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Original articles

Research article

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Probing molecular interactions, electronic properties, and reactivity of monoamine neurotransmitters in different protonation states via quantum chemical investigation

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Abstract

Amphetamine, dopamine, norepinephrine, serotonin, and tryptamine are a group of monoamine neurotransmitters that regulate diverse brain functions. This work examined these compounds' neutral, protonated, and deprotonated, structural, energetic, and optical properties using quantum chemistry methods. Noncovalent interactions (NCI) and reduced density gradient (RDG) investigations revealed weak intermolecular forces and electron density distribution. The RDG values were observed to span from 0.12 to 0.43, indicating varying degrees of repulsion or attraction. The hydrogen bonding patterns and their strength and nature were also investigated using the Atoms in Molecules (AIM) and B3LYP methods. The quantification was done using $\nabla^2 \rho(r)$, $H(r)$, and energy density values, which showed a variation from -0.014 to 0.026 Hartree/Bohr³, reflecting covalent or electrostatic interactions. A comparison was made between the compounds based on their physical and chemical attributes, such as polar surface area (ranging from 41.81 to 86.71 Å²), rotatable bonds (which were identical), and proton affinity (a measure of stability). Lewis structures and natural bond orbital (NBO) analysis showed resonance and electron delocalization. The study also examined their molecular orbitals (MOs) and found that protonation and deprotonation could significantly change their electronic characteristics, including the energies of the highest occupied (HOMO) and lowest unoccupied (LUMO), the energy gap, and the shape and size of their lobes. The nonlinear optical properties were also assessed, affected by polarizability and hyperpolarizability indices, ranging from 2.267 a.u. (Dopamine) to 7.891 a.u. (Protonated Serotonin). These properties pointed to the applications of these compounds in optical devices.

Keywords: Quantum chemistry, Molecular interactions, Monoamine neurotransmitters, electronic properties, and Protonation states

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Research article

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Formation of silver nanocrystals in Ag-Si composite films obtained by ion beam sputtering

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Abstract

Nanostructured composite films based on Ag-Si containing silver nanoparticles are used as a material for SERS (Surface-enhanced Raman spectroscopy) substrates, plasmonic back reflector, nanoplasmonic sensors, nonlinear optics devices, memristor structures, etc. Due to the widespread use of nanocomposite films based on Ag-Si, there is a need to develop simple and affordable methods for their production compatible with semiconductor technology. Therefore, this work is devoted to the production of an Ag₈₀Si₂₀ nanocomposite film with a high silver content (80 at.%) by ion-beam sputtering with simultaneous control of the morphology, structure, phase composition and electrical properties of the manufactured sample. As a result of complex studies using X-ray diffraction, ultra-soft X-ray emission spectroscopy, SEM and AFM microscopy, it was found that the film is a nanocomposite material based on silver nanoparticles with an average size of ~15÷30 nm. At the same time, some silver nanoparticles are in direct contact, while some Ag nanoparticles are isolated from each other by a shell of silicon dioxide SiO₂ and amorphous silicon *a*-Si. Such a nanogranulated structure of the Ag₈₀Si₂₀ film causes



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the presence in the test sample of the effect of switching from a high-resistance state (880 Ohm) to a low-resistance state (~1 Ohm) under the action of a voltage of ~ 0.2 V. As a result of the formation of conductive filaments (CF) of Ag atoms in the dielectric layer between the silver granules.

Keywords: Silver nanoparticles, Ag NPs, Ag-Si films, Ultra-soft X-ray emission spectroscopy, Ion-beam sputtering

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Research article

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Electrophysical properties of PIN photodiodes of the 2.2-2.6 μm range based on InGa(Al)As/InP heterostructures with a metamorphic buffer layer

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Abstract

Due to a large number of applications in the near and short-wave IR spectrum and a relatively high detectivity, PIN photodiodes based on epitaxial InGa(Al)As/InP heterostructures are of a great scientific interest. The operational spectral range of such photodetectors is up to 2.6 μm . However, to reach such wavelengths it is necessary to synthesize heterostructures with metamorphic buffer layers. In our study, we investigated the current-voltage and capacitance-voltage characteristics of PIN photodiodes based on InGa(Al)As/InP heterostructures with an original metamorphic buffer layer and an $\text{In}_{0.85}\text{Ga}_{0.15}\text{As}$ absorbing layer grown by means of molecular beam epitaxy.

