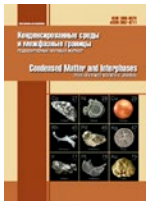

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Аннотации на английском языке

Special Issue
New materials for micro-, nano-, and optoelectronics: properties, structure, and growth mechanisms
Sergey A. Kukushkin
Website: http://www.ipme.ru/ipme/labs/phase/kukushkin.html
Institute for Problems in Mechanical Engineering of the Russian Academy of Sciences
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The editorial board of the journal Condensed Matter and Interphases is pleased to present a special issue dedicated to studying the fundamental and applied aspects of the synthesis and properties of new materials used for a wide range of purposes. The issue includes theoretical and review articles, as well as empirical studies that should be interesting for theorists, experimental scientists and technologists.

Review

Review article
https://doi.org/10.17308/kcmf.2023.25/11470
Surface energy in microwires. Review
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Abstract
The research involves using an analytical solution of the Gibbs–Tolman–Koenig–Buff equation to calculate the microwire surface tension. The classical theory of nucleation and the statistical theory of density were used to determine dependencies for the surface energy of a cylindrical particle. It was shown that within the linear theory, both approaches produce similar results. However, within the nonlinear theory, the results may differ. The article presents an analysis of the analytical solutions of equations for a cylindrical surface within the van der Waals linear and nonlinear theories.
Keywords: Gibbs–Tolman–Koenig–Buff theory, Tolman length, Van der Waals theory, Surface energy, Cylindrical surface
Funding: The study was supported by the Moldovan National Project and the project of Shevchenko Transnistria State University.
For citation: Baranov S. A. Surface energy in microwires. Review. *Condensed Matter and Interphases*. 2023;25(4): 484–493. https://doi.org/10.17308/kcmf.2023.25/11470

Original articles

Research article
https://doi.org/10.17308/kcmf.2023.25/11480
Relativistic model of interatomic interactions in condensed systems
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Abstract
A method was proposed to describe the dynamics of systems of interacting atoms in terms of an auxiliary field. The field is equivalent to the specified interatomic potentials at rest, and represents the classical relativistic field under dynamic conditions. It was determined that for central interatomic potentials, allowing for the Fourier transform, the auxiliary field is a superposition of elementary fields satisfying the Klein-Gordon-Fock equation with complex mass parameters.
Keywords: Interatomic potentials, Classical relativistic dynamics, Retarded interactions, Irreversibility phenomenon, Klein-Gordon-Fock equation
For citation: Zakharov A. Yu., Zakharov M. A. Relativistic model of interatomic interactions in condensed systems. *Condensed Matter and Interphases*. 2023;25(4): 494–504. https://doi.org/10.17308/kcmf.2023.25/11480

Research article
https://doi.org/10.17308/kcmf.2023.25/11473
Pair interaction of intersecting dilatation and disclination defects
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Abstract
An elastic interaction of the intersecting dilatation and disclination defects located in an infinite linear isotropic media is investigated. The eigenstrain approach is employed to obtain the analytical expressions describing the pair interaction between intersecting dilatational lines and intersecting wedge disclinations. It is demonstrated that the interaction energy strongly depends on the intersection angle between the defects. The energy reaches the maximum value if the defect lines are coincided while the energy reaches the minimum value if the defect lines are orthogonal. Besides, it is shown that interaction energy of intersecting wedge disclinations strongly depends on the elastic properties of the media: the less the Poisson ratio, the less the energy. The obtained analytical results seem to be applicable for the theoretical analysis of the residual stress relaxation mechanisms in heterostructures with pentagonal symmetry such as icosahedral particles.

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Keywords: Disclination, Dilatation line, Pair interaction
Funding: The study was supported by the Russian Science Foundation, project No 23-72-10014.
For citation: Krasnitckii S. A., Smirnov A. M. Pair interaction of intersecting dilatation and disclination defects. *Condensed Matter and Interphases*. 2023;25(4): 505–513. https://doi.org/10.17308/kcmf.2023.25/11473

