechanisms of interaction processes and characteristics, resulting in a material.

NOTES

Carbon nanotubes as a new material for the purification of alcohol-containing liquids

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Ethyl alcohol, which has a wide application in pharmaceutics, chemical, electronic and food-processing industry, practically always contains various impurities. Many of these impurities are found in quantities which are not sufficient to influence organoleptic effects and toxic potential of ethyl alcohol. However, the quantity of some of them, such as aldehydes, fusel oil, ethers and methyl alcohol is strictly regulated. The paper suggests a new effective method of purifying alcohol-containing liquids from undesirable impurities. At present, development in many areas of science and technology is associated with carbon nanotubes (CNTs) [1-6]. One of their remarkable features of is related to their unique sorption characteristics. The highly curved surface of CNTs can adsorb rather complex molecules including molecules of organic origin. The effectiveness of nanotubes with respect to organic molecules is ten times greater than the that one of graphite adsorbents, which are currently considered the most common means of purification. Therefore, nanotubes can be used for final purification of various liquids from extremely low concentrations of impurities. We performed quantum-chemical study of molecul adsorption of heavy alcohols (normal and isomeric propanol) on the outer surface of single-walled carbon nanotubes. We constructed energy curves of interaction of normal propanol and isopropanol molecules with the CNT's surface (6, 6). We also established the most effective adsorption centres for molecules of heavy alcohols. We also proved the feasibility of physical adsorption. We developed and implemented a method of alcohol liquids purification from impurities with CNTs. We carried out experimental study of water-ethanol mixtures taken before and after purification with carbon nanomaterials, applying molecular methods of IR spectroscopy, chromatography and chemical analysis and proved the positive effect of carbon nanotubes on the process of purifying alcohol liquids from adverse impurities.

NOTES

Effect of buckypaper properties on attenuation of electromagnetic radiation

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Two different procedures of carbon nanotube foils fabrication are discussed. The size, structural and optical characteristics as well as electrophysical properties of initial nanotubes and prepared buckypaper are studied. The parameters of electromagnetic radiation-buckypaper interaction are derived for the range 8.15 – 73.3 GHz. Strong reflection and attenuation of the radiation up to 40 dB are observed. Such results render this material promising for protection against electromagnetic radiation in sensitive devices and systems, especially in those experiencing elevated mechanical and thermal loads.

NOTES

Electrical and magnetic properties of thin films of cross-linked fullerene C60 polymers in micro- and nano-scale

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Thin (100-200 nm) films of fullerene C60 polymers were formed using the method of electron-beam dispersion of pristine fullerite in high vacuum with fullerene ions assistance. Material of the synthesized films represents a highly cross-linked random 3D network of covalently bonded fullerene molecules. Electrical properties of the films deposited onto the substrates with a thin-film interdigital electrode system have been measured in-situ in the vacuum chamber immediately after the deposition and after atmosphere exposure. It was shown that original conductance of the film is relatively high (about 50 Ohm cm). Upon atmosphere exposure, it decreases by approximately 3 orders of magnitude. However, even after the air exposure, the film conductance is still several orders of magnitude higher than that of the nonpolymerized C60 films. Electrical properties of the films in the micro- and nano-scale have been measured via the conductive atomic-force microscopy (C-AFM) technique. The measurement showed that the film conductance is enabled by a conducting network in a significantly less conductive matrix. The behavior and physical chemical processes in the film material upon C-AFM measurement is discussed. Magnetic properties of the synthesized films have been studied using magnetic force microscopy (MFM) technique. The films exhibit stable magnetic contrast highly correlated with the film topography, whereas the content of the ferromagnetic contaminants in the films is insignificant (less than 1 ppm as estimated by matrix-assisted laser desorption ionization mass spectrometry). Origin of the MFM signals and magnetic structure of the cross-linked C60 polymer films is being speculated about.