The photodiode chips were formed using standard post-growth processing techniques. The diameter of the photosensitive area of the obtained diodes was 140 μm . The dark currents and the shunt resistance were ~ 300 nA and ~ 25 k Ω at the voltage of -10 mV respectively. Therefore, the suggested metamorphic buffer layer effectively eliminates threading dislocations in the active area of the heterostructure. The obtained heterostructures with metamorphic buffer layers can be used to produce IR photodetectors for the spectral range of 2.2-2.6 μm .

Keywords: Molecular beam epitaxy, Metamorphic buffer layers, Near IR photodetectors, Current-voltage characteristic, Capacitance-voltage characteristic, Dark currents

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Research article

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Effect of plasmonic Au nanoparticles on IR luminescence of Ag₂S quantum dots

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Abstract

Luminescent manifestations of the interaction of Ag₂S quantum dots (QDs) with Au nanorods (NRs) depending on the overlap degree of the corresponding luminescence bands and plasmon resonance peaks have been experimentally established. Under spectral resonance conditions, the possibility of controlling the intensity of QDs luminescence by changing the interaction with Au NRs by varying the distance between the components of the plasmon-exciton mixture has been demonstrated. In turn it determines the influence of the near-field of metal nanoparticles on photoprocesses in Ag₂S QDs.

The detuning of the spectral resonance due to the change in the Au QDs length leads to the asymmetry of the spectral contour of the Ag₂S QDs luminescence band, which may be due to the manifestation of the Fano effect during plasmon-exciton interaction, taking into account the inhomogeneous broadening of the corresponding bands.

Keywords: Quantum dot, Plasmonic nanoparticles, Plasmon resonance, IR luminescence, Plasmon-exciton interaction

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Research article

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Formation of hybrid nanostructures based on Zn_{0.5}Cd_{0.5}S quantum dots and silver nanoparticles for nonlinear optical applications in the near ultraviolet

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Abstract

The goal of this study was to establish optimal conditions for the formation of hybrid nanostructures based on quantum dots and metal nanoparticles with a nonlinear optical response in the near ultraviolet. The relevance of this study is confirmed by the need to create passive devices for controlling the parameters of laser radiation in the presence of semiconductor colloidal quantum dots (QDs) and plasmonic nanoparticles (NPs). Manifestations of interaction in the nonlinear optical response of Zn_{0.5}Cd_{0.5}S QDs and spherical Ag NPs (10 nm) in the field of laser pulses of 10 ns duration at a probing radiation wavelength of 355 nm have been established using the Z-scan method. Manifestations of the formation of hybrid nanostructures have been established using transmission electron microscopy and optical absorption and luminescence spectroscopy. The interaction of colloidal QDs and NPs was manifested as the recombination luminescence quenching of the former with a peak at a wavelength of 450–480 nm. For ensembles of colloidal Zn_{0.5}Cd_{0.5}S QDs with an average size (2.0, 2.2, 2.4 nm), nonlinear refraction (defocusing) of 10 ns laser pulses in the near ultraviolet (355 nm) was established, the coefficient of which increased with increase in QDs. It has been established that during the interaction of Zn_{0.5}Cd_{0.5}S QDs with Ag NPs, the suppression of nonlinear refraction was observed against the background of a twelvefold increase in the nonlinear absorption coefficient. It was concluded that the most probable reason for the observed changes in the nonlinear optical response is the polarizing effect of plasmonic Ag NPs.

Keywords: Nonlinear refraction, Nonlinear absorption, Quantum dot, Zn_{0.5}Cd_{0.5}S, Plasmonic nanoparticle, Z-scan

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Research article

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Formation of smooth and microporous ZnO-based substrate material

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Abstract

The paper investigates the influence of the deposition temperature on the morphology and structural-phase composition of the ZnO-based substrate material with a thickness of over 50 μm during the magnetron sputtering of hot ceramic targets.