Research article
https://doi.org/10.17308/kcmf.2023.25/11477
Semi-polar GaN(11-22) on nano-structured Si(113): a structure for reducing thermal stresses
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Abstract
The article reports the growth of semi-polar GaN(11-22) layers using epitaxy from metal organic compounds on a nano-structured NP-Si(113) substrate. It was shown that upon the emergence of an island layer, elastic deformed structures of GaN(11-22)/NP-Si(113) form a nano-meter compliant silicon layer on a substrate while elastic stresses conditioned by the difference of temperature coefficients of GaN and Si in such a structure decrease.
Keywords: Semi-polar gallium nitride, Nano-structured silicon, Elastic and plastic structure deformation
Acknowledgments: The authors thank V. K. Smirnov for providing nanostructured Si(113) substrates, M. P. Shcheglov, M. E. Kompan for measurements.
***For citation*:** Bessolov V. N., Konenkova E. V., Orlova T. A., Rodin S. N. Semi-polar GaN(11-22) on nanostructured Si(113): structure for reducing thermal stresses. *Condensed Matter and Interphases*. 2023;25(4): 514–519. https://doi.org/10.17308/kcmf.2023.25/11477

Research article
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Structural and optical properties of composition-graded InGaN nanowires
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Abstract
At the moment, InGaN ternary compounds are of a great interest for the development of devices for sunlight driven water splitting. However, the synthesis of such materials is hindered by the fact that $In_xGa_{1-x}N$ layers are susceptible to phase decomposition at *x* from 20 to 80%. Nanowires can be a promising solution to this problem. The purpose of our study was to analyze the structural and optical properties of $In_xGa_{1-x}N$ nanowires with a gradient x content being inside the miscibility gap.
$In_xGa_{1-x}N$ nanowires were grown on silicon substrates using plasma-assisted molecular beam epitaxy. The structural properties of nanowires were studied using scanning and transmission electron microscopy. The chemical composition and optical properties of nanowires were analyzed using energy-dispersive microanalysis and photoluminescence spectroscopy.
It was shown for the first time that the composition-graded $In_xGa_{1-x}N$ nanowires with x from 40 to 60% can be grown using plasma-assisted molecular beam epitaxy. The grown samples exhibit photoluminescence at room temperature with a maximum at about 890 nm, which corresponds to an In content of about 62% according to the modified Vegard's rule and the transmission electron microscopy data. The obtained results can be of practical interest for the development of devices for water splitting induced by sunlight or sources of near IR radiation.
Keywords: InGaN, Structural properties, Miscibility gap, Molecular beam epitaxy, Optical properties, Photoluminescence, silicon
Funding: The synthesis of the experimental samples and the optical measurements were conducted with the financial support of the Russian Science Foundation, grant No. 23-79-00012. The study of the morphological properties of the grown samples was conducted with the financial support of the Ministry of Science and Higher Education of the Russian Federation, research project No. 2019-1442 (project reference number FSER-2020-0013). The structural properties of the grown samples were studied with the financial support of St. Petersburg State University, research grant No. 94033852.
For citation: Gridchin V. O., Reznik R. R., Kotlyar K. P., Kirilenko D. A., Dragunova A. S., Kryzhanoskaya N. V., Cirlin G. E. Structural and optical properties of composition-graded InGaN nanowires. *Condensed Matter and Interphases*. 20223;25(4): 520–525. https://doi.org10.17308/kcmf.2023.25/11475

Research article
https://doi.org/10.17308/kcmf.2023.25/11474
Confirmation of spontaneous doping of GaN nanowires grown on vicinal SiC/Si substrate by electron beam induced current mapping
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Abstract
This study is devoted to the confirmation of spontaneous doping of GaN nanowires grown on vicinal SiC/Si hybrid substrates by electron beam induced current mapping.