NOTES

Optical characterisation of nanostructured composite formed by Ag+ implantation into polyethyleneterephthalate

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Thin (40 μm) polyethylenterephthalat ($C_{10}H_8O_4$)n films were implanted with 30 keV Ag+ ions to fluencies of (0,25–1,5)10^17 cm^-2 at ion current density of 4 μA/cm^2. The maximum silver atomic concentration occurs at the projected range of 35 nm and the penetration depth (modified layer) extends to about 60 nm. Reflectance and transmittance spectra were measured for two opposite sides of the film (implanted and non-implanted) by Proscan MC-122 at the wave length range 200–1100 nm. Transmittance spectra show sharp increasing of penetration at λ=310 nm. The absorption increases with fluence increasing. Such behaviour indicates growing concentration of carbon clusters and metallic inclusions. Reflectance spectrum of virgin sample shows two weak peaks in UV region at λ1=205, λ2=260 nm which vanish on implanted and increase on non-implanted side because of carbonization of the irradiated surface and thermal modification of the film beyond the projected range. Independently of exposed side reflection increases with fluence increasing and shows maxima at λ≈620 nm due to surface plasmon resonance in silver nanoparticles. This maxima shifts continiously towards longer wavelength with fluence increasing because of growing of silver nanoparticles. Supposing two-layer structure of the implanted film numerous fitting reflection and extinction coefficients was made for refractive index determination. Refractive index for modified layer obtained in the range 1,4–2,8 depending on the fluence. The numerical estimation of the mean silver cluster size with «MiePlot v.4.2» computer program for obtained refractive index was made. The mean cluster sizes are in the range 5-20 nm. Validity of the two-layers structure for optical properties describing in a whole fluence interval is discussed.

NOTES

Surface plasmon resonance in silver nanoparticles formed in polyimide by ion implantation

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Thin (40 μm) polyimide ($C_{22}H_{10}O_5N_2$)n films were implanted with 30 keV Ag+ ions and fluencies of (0,25 – 1,5)□10^17 cm^-2 at ion current densitys of 4.0, 8.0 and 12 μA/cm^2. Reflectance and transmittance spectra in wavelength range of 200 – 1100 nm for both sides of the films (implanted and non-implanted) have been measured. Metal ion implantation into the polymers creates both carbonaceous clusters, responsible for enhanced optical absorption, and metallic inclusions leading to the additional absorption as well as strong reflection and scattering of light. Abrupt increasing of absorbance below λ=500 nm is observed in transmittance spectra. Three weak peaks in UV region at 210 nm, 254nm and 311 nm are clearly seen in reflectance spectrum of the virgin sample. In the visible light region reflectance for both sides of the samples increases with fluence and show maxima at λ=620 nm and λ=800 nm for implanted and non-implanted sides. These peaks are originated from surface plasmon resonance (SPR) in silver nanoparticles. The SPR peak positions shift continiously to longer wavelengths with fluence due to increase of silver nanoparticle sizes. Moreover the red shift of SPR peak for non-implanted side indicates non-uniform distribution of mean cluster sizes along the depth of modified layer. Three UV peaks mentioned above haven't been observed for implanted side whereas their intensities were increased for non-implanted one. Such behavior is explained by complete carbonization of the near-surface region and heating induced modification of the film beyond the ion projected range. It was observed also that peak at λ=254 nm shifts to shorter wavelengths with fluence. Optical parameters of modified layers, mean sizes of silver clusters and origin of the peak shifts are discussed.

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Interaction of Aligned Carbon Nanotube Arrays with the Electromagnetic Radiation of the 78-118 GHz Frequency Range