The study revealed the influence of the deposition temperature on the growth rate, morphology, and structural parameters of the ZnO single crystal precipitate. It was shown that the ZnO deposition rates during the spluttering of hot ceramic targets were ultra-high (up to 1.5 μm/min). The authors propose a method for the formation of both smooth and microporous ZnO-based substrate materials without using template technologies.

The results obtained in the work can be widely used in optoelectronics and nitride technologies.

Keywords: Zinc oxide, Hot target, Magnetron sputtering, Microporous Structure, substrates, Nitride technologies

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Research article

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Influence of the nature of the organic acid salt on the current-voltage characteristics and electrochemical impedance spectra of anion-exchange membranes

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Abstract

To improve the processes of obtaining and isolating organic acids from solutions, it is necessary to understand the processes occurring on heterogeneous and homogeneous anion-exchange membranes in contact with solutions of salts of organic acids when electric current flows through the membrane system.

The purpose of this paper was to study the effect of sodium salts of acetic, malonic, and citric acids on the current-voltage characteristics (CVC) and electrochemical impedance (ECI) spectra of heterogeneous and homogeneous anion-exchange membranes.

Heterogeneous Ralex AMH (Mega, Czech Republic) and homogeneous Lancyтом® AHT (LANRAN, China) membranes in contact with 0.1 mol-eq/L solutions of neutral and acidic sodium salts of acetic, malonic and citric acids were studied. In solutions of neutral salts, the current-voltage characteristics of both membranes have a traditional form typical for mineral salt solutions, with the exception of the homogeneous Lancyтом® AHT membrane in a sodium malonate solution. In the latter case and in solutions of acidic salts of these acids CVC of both membranes are nonlinear at currents less than the limiting. This is caused by proton transfer reactions between water molecules and carboxyl groups of acid anions or acid molecules and, as a result, the rate constant of dissociation of water molecules in solutions of

organic acidic salts increased by many orders of magnitude. By the appearance of additional semicircles in the spectra, ECI frequency spectra allow identifying the occurrence of new processes in the membrane system when an electric current flows through it.

In most cases, the results of impedance measurements of the studied systems are consistent with the results of voltammetry, although the protonation-deprotonation processes in solution with the participation of organic acid anions are not reflected in the frequency spectra of a heterogeneous membrane. This feature may have been caused by a greater intensity of electroconvection near the surface of heterogeneous anion-exchange membranes as compared to homogeneous anion-exchange membranes.

Keywords: Anion-exchange membrane, Voltammetry, Impedance measurement, Organic acid, Protonation-deprotonation reaction

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Research article

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Synthesis of nanoscale nickel (II) ferrite and a study of its catalytic and sorption activities towards methyl orange

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Abstract

Nanoscale magnetic spinel ferrites are attracting an increased attention as functional materials for catalysis and sorption. Such catalysts and sorbents are advantageous due to their chemical stability in aggressive media, their thermal stability, a large area of specific surface, and high saturation magnetization, which allows using them to create magnetically controlled functional materials. This article presents the results of the synthesis of nickel (II) ferrite nanopowder, its characterization, and a study of its catalytic and sorption activities towards methyl orange dye.

X-ray diffraction (XRD), transmission electron microscopy (TEM), and scanning electron microscopy (SEM) were used to characterize nanocrystalline NiFe₂O₄ synthesized by citrate combustion. The nickel spinel was tested as a catalyst of Fenton-like reaction of oxidative degradation of methyl orange under UV irradiation of $\lambda = 270$ nm. The study involved differentiation of oxidation during dye sorption on a NiFe₂O₄ nanoscale catalyst. The oxidative degradation of the pollutant under ultraviolet irradiation in the presence of a catalyst was satisfactorily described by a pseudo-first-order model, the rate constant of the reaction was 0.0191 min⁻¹. The degree of methyl orange destruction reached 99% 150 minutes after the beginning of the reaction. A parallel experiment without the addition of hydrogen peroxide to the dye solution allowed assessing the sorption capacity of nanoscale nickel (II) ferrite. After 150 minutes, the concentration of the dye decreased by 7.5% due to its sorption, the equilibrium sorption capacity of NiFe₂O₄ was low (0.132 mg/g). This indicates that the methyl orange solution decolorizes mainly due to its catalytic oxidative degradation according to the Fenton reaction.