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GaN nanowires (NWs) were grown on singular and vicinal SiC/Si substrates by molecular beam epitaxy with nitrogen plasma activation. The morphological properties of the NWs were studied by scanning electron microscopy. The electrophysical properties of the obtained nanostructures were studied by electron beam induced current mapping.
By electron beam induced current mapping, we confirmed the spontaneous doping of the GaN NWs grown on vicinal SiC/Si wafers. It was also shown that the GaN NWs grown on singular SiC/Si substrates did not exhibit an induced current signal, indicating that they were not doped.
Keywords: Semiconductors, GaN, Nanowires, Molecular beam epitaxy, Spontaneous doping, Silicon, Silicon carbide, Electron beam induced current method
Funding: The synthesis of the experimental samples was financially supported by the Russian Science Foundation, Grant No. 23-79-00012. The morphological studies of the obtained samples were financially supported by the Ministry of Science and Higher Education (FSRM 2023-0007). The electrophysical studies of the obtained samples were supported by PHC KOLMOGOROV project No. 43784UJ (2019).
For citation: Reznik R. R., Gridchin V. O., Kotlyar K. P., Neploh V. V., Osipov A. V., Kukushkin S. A., Saket O., Tchernycheva M., Cirlin G. E. Confirmation of spontaneous doping of GaN nanowires grown on vicinal SiC/Si substrate by electron beam induced current mapping. *Condensed Matter and Interphases*. 20223;25(4): 526–531. https://doi.org/10.17308/kcmf.2023.25/11474

Research article
https://doi.org/10.17308/kcmf.2023.25/11482
GaN micro- and nanostructures selectively grown on profiled sapphire substrates using PA-MBE without lithography
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Abstract
Purpose: Development of technology for the formation of ordered arrays of nanocolumns (NCs) of GaN microcrystals using plasma-activated molecular beam epitaxy from nitrogen (PA-MBE) on profiled sapphire substrates (SPS) of large diameter with a micro-cone profile. The proposed method eliminates the use of low-performance and expensive nanolithography methods. The article is aimed at a deeper understanding of the processes that determine the growth kinetics of III-N nanocolumns using PA MBE on patterned sapphire substrates with multiple orientations of various non-polar and polar planes.
A new technological process for the fabrication of GaN NCs using PA-MPE is proposed, which ensures selectivity of their growth at the tops of PPS micro-cones and suppresses growth on the semipolar planes of these substrates. GaN NCs and microcrystals were grown using PA-MBE on commercially available PPS.
A technology has been developed for the formation of discharged arrays of GaN nanocolumns without the use of lithographic procedures. Modes have been established that allow the formation of microcrystals and NCs with different diameters: from 30 nm to several microns. A diagram of the growth of GaN by the PA MBE method on PPS has been constructed, demonstrating the boundaries of the technological regimes for the formation of GaN NCs and microcrystals with different surface topography.
Keywords: Selective area growth, Whiskers, Microcrystals, Nanocolumns, Plasma-activated molecular beam epitaxy, Wide-gap semiconductor compounds A^3N
Funding: The research was carried out with financial support from the Ministry of Science and Higher Education Higher Education of Russian Federation (agreement 075-15-2022-1224 “Bio-Light”).
For citation: Semenov A. N., Nechaev D. M., Troshkov S. I, Berezina D. S., Abbas A. S., Jmerik V. N. Micro- and nanostructures of GaN selectively grown on patterned sapphire substrates by PA-MBE without lithography techniques. *Condensed Matter and Interphases*. 2023;25(4): 532–541. https://doi.org/10.17308/kcmf.2023.25/11482

Research article
https://doi.org/10.17308/kcmf.2023.25/11476
Fabrication of α-Ga_2O_3:Sn/α-Cr_2O_3/α-Al_2O_3 heterostructure by mist CVD and HVPE
P. N. Butenko[1], R. B. Timashov[1], A. I. Stepanov[1], A. I. Pechnikov[1,2], A. V. Chikiryaka[1], L. I. Guzilova[1], S. I. Stepanov[2], V. I. Nikolaev[1,2]
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Abstract
Corundum-structured chromium oxide (α-Cr_2O_3), exhibiting *p*-type conductivity, is a highly attractive candidate for forming high-quality *p-n* heterojunctions with α-Ga_2O_3. Two CVD growth techniques were employed in the fabrication of the heterostructure. A ~ 0.2-micron α-Cr_2O_3 layer was grown on a (0001) sapphire substrate using mist CVD at 800 °C. It possesses high morphological homogeneity and low roughness, which is acceptable for further epitaxial processes. Subsequently, Sn-doped α-Ga_2O_3 with a thickness of ~ 1.5 μm was grown on the α-Cr_2O_3 layer using HVPE at 500 °C. The feasibility of fabricating this heterostructure with the specified layer thickness and acceptable surface morphology using CVD techniques has been demonstrated.
Keywords: Gallium Oxide, Sapphire substrate, Heteroepitaxy, CVD, Mist-CVD, HVPE
Funding: P.N. Butenko, A.I Pechnikov, and L.I. Guzilova gratefully appreciate the Russian Science Foundation for financial support (grant No. 23-29-10196).
For citation: Butenko P. N., Timashov R. B., Stepanov A. I., Pechnikov A. I., Chikiryaka A. V., Guzilova L. I., Stepanov S. I., Nikolaev V. I. Fabrication of α-Ga_2O_3:Sn/α-Cr_2O_3/α-Al_2O_3 heterostructure by mist CVD and HVPE. *Condensed Matter and Interphases*. 2023;25(4): 542–547. https://doi.org/10.17308/kcmf.2023.25/11476