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Great potential of carbon nanotubes (CNTs) for electromagnetic interference (EMI) shielding applications has been undoubtedly acknowledged due to their high conductivity, small diameter, high aspect ratio, large specific surface area, chemical stability, and low weight. In this work we report on the EMI shielding properties of aligned CNTs in the 78-118 GHz frequency range. The samples of CNT arrays aligned perpendicularly to the Si substrate were grown by the floating catalyst chemical vapor deposition. The advantage of this technique is that CNTs are naturally formed with iron phases inclusions of catalyst nanoparticles, what gives rise to magnetic losses along with the dielectric ones. It was revealed that the interaction of electromagnetic radiation (EMR) with the CNT arrays is characterized by a resonant behavior, and all the CNT samples possess high shielding efficiency (SE) of EMR. The influence of the percentage content of magnetic inclusions, as well as the height of the CNT arrays on the absorbing properties of the obtained CNT arrays was investigated. It was found that the higher is the catalyst precursor loading during the CNT synthesis, the higher attenuation of EMR by the samples would be. In particular, the highest attenuation (18-29 dB) was reached for the 35 μm CNT array obtained at a 10 wt.% concentration of the feeding solution, what was the result of both the high reflection and absorption of electromagnetic waves by CNTs. Approximately the same values (16-26 dB) of attenuation was obtained by a 110 μm CNT array, obtained at a 1 wt.% concentration of the feeding solution. The possible mechanisms of interaction of EMR with the CNT arrays, the origin of resonance behavior, as well as the future applications of the investigated material were discussed.

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Dielectric properties of lead-barium zirconate titanate, alloyed with copper and nickel

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Piezoceramics are as a rule inorganic dielectrics with high value of dielectric permittivity depending on an electric field strength. Among these materials the most known are the ceramics based on $PbZrO_3$—$PbTiO_3$ (PZT) systems[1]. Piezomaterials based on PZT ceramics have widespread applications as electromechanical and electroacoustic transducers [1]. In this work we investigate the dielectric properties of Pb0.75Ba0.25Zr0.53Ti0.47O3 (PBZT) – metal nanocomposites in wide frequency range from 20 Hz – 1 MHz. The complex dielectric permittivity of all investigated composites at higher temperatures and low frequencies is mainly caused by the high electric conductivity, wich similarly to the pure PZT is mixed electronic-ionic. Only at the highest frequency - 1 MHz the real part of complex dielectric permittivity is much higher as imaginary part, therefore the dielectric permittivity at this frequency is static and can be fiited with Curie-Weiss law. Obtained Curie-Weiss law parameters indicate nearly the second order displacive phase transition driven by resonant soft mode in all investigated composites. The ferroelectric phase transition temperature is higher for composites with Ni addition and lower in composites with Cu addition in comparison with pure PBZT. Below the ferroelectric phase transition temperature the dielectric dispersion is mainly caused by ferroelectric domains dynamic. The activation energy of domains dynamics is lower in composites in comparison with pure PBZT, it can be explained by decreasing of domains size in PBZT composites.

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NOTES

Reorientation of magnetization in a single-domain cobalt particle by a laser beam

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We have theoretically observed switching and oscillations of magnetization in a single domain nanodisk in a ferromagnet/non-magnetic metal/ferromagnet nanostructure being irradiated by laser pulses with linear and circular polarization. A macrospin approximation and the generalized Landau-Lifshitz-Gilbert equation were used. The interaction of the laser radiation with the ferromagnetic metal is supposed to be followed by: (i) the change the energy of magnetic crystallographic anisotropy, (ii) saturation of magnetization, (iii) generation of a spin-polarized current by photon pressure. Moreover, the circular-polarized laser radiation is considered to initiate the inverse magneto optical Faraday effect in the nanodisk. Switching of the magnetization of the nanodisk under linear-polarized laser radiation was found to be controlled by a change of the magnetic anisotropy energy due to heating of the nanostructure. This process is accompanied by oscillations of the magnetization with a frequency of 5 – 20 GHz damped within few to tens nanoseconds. Thermal fluctuations lead to an increase of both the damped period and the frequency of oscillation. In the case of the circular-polarized light irradiation the magnetic field arising from the inverse Faraday effect increases the frequency and amplitude of magnetization oscillations.