This allows considering nanoscale nickel ferrite as a promising material for wastewater treatment by deep oxidation of organic pollutants.

Keywords: Nickel ferrite, Nanopowder, Photocatalysis, Fenton reaction

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Research article

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Features of the local activation of aluminum in the presence of bicarbonate ions

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Abstract

The purpose of the article is to study the effect of bicarbonate ions on the local activation of aluminum at a temperature of 25 °C.

The features of local activation of aluminum in the presence of bicarbonate ions ($2 \cdot 10^{-4}$ – $4 \cdot 10^{-5}$ M) were studied using the methods of voltammetry, chronoamperometry, optical and scanning electron microscopy, and X-ray spectral microanalysis.

As a result, we established the range of sodium bicarbonate concentrations, in which there is local activation of aluminum; obtained experimental data on the dependence of the main quantitative characteristics of the process (potential of pitting formation, potential of local activation, and induction period) on the concentration of sodium bicarbonate. Formal kinetic approach was used to propose a mechanism for the local activation of aluminum in hydrocarbonate media.

Keywords: Sodium bicarbonate, Aluminum, Local activation, Passivation, Voltammetry, Chronoamperometry, Scanning electron microscopy

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Research article

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The effect of the chemical compositions of palladium alloys on their hydrogen permeability

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Abstract

The purpose of the article is to identify the effect of the alloying element in palladium alloys on their parameters of hydrogen permeability. Cyclic voltammetry and anodic-cathodic chronoamperometry were used to study the electrochemical behavior of cold-rolled alloys of Pd-5Pb, Pd-6Ru, and Pd-7Y systems (wt. %) in the processes of atomic hydrogen injection and extraction in a deaerated aqueous solution of 0.1 M H₂SO₄.

The study identified the role of lead, ruthenium, and yttrium in the processes of atomic hydrogen injection and ionization. Voltammetry and chronoamperometry data indicate a higher ionization rate for the Pd-6Ru alloy. The parameters of hydrogen permeability calculated from the cathodic current drops show that the hydrogen permeability of alloys varies in the series: Pd-6Ru > Pd-7Y > Pd-5Pb. The effective constant of the injection rate coincides for all alloys within the measurement error, whereas the effective constant of the extraction rate of atomic hydrogen is higher for Pd-5Pb. The marginal solubility of ruthenium in the Pd-6Ru alloy contributes to the passivation of grain boundaries in the alloy with excess ruthenium. As a result, there is preferential movement of hydrogen solely along the grain body. This results in higher hydrogen permeability.

Keywords: palladium, Pd-7Y, Pd-5Pb, Pd-6Ru alloys, hydrogen permeability, atomic hydrogen, phase-boundary transition, membrane separation

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Research article

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Mechanical properties and catalytic activity of the Cu-36Pd (at. %) alloy foil surface after cleaning

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Abstract

The purpose of the study was to evaluate the effect of mechanical treatment and ion sputtering on hydrogen sorption and the mechanical properties of the surface of the membrane foil of the Pd-Cu solid solution system obtained by rolling.

The efficiency of mechanical and ion beam treatment in cleaning of the surface of membrane foil of the Pd-Cu solid solution system obtained by rolling was assessed using cyclic voltammetry, Auger electron spectroscopy and atomic force microscopy.

It was established that ion beam treatment (Ar⁺) and mechanical treatment reproduce the elemental composition of the surface, corresponding to the original composition of the solid solution, and forms a developed relief. The change in the asymmetry of the relief roughness after ion-beam treatment indicates the formation of microcracks on the foil surface, which reduce hardness and plasticity. Ion-beam surface treatment also contributes to the cleaning of the surface from rolling artefacts, which leads to a twofold increase in the ionization rate of atomic hydrogen, compared to a sample subjected to mechanical treatment.