Аннотации на английском языке

Research article
https://doi.org/10.17308/kcmf.2023.25/11484

A study of gallium oxide by using the piezoelectric composite oscillator technique at a frequency of 100 kHz

V. V. Kaminskii, D. A. Kalganov, D. I. Panov, V. A. Spiridonov, A. Yu. Ivanov, M. V. Rozaeva, D. A. Bauman, A. E. Romanov
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Abstract

The article presents the results of the study of the mechanical properties and defect structure of gallium oxide (Ga_2O_3) by using the piezoelectric composite oscillator technique. Bulk samples of the Ga_2O_3 beta phase in the form of single crystals and their intergrowths were obtained by growth from a melt with a shaper (Stepanov technique). The research involved studying the dependences of the longitudinal elastic modulus and the damping of elastic vibrations at a frequency of 100 kHz on the strain amplitude. Changes in the elastic and microplastic properties of the samples at different temperatures were attributed to possible relaxation phenomena in the structure of the material.

Studying the defect structure in samples of pure and doped Ga_2O_3 is necessary to improve the technology for the production of large single crystals. The fundamental questions in this area are the influence of defects on the anisotropy of electrical conductivity, band structure, and other functional properties of the resulting semiconductor material. The purpose of this article is to establish the features of sample preparation, research, and interpretation of the results obtained by the piezoelectric composite oscillator technique for gallium oxide samples.

In the studied samples, the first longitudinal vibration mode was excited, which corresponded to a length of about 27 mm and a small cross-section of the sample. The temperature dependences in the region of low and high strain amplitudes were determined separately. The crystalline quality of the prepared samples was assessed by X-ray diffraction with the analysis of the rocking curve.

The value of Young's modulus obtained along the growth axis (crystalline orientation <010>) in Ga_2O_3 crystals E≈260 GPa is in line with the results of previous studies. Relaxation peaks corresponding to various dislocation interactions were found on the temperature dependences of internal friction at a temperature of 280 K.

Keywords: Gallium oxide, Single crystal, Defect structure, Real structure, Semiconductor, Piezoelectric composite oscillator technique
Funding: This work was supported by the grant of Russian Science Foundation No. 19-19-00617.
For citation: Kaminskii V. V., Kalganov D. A., Panov D. I., Spiridonov V. A., Ivanov A. I., Rozaeva M. V., Bauman D. A., Romanov A. E. A study of gallium oxide by using the piezoelectric composite oscillator technique at a frequency of 100 kHz. *Condensed Matter and Interphases*. 20223;25(4): 548–556. https://doi.org/10.17308/kcmf.2023.25/11484

Research article
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Phase transformations during the annealing of Ga_2O_3 films

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Abstract

A growth technique has been developed to obtain the three main crystalline phases of Ga_2O_3, namely: α-phases, ε-phases, and β-phases using hybrid vapour phase epitaxy (HVPE). The substrate temperatures and precursor fluxes were determined at which only the α-phase, only the ε-phase, or only the β-phase were deposited. It was found that the annealing of the metastable α- and ε-phases led to completely different results. The ε-phase quickly transforms into the stable β-phase as a result of annealing, while the α-phase, upon annealing, transforms into an intermediate amorphous phase, after which it peels off and is destroyed. The obtained result is explained by the fact that the reconstructive phase transition from the α-phase into the β-phase is accompanied by too large an increase in density (~10%), leading to enormous elastic stresses and, consequently, an increase in the height of the phase transition barrier.