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Modified flame pyrolysis method for magnetic nanoparticles synthesis

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The potential of magnetic nanoparticles has been recognized in recent years, and new commercial applications were clearly identified. Together with usage as catalysts, sensors, composites and others, they got broad usage at illness diagnostics and treatment, in particular, tumor hyperthermia, drug delivery, in MRT image contrast enhancement agents. In all these applications, it is important for the particles to not only be small, but also to be non-agglomerated. The latter is a quite complex task to solve for powder magnetic materials. So, there are special synthesis methods being developed for obtaining such nanoparticles. One of these is the flame pyrolysis method. Though it has many benefits, the processes of aggregation of particles are still occurring. To avoid this, precise control of burning temperature and spraying speed is required. Besides, many of properties of nanoparticles obtained by this method depend on size of the sprayed droplets. To avoid these problems, in this work we propose to use ready-made sols of the source components instead of solutions, as precursor in flame pyrolysis. In this case, crystallization center formation and solid phase germ growth stages take place not in flame. Size, shape and crystal structure of the particles in this case are mostly determined by the conditions of the corresponding sol synthesis. The flame pyrolysis stage allows the transformation of sols into powders minimizing the risk of agglomeration of the particles. Simultaneously, this provides thermal treatment of the material. Non-agglomerated spherical particles (d ~ 80 nm) of γ-Fe2O3 doped with Co (2.6 mol %) were obtained by this approach. This material has a structure of CoxFe2–xO4 solid solution and can be potentially used for magnetic hyperthermia of tumors.

NOTES

Formation of the EM-absorbing polimer films

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In this talk we analyse different approaches to the formation of composite thin-film materials with carbon nanopparticles as filler, and present-day technologies for the deposition of shielding coatings. The interest to the work is dictated by that polymer materials with nanocarbons embedded manifest unique properties on attenuation (reflection and absorption) of electromagnetic radiation without essential damage of physical chemical characteristics of polymer matrixes. Nano-dimensional fillers drastically differ from mcrostructured ones in mechanical and electric properties. Structure formation in nano-scale systems is dictated not only by the energy of intermollecular and inter-partical interaction but also the mobility of macromolecules. That should be taken into account under design of polymer compositions. To optimize the cost and thickness of shielding materials without the effectiveness loss, the multilayer polymer systems can be applied. Each polymer layer is formed by several compositions and can include its own set of nanoparticles differing in size, structure, shape, concentfration, etc. Multilayer systems are very promising from the point of view of tunability snd control of working characteristics.

The work has been partially supported by theISTC project B-1708.

NOTES

Method of vacuum deposition of carbon nanotube thin film nanocomposites

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Carbon nanotubes (CNT) nanocomposites are one of the most attractive near-term means to exploit the unique properties of carbon nanotubes. This is particularly true for composites aimed at electronics, electromagnetics and photonics, where a number of possible promising applications have already been demonstrated [1]. The main method for producing of CNT nanocomposite films is deposition from CNTs liquid-phase suspension. This technology limits the range of materials suitable for forming the composite matrix. We have demonstrated the possibility of vacuum sublimation (10-4 Pa) of few-wall CNT (FWNT) short fraction (100 ÷ 500 nm) with a diameter of 2 ÷ 10 nm, which makes it possible to obtain nanocomposite films by vacuum co-deposition of thermally sublimed FWNTs with thermally sublimed matrix composite material. Vacuum formation technology of nanocomposite films may be used as a template, except for organic matter, metals and metal oxides, which opens up new opportunities for their applications in electronics and electromagnetism. Studies using scanning and transmission electron microscopy in conjunction with Raman spectroscopy showed that the vacuum deposited FWNT thin films on substrate had been formed, consisting of individual FWNT and not fully ordered transition forms of carbon. The processes for obtaining the fraction of short FWNTs using chemical treatments, laser cutting and mechanical degradation as well as the relationship between macroparameters of vacuum sublimation process and the parameters of the FWNTs thin film will be discussed. The direction and criteria for the FWNT-cut and vacuum deposition process optimization to create on their basis thin film nanocomposites will be discussed.