Keywords: Cu-36Pd (at. %) solid solution, thin foil, surface cleaning, voltammetry, atomic force microscopy, nanoindentation

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Research article

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Photoluminescence of GaPNAs/GaP(N) superlattices and bulk GaPN layers on GaP substrates

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Abstract

The addition of a few percent of nitrogen to GaP or GaPAs allows obtaining GaPNAs solid solutions that are lattice-matched to the silicon substrate over a wide range of band gaps, which makes it possible to obtain optoelectronic silicon integrated circuits. However, materials with a small fraction of nitrogen are understudied due to the difficulty in epitaxial growth of quaternary solid solutions with three materials of group V. The purpose of the study was the investigation of the influence of the substrate temperature during the epitaxial growth of dilute nitride materials (GaPN solid solution and GaPNAs/GaP(N) superlattices) on their optical properties, as well as the influence of the growth temperature and superlattice design on the bandgap of the resulting material.

It was shown that there is an optimal growth temperature for samples: at temperatures below the optimal, non-radiative recombination at defects predominates, and at a temperature higher than the optimal one, the solid solution of the GaPN layer material decomposes into components with a larger and smaller fraction of nitrogen. Studies were also carried out on the decay of photoluminescence intensity over

time in the studied structures at room temperature, which allowed us to evaluate the influence of growth parameters and structure design on the lifetime of nonequilibrium charge carriers. The best lifetime for structures with superlattices was obtained for the GaPNs/GaPN superlattice and amounted to ~0.2 ns.

As a result, the optimal growth temperatures were determined for bulk GaPN layers and for GaPNs/GaP(N) superlattices, which leads to an increase in the PL intensity and lifetime of the carrier.

Keywords: GaPN(As), Superlattices, Photoluminescence

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Research article

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A molecular dynamics simulation of the release of desloratadine from alloys containing polyvinylpyrrolidone

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Abstract

Computer modeling is currently a promising technique used in pharmaceutical technologies to develop drug compositions. Molecular dynamics has provided space and time resolutions unavailable during experiments and thus has greatly extended the capabilities of chemistry and some other areas. Molecular dynamics stimulations are very important for the development of solid drug dispersions. The purpose of this study is to simulate the molecular dynamics of the release of desloratadine from alloys containing polyvinylpyrrolidone-10000 into the dissolution medium.

The release of desloratadine from alloys containing polyvinylpyrrolidone-10000 was simulated by the method of molecular dynamics (Gromacs 2023 program, Amber 99 force field). The study involved calculating van der Waals energies of interaction between desloratadine and PVP and desloratadine and water and the proportion of desloratadine molecules that lost their bonds with PVP. The desloratadine molecule was considered released into water provided that it did not bind either to the polymer or water.

It was found that the degree of desloratadine release from PVP into the aqueous medium was the highest at a ratio of 1:1 (24.56±2.08%), and the lowest at ratios of 1:2 and 1:5 (8.27±1.79 and 8.65±0.98%, respectively). At a ratio of 1:1, the average energy of interaction between desloratadine with PVP per one molecule of desloratadine was the highest (−36.13±0.62 kJ/mol) when the energy of interaction between desloratadine and water was low (−52.03±0.82 kJ/mol), which indicates that desloratadine involvement in the solvation and desorption processes was the highest at this ratio. The average energy of interaction between desloratadine and the polymer was the lowest at a ratio of 1:5 (−52.03±0.82 kJ/mol) when the energy of interaction between desloratadine and water was −44.45±1.60 kJ/mol. This fact indicates a low intensity of the desorption and solvation processes at this ratio.

Keywords: release, desloratadine, polyvinylpyrrolidone, molecular dynamics

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Research article

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Preparation and properties of conversion phosphate-containing coatings on magnesium alloys doped with rare earth elements

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Abstract

The purpose of our study was to synthesize and analyze the structure, qualitative and quantitative composition, and protective properties of phosphate-containing conversion coatings on WE43, ZRE1, and QE22 magnesium alloys doped with rare earth elements in the Hank's Balanced Salt Solution.

Scanning electron microscopy, energy dispersive X-ray analysis, and X-ray phase analysis methods were used to study the morphology, microstructure, the elemental and phase compositions of QE22, ZRE1, and WE43 magnesium alloys doped with rare earth elements, as well as conversion coatings formed on their surface during phosphating. Linear voltammetry and electrochemical impedance spectroscopy were used to study the kinetic properties of corrosion of the analyzed samples in the Hank's Balanced Salt Solution (pH = 7.4) imitating the human body environment before and after phosphating.

