1. NANOPHYSICS

1.2. Properties of Materials and Structures

3.1.2.1. The effect of high-amplitude deformation and high-frequency magnetic field exposure on the elastic/inelastic properties of PTFE-based hybrid nanocomposite filled with Fe cluster-doped CNTs. /E. Kutelia, G. Darsavelidze, T. Dzigrashvili, D. Gventsadze, I. Kurashvili, O. Tsurtsumia, L. Gventsadze, L. Nadaraia, L. Rukhadze, T. Kukava, S. Bakhtiyarov/. Bulletin of the Georgian National Academy of Sciences. – 2021. – v. 15. – #1. – pp. 38-44. – eng.; abs.: eng., geo.

The influence of high-amplitude torsional deformation ($\varepsilon \sim 10^{-1} \div 10^{-2}$) and high-frequency (2.4 GHz) magnetic field treatment on elastic/inelastic properties of PTFE-based new hybrid nanocomposites modified with a two-component filler (2.5 wt% Fe-cluster-doped CNT nanopowder + 5wt% chalcopyrite micropowder) was studied using low-frequency amplitude-independent (AIIF) and amplitude-dependent (ADIF) internal friction measurements. The behavior of elastic/inelastic properties of the new trial PTFE-based hybrid nanocomposite modified by a two-component filler (Fe-cluster-doped CNTs + chalcopyrite micro-particles) was investigated in dependence on highamplitude torsional deformation ($\varepsilon \sim 10^{-1} \div 10^{-2}$) and post-deformation high-frequency (2.4 GHz) magnetic field exposure and additional thermal treatment, using AIIF and ADIF measurements. It is shown that self-healing of micro/nano-cracks nucleated in the deformed samples of the nanocomposite may be properly performed via their exposure to high-frequency magnetic field and the additional annealing at 200˚C that leads to the recovery of the values of microplastic deformation beginning critical amplitude (ε_c) to the values even exceeding its initial magnitude by ~38%. Fig. 3, Tab. 2, Ref. 10.

Keywords: PTFE, hybrid nanocomposite, Fe-cluster-doped CNTs, chalcopyrite, magnetic field, internal friction

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3.1.2.2. Nonmonotonic carrier dispersion in dimensionally quantized nanostructures with broken symmetries. /H.S. Nikoghosyan, S.L. Harutyunyan, V.F. Manukyan, G.H. Nikoghosyan/. Proceedings of NAS RA. Physics. – 2020. – vol. 55. – #4. – pp. 537-549. – rus.; abs.: rus., arm., eng.

The features of the energy spectrum and carrier motion in one-dimensional asymmetric semiconductor nanosystems are considered. Asymmetric structures with an additional dip in the potential profile in quantum wells make it possible to vary the positions of size-quantized levels. And the additional influence of an external magnetic field leads to non-monotonic dispersion and a transverse local carrier drift. Such violations of fundamental symmetries will entail corresponding changes in the nature of electronic transitions. The dynamic properties of the electronic system of the nanostructure with the asymmetry of the quantum profile are analyzed, depending on the strength of the external magnetic field. Fig. 4, Ref. 12.

Keywords: energy spectrum, one-dimensinal assymetric semiconductor nanosystems, fundamental simmetries, quantum profile, external magnetic field

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3.1.2.3. Physical adsorption of single-stranded DNA on carbon nanotube. /D.G. Khechoyan, V.F. Morozov/. Proceedings of NAS RA. Physics. – 2021. – vol. 56. – #1. – pp. 100-105. – rus.; abs.: rus., arm., eng.

The results of simulation modeling of single-stranded DNA adsorption on the surface of a single-walled carbon nanotube performed by the molecular dynamics method using the GROMACS software package are presented. The dependence of the timescale and degree of DNA adsorption was studied in dependence on the chirality of the carbon nanotube and the DNA sequence. Fig. 4, Ref. 16.

Keywords: simulation, single-stranded DNA, single-walled carbon nanotube, GROMACS software package, DNA adsorption

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3.1.2.4. Geometric features and numerical analysis of InAsSbP composition micro- and nano-structures shape transformation at nucleation from liquid phase. /K.M. Gambaryan, V.M. Aroutiounian/. Proceedings of NAS RA. Physics. – 2021. – vol. 56. – #2. – pp. 208-217. – rus.; abs.: rus., eng.