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Ag Displacement Deposition on Porous Silicon for SERS Substrate Fabrication

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Displacement technique was applied to deposit Ag on porous silicon (PS) template that provided a metal film nanoroughness. Morphology and strycture of the obtained samples were studied with scanning electron microscopy. The Ag layer on the PS surface presented quasi-continuous film consisted of the particles of the 70-150 nm diameter. An average distance between such nanoparticles (NPs) varied in the range 100-200 nm and the gaps between them were filled with NPs of the 15-25 nm diameter almost touched each other. The connection of NPs should promote plasmon's coupling that cause the strong local field enhancement areas (so-called “hot spots”) emergence. The enhancement of Raman signal was estimated at 441,6 nm laser excitation from the intensity of the 1366 cm–1 line in the spectrum of water-soluble cationic copper porphyrin (CuTMPyP4) adsorbed on the Ag/PS substrates.The level of the signal was found strongly dependent on PS morphology, composition of the solution for metal deposition and regimes of the Ag films fabrication. The present research was funded under the followed projects: F11MC-019, T10M-089 and T11OB-057.

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Ion Beam Synthesis and Characterization of A3b5 Nanocrystals in Si And SiO_2/Si for Optoelectronic Systems

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We have studied the ion-beam synthesis of InAs, InSb and GaSb nanocrystals in Si and SiO_2/Si by high-fluence implantation of (As + In), (Sb + In) and (Ga + Sb) ion followed by furnace and rapid thermal annealings. In order to characterize the implanted samples Rutherford backscattering spectrometry in combination with channeling (RBS/C), transmission and cross-sectional electron microscopy (TEM, XTEM), Raman spectroscopy (RS) and low-temperature photoluminescence (PL) techniques were employed. It was demonstrated that by introducing getter, varying the ion implantation temperature, ion fluences and post-implantation annealing duration and temperature it is possible to form InAs, InSb and GaSb nanocrystals in the range of sizes of (2 - 80) nm. TEM and RS results confirm the crystalline state of the clusters in the silicon matrix after high-fluence implantation of heavy (As + In), (Sb + In) and (Ga + Sb) ions. Significant redistribution of implanted species has been revealed after “hot” implantation and post-implantation annealing. We have suggested that it caused by non-equilibrium enhanced diffusion. A broad band in the spectral region of 0.7 – 1.1 eV is detected in the photoluminescence (PL) spectra of the samples. The nature of this PL band as well as potential applications of the fabricated structures with quantum dots in optoelectronics and nanophotonics are discussed.

NOTES

Characterization of ferromagnetic metal – carbon nanocomposites prepared by solid-phase pyrolysis of metall-phthalocyanine

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We have developed a simple one-stage method for solid-phase pyrolysis of metal-phthalocyanines (MPc) used for preparation of ferromagnetic metal-carbon nanocomposites (M = Ni, Co). By changing the pyrolysis conditions (temperature, time, and pressure in the reaction ampoule) we synthesized ferromagnetic and superparamagnetic Ni and Co nanoparticles in different carbon matrices. The mean sizes of nanoparticles are varied from 5−10 nm to 300−400 nm. Prepared samples were investigated by SEM and TEM microscopy, energy-dispersive X-ray microanalysis, Raman spectroscopy, and ferromagnetic resonance technique. The nanocomposites can be used in biomedicine, as catalysis, filters, magnetic paints, and electromagnetic field energy absorbers.

NOTES

Development of anisotropic composite materials for electromagnetic applications

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Composite materials, consisting of carbon nanotubes (CNTs) and polymer matrix, are promising materials for electromagnetic (EM) shielding. Anisotropic composite materials, which can selectively absorb EM radiation, attract especial interest. Such composite materials can be demanded in creation of strong and thin EM screens with the required values of the absorption coefficient. Here we discuss two methods for development of anisotropic composites. In the first method, multiwall CNTs synthesized by chemical vapor deposition (CVD) method were deposited on quartz, glass or Si substrate by solvent evaporation or by spin-coating method. CNTs orientation on the dielectric surfaces was achieved by applying the directional force. After that polymer solution was applied on the obtained CNTs layer and dried until complete solvent evaporation. Finally, polymer material with CNTs was carefully detached from the dielectric substrate. In the second method CNTs were mixed with polystyrene taken in the required proportion, dispersed in toluene and carefully stirred for complete dissolving of polystyrene. The obtained composite slush was applied over metallic plate and dried at ambient conditions. The forge-rolled method or stretching method was used for orientation of CNTs in polymer matrix. CNTs length was predominantly about 100 μm which is equal to the wavelength of terahertz radiation. Reorientation of CNTs in predominant direction on the dielectric surfaces and in the polymer matrix as a result of applied force was shown. Occurrence of anisotropic dielectric response in the obtained samples was demonstrated.