The study showed that the phosphating of magnesium alloys doped with rare earth elements results in the formation of low-soluble fine-grained coatings with a pronounced crystal structure and a thickness from 16 to 21 μm. The obtained conversion coatings are characterized by the following elemental composition: Ca ≈ 40 wt.%; P ≈ 15 wt.%; and O ≈ 35 wt.%. The crystal structure of phosphate-containing coatings is presented by the brushite phase (CaHPO₄·2H₂O).

The electrochemical studies of the corrosion behavior of magnesium alloys in the model Hank's Balanced Salt Solution (pH = 7.4) demonstrated that the corrosion current density decreases in the sequence QE22, ZRE1, WE43 and is i_{corr} , A/cm²: 5.2·10⁻⁵; 2.5·10⁻⁵; 2.0·10⁻⁵. The obtained conversion coatings based on brushite reduce the corrosion rate of QE22, ZRE1, and WE43 magnesium alloys by 15.2, 7.8, and 6.3 times, respectively.

Keywords: Magnesium, Rare earth elements, Conversion coating, Brushite, Corrosion

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Research article

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Residual strain evaluation in GaN/AlN multiperiod superlattices grown on SiC/Si

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Abstract

In our study, we formed a multilayer heterostructure consisting of periodic GaN and AlN layers by means of chloride-hydride epitaxial growth on a hybrid SiC/Si substrate synthesized using the method of the coordinated substitution of atoms.

A comprehensive study of the heterostructure by means of nanoscale mapping of elastic strain demonstrated that in the upper GaN layer the dual-axis strain σ_{xx} is minimal (~ -0.12 GPa). There is practically no strain in the superlattices located in the upper part of the heterostructure.

Keywords: GaN, AlN, Superlattice, Raman spectroscopy

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Research article

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Structural and spectroscopic studies of epitaxially overgrown GaN, n-GaN, and n⁺-GaN contact layers

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Abstract

The paper demonstrates that the technology of plasma-assisted molecular beam epitaxy (PA MBE) can be used to form epitaxially overgrown GaN, n-GaN, and n⁺-GaN contact layers with a high structural quality on virtual GaN/c-Al₂O₃ substrates under Ga-enriched conditions at relatively low growth temperatures of ~ 700 °C.

It was shown that the initial stage of growth of the contact layers was accompanied by effective filtration of dislocations threading from the buffer GaN layer of the virtual substrate formed by MOCVD.

The values of residual stresses calculated using the data of Raman microspectroscopy indicate a high structural quality of GaN, n-GaN, and n⁺-GaN contact layers regardless of the level of silicon doping.

The contact resistance reduced to the pad width determined using the transmission line method for the structure with n⁺-GaN contact layer was ~ 0.11 Ohm-mm and for the n-GaN contact layer it was ~ 0.5 Ohm-mm.

Keywords: Molecular beam epitaxy, GaN, n-GaN, and n⁺-GaN contact layers, Virtual substrate, Raman microspectroscopy

Funding: The study was carried out within the framework of the grant of the Ministry of Education and Science of the Russian Federation (grant No. FZGU-2023-0006). GaN, n-GaN, and n⁺-GaN contact layers were synthesized in the framework of the grant of the Ministry of Education and Science of the Russian Federation No. FSRM-2023-0006.

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Research article

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Nanocrystalline films based on YCrO₃ and LaCrO₃ yttrium and lanthanum chromites doped with strontium ions Sr²⁺ as a basis for semiconductor gas sensors

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Abstract

For the production of gas-sensitive sensors, easily obtained nanostructured substances are required. Therefore, one of the most important scientific problems is the search for new compositions and an improvement in the used materials. The aim of this study was the creation of thin-film materials based on yttrium and lanthanum chromite nanopowders YCrO₃ and LaCrO₃, doped with strontium ions, and the identification of their gas-sensitive properties.

The synthesis of nanopowders was carried out by the sol-gel method for LaCrO₃ and the citrate method for YCrO₃. Doped powders were obtained using the same synthesis methods as the original samples. The phase and elemental composition of the obtained samples was determined. The result of this study demonstrated that the actual composition of the nanopowders is close to the nominal one. Gas-sensitive properties were determined by measuring the specific surface resistance of the obtained samples to the content of carbon monoxide CO with a concentration of 50 ppm.