Results of the characterization and numerical analysis of InAsSbP composition strain-induced micro- and nanostructures shape transition are presented. Nucleation is performed from In–As–Sb–P quaternary composition liquid phase in Stranski–Krastanow growth mode. Geometric features and the shape transformation chronology of truncated pyramidal islands, lens-shape and pyramidal quantum dots (QDs) are under consideration, which opens up new possibilities at nanoscale engineering and nanoarchitecture of several types of nanostructures. High-resolution scanning electron (HR-SEM) and transmission electron (TEM) microscopes are used for micro- and nanostructures characterization. We show that as the islands volume decreases, the following succession of shape transitions are detected: truncated pyramid, {111} facetted pyramid, {111} and partially {105} facetted pyramid, completely unfacetted “prepyramid”, which gradually evolve to hemisphere and then again to pyramidal QD but with higher facet indexes. Critical sizes of islands shape transformation from “pre-pyramid” to hemisphere (500–550 nm) and then from lens-shape again to pyramidal QDs (5–7 nm) are experimentally detected and theoretically evaluated. It is shown that theoretically calculated values coincide with experimentally obtained data. Fig. 2, Tab. 1, Ref. 21.

Keywords: numerical analysis, InAsSbP, Stranski–Krastanow growth mode, pyramidal quantum dots (QDs), truncated pyramid, facetted pyramid, pyramidal QDs

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3.1.2.5. Monovalent and diavalent impurity states in a semiconductor nanoplatelets. /V.A. Harutyunyan, H.A. Sarkisyan/. Proceedings of NAS RA. Physics. – 2021. – vol. 56. – #3. – pp. 348-355. – rus.; abs.: rus., arm., eng.

Within the framework of the variational method, hydrogen-like impurity states in the semiconductor nanoplatelets with the shape of a rectangular parallelepiped of a small thickness are investigated. Due to the small thickness of the nanostructure, it is shown that, the impurity can be considered two-dimensional. In the case of a divalent impurity, the electron-electron interaction is also considered two-dimensional and taken into account as a perturbation. By the analogy with the theory of the helium atom, the electron-electron interaction energy is determined for the para-state. Fig. 4, Ref. 16.

Keywords: variational method, semiconductor nanoplatelets, nanostructure, divalent impurity, helium atom, electron-electron interaction

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3.1.2.6. Electrical characteristics and photoresponse of the "carbon nanofilm on silicon" heterostructure. /G. A. Dabaghyan, L.M. Matevosyan, K.E. Avjyan/. Proceedings of NAS RA. Physics. – 2021. – vol. 56. – #3. – pp. 374-383. – rus.; abs.: rus., eng.

The electrical characteristics and photoresponse of the “carbon nanofilm on silicon” heterostructure obtained by pulsed-laser deposition, where the thickness of the carbon nanofilm is selected from the condition of the maximum antireflection effect of the substrate, have been investigated. It was found that the obtained heterostructure is rectifying with a rectifying coefficient of 35 at 1 V. The direct current-voltage characteristic from 0.1 V to 0.35 V is in satisfactory agreement with the expression $J = J_0 \exp(eU/\eta kT)$. An increase in the voltage in the forward direction leads to the appearance of the space charge-limited currents ($J = AU^2$). Linearization of the C^{-2} - U dependence indicates the sharpness of the impurity distribution in the space charge region. The mechanism of the photoresponse of the

heterostructure is similar to the photoresponse of anisotype heterostructures with the “window” effect. The longwavelength edge (1.1 μm) of the photosensitivity is determined by the silicon substrate, and absorption in the carbon nanofilm leads to an additional expansion of the photosensitivity region. The heterostructure has uniform photosensitivity at the level 0.8 of a relative photoresponse in the wavelength range of 0.55–1.1 μm. The short-wavelength tail reaches up to 0.4 μm. Fig. 8. Ref. 17.

Keywords: “carbon nanofilm on silicon” heterostructure, maximum antireflection effect of the substrate, space charge-limited currents, short-wavelength tail

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3.1.2.7. Investigation of properties of graphene quantum dots and carbon nanotubes synthesized in a colloid solution. /N.B. Margaryan, N.E. Kokanyan, E.P. Kokanyan/. Proceedings of NAS RA. Physics. – 2021. – vol. 56. – #3. – pp. 392-398. – rus.; abs.: rus., eng.