NOTES

Fabrication and characterization of Er- and Gd-implanted tin dioxide films

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Tin dioxide (SnO_2) is wide band gap semiconductor that is widely used in gas sensors and different optoelectronic applications [1]. Doping of semicondiuctors by rare-earth elements provides possibility of their use as active optical elements due to existence of radiative transitions in a wide wavelength range [2]. We report here fabrication procedure and optical properties of polycrystalline SnO_2 films implanted with Gd3+ and Er3+ions. DC reactive magnetron sputtering from tin sputtering target in the gas mixture of Ar and O_2 was used for tin dioxide films preparation. After sputtering process samples were subjected to heat treatment in air in the temperature range 200-600 ^{0}C. Optical absorption spectra of tin dioxide films were measured using UV-Vis spectroscopy within 220-900 nm range of wave length. Estimation of the band gap transition energy gives value of about 3.6 eV. Than samples were implanted by Gd3+ and Er3+ions with a dose in the range 1012-1014 cm-2 and rapid thermal annealing at 700 ^{0}C during 1 minute in nitrogen atmosphere. Photoluminescence spectra of Er- and Gd-doped tin dioxide films was measured with UV laser (325 nm) as excitation source. Emission at ~550 nm was observed SnO_2 films implanted both by Gd3+ and Er3+ions. The origin of visible emission might be related to 4f transition in rare-earth (RE3+) ions or to defect levels associated with oxygen vacancies. References

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NOTES

Bistable states of 5-7 defects in graphene

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Defects of a graphene sheet of a 5-7 type are considered, when instead of hexagons the 5- and 7-gons are present while dangling C–C bonds (radicals) are absent. Defects in graphene were experimentally found and an increase in density of π-electron states in the vicinity of such defects was mentioned in [1].
The block-regular method, developed by the authors [2], allows calculation of 5-7 defects employing methods of differential geometry and topology for description of the properties of carbon surfaces containing such defects. It was previously shown (see, e.g., [3]) that in the graphene sheet the 5-7 defect being the convexity of the carbon hexagonal lattice leads to the redistribution of π-electron charges and to the appearance of the local electric dipole moment. There is a possibility of the 5-7 defect turning inside out (inversion relative to the graphene plane) by using the external electric field, which leads to the change in a direction of the electric dipole. Moreover, the graphene plane with the defects of convexity (or concavity) type can be formed on an engineering surface (matrix) which contains convexities and concavities of nanometer size in both vertical and in-plane directions.
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NOTES

Effect of annealing and biaxial deformation on the dielectric properties of composites of multiwall carbon nanotubes and poly(ethylene terephthalate)

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The dielectric properties of composites of PET with MWCNTs were investigated over a wide frequency and temperature range below the electrical percolation threshold. In composites with 1 wt% MWCNT inclusions the dielectric properties below room temperature are mostly determined by β relaxation, as a consequence of the rotation of PET molecules. In bi-axially stretched samples the CNTs are oriented at about 45o to the stretch direction. Such deformation increased the potential for molecular rotation. However, annealing after stretching increased homogeneity of the composite and decreased the potential barrier for polymer chain rotation. Electrical conductivity effects and Maxwell–Wagner polarization mostly cause the dielectric properties of the samples with 2 wt% MWCNT inclusions. The potential barrier for carrier tunnelling is lowest in the annealed sample.