It was found that the obtained samples possess *n*-type of conductivity and a good response to the presence of traces of carbon monoxide. Yttrium chromite-based nanofilms exhibit better gas-sensitive response compared to LaCrO₃. The maximum value was obtained for Y_{0.9}Sr_{0.1}CrO₃, demonstrating a gas sensitive response of 2.83 at a temperature of 200 °C.

Keywords: Semiconductors, Gas sensitivity, Yttrium chromite, Lanthanum chromite, Doping, Nanofilms, Nanopowders

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Research article

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Preparation of composite micro-nanofibers based on nano-sized magnetite by electrospinning

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Abstract

Composite materials with magnetic fillers play an important role in a number of industries, from functional coatings in electronics to electromagnetic wave absorption and microwave-shielding materials. An important feature is the selection of a magnetic nano-sized filler that does not cause increased degradation of the polymer binder, and the selection of a polymer that ensures the weather resistance of the nanocomposite material. In this study, composite samples of micro- and nanofibers based on fabricated particles of nanosized magnetite (Fe₃O₄) as a cheap electromagnetic wave absorption material were investigated.

Magnetic polymer-dielectric fibers polystyrene-Fe₃O₄ were obtained by electrospinning. The X-ray diffraction analysis showed that the synthesized Fe₃O₄ nanoparticles have a cubic space group structure *Fd3m* with crystal lattice parameter *a* = 8.422±0.026 Å. The analysis of the ferromagnetic resonance spectrum showed the ferromagnetic nature of the obtained magnetite nanoparticles. It has been shown that during the production of composite fibers by electrospinning, a dispersion of nano-sized magnetite powder can be included in the spinning solution, which, as a result of the electrospinning process, allows obtaining magnetic composite micro- and nanofibers. The average size of the included magnetite particles was 15±3 nm.

The resulting non-woven magnetic material is predominantly composed of two types of fibers with an average diameter of 680±280 nm and larger associated fibers with a diameter of 1500±300 nm. Based on a certain frequency dependence of losses upon reflection *RL* in the frequency range 15 MHz – 7.0 GHz, the synthesized fibrous material can be considered to be an effective electromagnetic wave absorption material.

Keywords: Nano-sized magnetite, Electrospinning, Composite fiber, Structural characteristics, Magnetic materials, Radio absorption

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Research article

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XPS investigations of thin epitaxial and magnetron tin layers surface physico-chemical state

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Abstract

Thin layers of the tin-oxygen system with nanometer thicknesses and structures based on them are relevant objects of development for use in modern devices, for example in microelectronics. The general miniaturization of electronic devices, the achievement of energy efficiency in the operation of such devices, and the optimal modes of their operation determine the strategies for using the tin-oxygen system structures. First of all, the justification of the tin-oxygen system nanolayers formation technique. The dependence of the formed nanolayers properties on the state of their surface is significant.

The article contains the results of direct experimental studies of the composition and physico-chemical state of the tin-oxygen system thin nanolayers surface. To form the studied structures, the popular and in-demand methods of magnetron sputtering and molecular beam epitaxy were used. The X-ray photoelectron spectroscopy was applied with the use of the synchrotron radiation which has a high intensity and the possibility of spectrum excitation energy optimal selection, which is important for a small amount of the studied material. After formation, the research objects were stored in laboratory conditions for several weeks before synchrotron studies.

Differences in the surface composition and physico-chemical state of the thin tin layers formed by magnetron sputtering or epitaxially, and then oxidized naturally, are shown. Five monolayers of tin formed by the molecular beam epitaxy make it possible to diffuse atmospheric oxygen, which oxidizes the Si buffer layer located under the Sn nanolayer on a silicon substrate. At the same time, the surface of the tin film obtained by magnetron sputtering is close to the natural oxide SnO_{2-x} in its physico-chemical state.

The results of the work can be useful for determining the optimal approaches to the formation and subsequent modification of thin and ultrathin layers of tin oxides for the tasks of creating active layers of modern electronic devices.

Keywords: Tin and its oxides, Physico-chemical state, Composition, Epitaxial nanolayers, Magnetron nanolayers, X-ray photoelectron spectroscopy, Synchrotron studies

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