Keywords: Reconstructive phase transitions, Gallium oxide, Polymorphs, X-ray diffraction, Spectroscopic ellipsometry, Raman spectrum
Funding: A. V. Kremleva carried out her part of the study with financial support Russian Science Foundation (grant No. 21-79-00211).
For citation: Osipov A. V., Sharofidinov Sh. Sh., Kremleva A. V., Smirnov A. M., Osipova E. V., Kandakov A. V., Kukushkin S. A. Phase transformations during the annealing of Ga_2O_3 films. *Condensed Matter and Interphases*. 20223;25(4): 557–563. https://doi.org/10.17308/kcmf.2023.25/11479

Research article
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Crystallization features and physical properties of the thin-film heterostructure of lead zirconate titanate – lead oxide

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Abstract

Various diagnostic techniques aimed at studying the structure and physical properties (synchronous thermal analysis, atomic force microscopy operating in the current measurement mode, electron-probe X-ray spectral microanalysis, dynamic method for determining the pyroelectric response) were used to study the crystallization features and physical properties of the thin-film heterostructure PZT – PbO_{1+x} formed by a two-stage technique of RF magnetron sputtering of a ceramic target.

During the first stage, amorphous films were deposited on a "cold" platinized silicon substrate, while the second stage involved high-temperature annealing in air. It was shown that annealing of amorphous films and crystallization of the intermediate pyrochlore phase are accompanied by additional oxidation of the structure resulting in the formation of lead orthoplumbate and lead dioxide and additional oxidation of organic inclusions. The presence of a liquid phase of lead oxide contributes to the formation of the pyrochlore phase.

It was found that lead oxide layers have significantly higher through conductivity than perovskite blocks. It was assumed that the increased conductivity of lead oxide layers is associated with lead dioxide, which has high conductive properties. Self-polarized thin films were

detected to have an abnormal electrical response to the strobing thermal exposure, including the typical pyroelectric response, local photoconductivity shunted by layers of the perovskite phase, and through photoconductivity. The presence of photoconductivity is also associated with the conductive properties of lead dioxide.

Keywords: Thin film heterostructure of lead zirconate titanate and lead oxide, Crystallization of pyrochlore and perovskite phases, Differential scanning calorimetry, Thermal analysis, Atomic force microscopy, Pyroelectricity

Funding: The study was supported by Herzen State Pedagogical University of Russia (internal grant No. 25 VN).

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Research article

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Anomalous electron channeling in PZT thin films

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Abstract

The study of the surface of lead zirconate-titanate (PZT) thin films using a scanning electron microscope (SEM) identified the patterns of electron channeling on the surface of the perovskite phase crystals. However, the observation conditions were completely uncommon and contradicted model representations. Thus, there was enough evidence to believe that the observed patterns of electron channeling were an anomaly. It was necessary to conduct an additional detailed study of the perovskite crystal in a PZT thin film in order to clarify which conditions could cause this anomaly.

In particular, the method of electron backscatter diffraction (EBSD) in SEM was used to study the crystallographic specific features of the crystal. The method is based on the collection and automatic processing of electron diffraction patterns which calculate a corresponding crystallographic orientation for each point on the scanned crystal surface.

As a result, the study revealed the unusual features of the crystallographic structure of perovskite in a PZT thin film that provided an opportunity for the manifestation of anomalous electron channeling. The research showed that the crystal lattice of perovskite experienced an axially symmetric monotone bend, which determined the round shape of the crystal. The study demonstrated the possibility of producing ferroelectric crystals with a curved crystallographic surface. In order to describe the growth of round perovskite crystals from the amorphous phase in PZT thin films, the author provided a dislocation model where the continuous bending of the perovskite crystal lattice could be explained by the accommodation of mechanical stresses with a decrease in the phase volume of the film material. In addition, it was shown that the bands observed in the electron channeling patterns corresponded to crystallographic planes, while any distortions of the pattern indicated a local deformation of the lattice in a highly symmetrical uniformly curved perovskite crystal in a PZT thin film.

Keywords: Anomalous electron channeling, Channeling, Thin films, Lead zirconate-titanate, PZT, Perovskite, Deformed crystals, EBSD

Acknowledgements: Experimental studies were performed using the equipment of the Center for the Collective Use of Scientific Equipment "Composition, structure, and properties of structural and functional materials" of the National Research Center Kurchatov Institute – Central Research Institute of Structural Materials "Prometey".