NOTES

Ultrasensitive detector of modulated terahertz radiation based on double-carbon nanotube system

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The new scheme of a detector of modulated terahertz radiation based on the system of two parallel single-walled carbon nanotubes (SWCNTs) with the metallic conductivity is proposed. In this scheme, the electric field of the incoming modulated THz wave excites plasma oscillations in the CNTs [1,2]. In turn, the redistribution of the electric charge in the nanotubes causes repulsion between them that is quadratic on the incoming signal. Due to this nonlinearity one can separate the modulation signal harmonics and then they can be amplified by the mechanical resonance in the CNTs [3-5]. The ways to measure the deformation of the CNTs in time-domain are discussed. The sensitivity of the detector of modulated THz radiation based on the scheme in question is estimated to be about 106 V/W.

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NOTES

General Session IX

Time Dependence of the Intensity of Parametric (Quasi-cherenkov) Radiation Produced by Relativistic Particles Passing Through Photonic Crystals

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Time evolution of parametric (quasi-cherenkov) radiation produced by a relativistic charged particle passing through a photonic crystal is studied. It is shown that the duration of radiation pulses, consisting of a sequence of peaks with decreasing amplitude, can be much longer than the time of particle flight through the crystal. This makes possible a detailed experimental investigation of the influence of the photonic crystal structure on the time characteristics of parametric (quasi-cherenkov) pulses generated by electron bunches. This makes possible to use the time-dependence of the parametric radiation for studying artificial periodical matter (photonic crystals) properties.

NOTES

The electrodynamic modeling of nanostructures and metamaterials on the basis of the method of minimal autonomous blocks

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On the basis of the method of minimal autonomous blocks (MAB) the complex approach to calculation of electrodynamic characteristics of composites, metamaterials and systems which structure includes any on geometry and material objects is developed. The basic algorithms of realization of the MAB method and features of the solving of internal and external electrodynamic problems are considered. It is established that the MAB method possesses high computing stability and allows to analyze systems with the big range of the wave sizes of structural elements. Various approaches to modeling of the systems containing composites and metamaterials are described: direct modeling by the MAB method, use of effective electromagnetic parameters, multichannel scattering matrixes of structurally non-uniform macroblocks, average scattering matrixes of non-uniform blocks. The technique of the analysis of electromagnetic properties of systems with the multiscale organisation of structure is considered. It is based on use of the MAB method and average scattering matrixes of dispersion which recurrently calculated at each scale level. Problems and features of calculation of scattering matrixes of MABs on nanoscale level are considered. Algorithms of the account of nonlinear properties of materials are presented. Results of modeling of interaction of electromagnetic radiation with various types of nanocomposites and metamaterials are presented. Possibility of use a system of nanosize metal particles in a plasmonic resonance modes for formation of the different types of electromagnetic fields distributions on a surface of a dielectric substrate is considered.

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Nanoscale investigation of microstructure effects on hydrogen behaviour in rapidly solidified aluminium alloys

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A key breakthrough in hydrogen embrittlement (HE) studies in Al-based systems is considered to be nanoscale and sub-micrometer characterization of their local composition and structure accompanying H measurements. While embrittlement mechanisms remain controversial regarding Al alloys of commercial interest as liner materials for efficient storage of compressed hydrogen gas, it should be highlighted that a lack of information on H behaviour in rapidly solidified (RS) Al materials prepared at exceptionally high cooling rates provides a renewed stimulus to developing a deeper mechanistic understanding of H/microstructure interactions in high strength Al alloys aimed to control the problem of HE in Al materials. This work presents an overview of our recent results on diffusion and trapping of hydrogen with emphasis on nano-scale microstructural evolution in RS Al-based alloys. Application of ion beam analysis techniques provided direct observations of elemental composition and microstructure with nanoscale precision (20-40 nm depth resolution) within the near-surface regions in the RS alloys. Thermal desorption spectroscopy was employed to analyse H trap states in the specimens. It was found out that H behaviour in RS Al binary alloys (with V, Cr, Fe, etc.) is strongly affected by alloying elements trapping at vacancies in respect to observed nonuniform dope distribution below the foil surface (up to 2.0 μm depth). Based on obtained patterns of H evolution as well as revealed enrichment/impoverishment behaviour of solutes at thin surface layers in foils it can be concluded that the role of lattice defects on solute/microstructure interactions represents key contribution to the understanding of H trapping in RS Al alloys.