In this paper, a simple and effective method for the synthesis of carbon nanotubes, graphene-based quantum dots is described. The topological properties of these nanostructures are studied by atomic force and scanning electron microscopes. The potential of quantum dots is investigated by the Kelvin probe method. To study the formed bonds and for a detailed structural analysis, Raman spectroscopy is performed. Other self-organized structures based on graphene are also disclosed using Raman spectroscopy. The effect of photon-phonon scattering on the Raman scattering spectrum is discussed. Fig. 4, Ref. 26.

Keywords: synthesis of carbon nanotubes, graphene-based quantum dots, Kelvin probe method, Raman spectroscopy, photon-phonon scattering

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3.1.2.8. Physicomechanical properties of nanocomposites based on copolymers of ethylene with α-olefins and clinoptilolite. /N.T. Kakhramanov, I.V. Bayramova, V.S. Osipchik, A.D. Ismayilzade, S.R. Abdalova, I.A. Ismayilov, U.V. Namazli/. Azerbaijan Chemical Journal. – 2020. – #4. – pp. 22-27. – eng.; abs.: eng., az., rus.
DOI: https://doi.org/10.32737/0005-2531-2020-4-22-27

The results of studying the effect of clinoptilolite concentration on the properties of nanocomposites based on of ethylene with butylene and of ethylene with hexene copolymer are presented. The effect of clinoptilolite particle size on ultimate tensile stress, elongation at break, flexural modulus, heat resistance, and melt flow index of composites was studied. It is shown that nanocomposites based on ethylene copolymers are characterized by higher values of physicomechanical properties. The additional use of ingredients such as alizarin and calcium stearate contributes to a significant improvement in the complex of properties of nanocomposites based on ethylene copolymers and clinoptilolite. Tab. 3, Ref. 12.

Keywords: ultimate tensile stress, elongation at break, heat resistance, flexural modulus, composite, copolymer

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The influence of additives of nanofillers containing nanoparticles of copper oxides stabilized by a polymer matrix of maleinized high-pressure polyethylene obtained by the mechano-chemical method on the structure and properties features of metal-containing nanocomposites based on isotactic polypropylene and butadienenitrile rubber by X-ray phase and differential thermal analyses is studied. The improvement of strength, deformation and rheological parameters, as well as thermal-oxidative stability of the obtained nanocomposites was revealed, that is probably due to the synergistic effect of interaction of copper-containing nanoparticles with maleic groups of maleinated high-pressure polyethylene. It is shown that nanocomposites based on isotactic polypropylene and butadiene-nitrile rubber can be processed both by pressing method and by injection molding and extrusion methods. The prospects of using a nanofiller containing NPs of copper oxide stabilized by a high-pressure polyethylene matrix obtained by the mechanochemical method as an additive to TPE based on PP/BNR is shown to contribute to the creation of a fine-crystalline structure of the composition, and therefore its properties are improved and thereby expand scope of the obtained nanocomposite. Fig. 4, Tab. 1, Ref. 18.

Keywords: isotactic polypropylene, butadiene-nitrile rubber, metal-containing nanocomposites, copper oxide nanoparticles, maleinized high-pressure polyethylene, thermal properties, XRD, SEM analyses

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The effect of nanofilles additives containing copper oxide nanoparticles stabilized by a polymer matrix of high-pressure polyethylene obtained by the mechanochemical method on features of the structure and properties of metal-containing nanocomposites based on isotactic polypropylene and high-pressure polyethylene was studied using differential thermal (DTA) and X-ray phase (XRD) analyzes. The improvement of strength, deformation and rheological parameters, as well as thermal-oxidative stability of the obtained nanocomposites was revealed, that apparently, is associated with the synergistic effect of

interfacial interaction of copper-containing nanoparticles in the PE matrix with the components of the PP/PE polymer composition. Fig. 2, Tab. 2, Ref. 19.

Keywords: isotactic polypropylene, high pressure polyethylene, copper oxide nanoparticles, thermal properties, DTA and XRD analysis

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