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Session «Electromagnetic shielding II (ISTC Workshop)»

Glasses with PbS and PbSe nanoparticles as saturable absorbers for mode-locked solid state lasers

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Non-linear optical devices can be designed on the basis of various nanostructures. Semiconductor nanoparticles (quantum dots) within dielectric matrices are of interest due to their strong interaction with light (absorption, scattering, luminescence, etc.) and opportunity to control both linear and non-linear optical features through chemical composition and size of nanoparticles and stabilization in solid matrices. An intense light generates electrons and holes (and excitons) providing transient states of quantum dots, thus influencing the light absorption. In the present work, we consider fabrication of glasses doped with lead chalcogenide quantum dots and their application for construction of saturable absorbers for mode-locking and Q-switching devices in the near IR-range. The glasses were prepared using an original technique on the basis of silicate glass-forming system doped with lead compounds and chalcogenes. The melting of all components was done in the reducing environment followed by cooling and secondary heat treatment at 450-600oC in air. PbS and PbSe nanoparticles of the size range of 5-50 nm were formed within the transparent glass providing optical response of materials. They were characterized by XRD, SAXS, TEM and optical spectroscopy. An explicit correlation between particle size and exciton energies was established evidencing the quantum confinement effect. The glasses can successfully function within IR lasers as efficient mode-locking elements.

NOTES

Local field effects and interference quenching of light in planar plasmonic nanostructures

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Unique optical properties of metal nanoparticles originated from localized surface plasmon resonance (LSPR) excitations have already found practical applications in various fields of science and technology. Spectral manifestations of the LSPR can be affected by particle sizes, shapes, materials and even more dramatically by collective interactions in particle arrays. Already in two-dimensional (2D) arrays of small nanoparticles (with sizes of some nm) lateral electrodynamic coupling leads to a strong change in local field characteristics and results in the red concentration shift of the LSPR absorption band. On the other hand, for 2D arrays of silver nanoparticles with sizes of about one hundred nanometers the strong suppression of dipole plasmon band and the appearance of an intense and sharp extinction peak at the frequency near a quadrupole plasmon mode were experimentally revealed [1] for intermediate concentrations of nanoparticles. We analyze these phenomena on the base of universal mechanisms of scattered waves interference and especially the local field effects. As soon as submicron particles have an essentially radiative type of the plasmon excitations decay, short-range ordering of these strong scatterers in densely packed monolayers leads to the partial coherence of scattered light waves. It amplifies the role of local field effects, which have a strong influence on amplitudes and phases of radiation scattered by particles. Employing the statistical theory of multiple scattering of waves, we examine the role of interference quenching in the formation of a strong and narrow extinction band in a monolayer of metal nanoparticles and determine the conditions of the quenching enhancement.

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Microwave absorption by magnetic nanocomposite of disordered carbon nanotubes arrays

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The interaction of electromagnetic radiation in the X and Ka bands with magnetic nanocomposite of disordered carbon nanotubes arrays has been investigated both experimentally and theoretically. Samples were synthesized on the quartz reactor walls by decomposition of ferrocene and xylene which provided random intercalation of iron phase nanoparticles in carbon nanotube array. We found that the absorption of the electromagnetic wave monotonically increases with the frequency. To describe these experimental data, we extended the Bruggeman effective medium theory to a more complex case of magnetic nanocomposite with randomly distributed spherical ferromagnetic nanoparticles in conducting medium. The essential feature of the developed model is the consideration of the complex nature of the studied material. In particular, such important parameters as magnetic and dielectric properties of both the carbon nanotube medium and the nanoparticles, the volume concentration and the dimensions of the nanoparticles, the wave impedance of the resistive-capacitive shells of the conductive nanoparticles, are explicitly taken into account in our model. Moreover, analysing the experimental results, we were able to obtain the frequency dependencies of permittivity and permeability of the studied nanocomposite.

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