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Brief review

https://doi.org/10.17308/kcmf.2023.25/11472

Natural ferromagnetic resonance in microwires and its applications. Brief review

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Abstract

The paper analyzes technological aspects of the Taylor–Ulitovsky method used to produce microwires of various structures.

Natural ferromagnetic resonance (NFMR) in cast glass-coated amorphous magnetic micro- and nanowires was theoretically and experimentally studied. The NFMR phenomenon is due to the large residual stresses appearing in the core of the microwire during the casting process. These stresses, along with magnetostriction, determine magnetoelastic anisotropy. Besides residual stresses, the NFMR frequency is influenced by externally applied stresses on the microwire or the composite containing the so-called stress effect (SE).

The dependence of the NFMR frequency on the deformation of microwires and the external stresses on them is proposed to be used for remote diagnostics in medicine.

Keywords: Cast glass-coated amorphous magnetic micro- and nanowire, Magnetostriction, Natural ferromagnetic resonance

Funding: The study was supported by the Moldovan National Project and the project of Shevchenko Transnistria State University.

For citation: Baranov S. A. Natural ferromagnetic resonance in microwire and its application. Brief review. *Condensed Matter and Interphases*. 2023;25(4): 581–586. https://doi.org/10.17308/kcmf.2023.25/11472

Research article

https://doi.org/10.17308/kcmf.2023.25/11478

Electronic structure of germanium dioxide with rutile structure according to ab initio computer simulation data

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Abstract

The article focuses on the electronic structure of the tetragonal crystalline modification of germanium dioxide. The electronic structure was theoretically studied by means of the full-potential linearized augmented plane wave method using the Wien2k software.

Аннотации на английском языке

Total and partial densities of electronic states were calculated. The spectra of the X-ray absorption near edge structure were simulated for various absorption edges of germanium and oxygen atoms. The Z+1 approximation method was used to calculate Ge K-, Ge L_3- and O K absorption edges for the tetragonal modification of GeO_2. The result obtained for the Ge K absorption edge is in good agreement with the experimental data.
The Ge L_3 spectrum was calculated for the first time, and the result is of predictive nature. In order to obtain a better agreement with the experimental calculations of the oxygen K absorption edge, besides the Z+1 approximation method, we also used the core hole method, including the simulation of a partial core hole. The study demonstrated that the use of a core hole with an electron charge of 0.7 results in a better agreement between the calculations and the experiment.
Keywords: Computer simulation, Germanium dioxide, Electronic structure, Density of states, XANES, Core hole, Rutile
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Brief review
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Solid wetting layer, interphase formation, and thin-film nanomaterials. Brief review
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Abstract
A review of the results on the formation of the interface between 3*d* metals and silicon silicides under identical conditions for various parameters of the deposited vapor, crystallographic orientation and substrate temperature is presented. A generalization of the results has been carried out, which consists of the fact that during the process of deposition of hot vapor on a colder substrate, the transition from the surface phase to the bulk phase occurs through a solid wetting layer (SWL). A classification of substrate-stabilized phases, including SWL, is proposed. It has been shown that SWL has an electronic density different from bulk phases, a smooth or nanostructured morphology, optical, electrical, and magnetic properties, and plays an important role in the formation of interfaces between bulk phases, their epitaxial films and multilayer nanostructures. These studies suggest the promise of SWL as a new nanotechnology object for the creation of thin-film nanomaterials.
The studied problem is the formation of interfaces in thin-film nanomaterials. The purpose of the article is to substantiate the discovery of nonequilibrium solid wetting layers, their uniqueness and their role in the formation of the above-mentioned interfaces. This is important research for nanomaterial technologies.
A review and generalization of the results of the study of the metal–silicon interface obtained under identical conditions was carried out. The review shows the detection a new type of transition state of the film under nonequilibrium conditions, a solid wetting layer, and the generalization justifies its role in the formation of the interface. Solid wetting layers are important as a new concept for the development of the theory of thin film growth, as well as a new object of nanotechnology for the production of thin-film nanomaterials.
Keywords: Solid wetting layers, Growth, Electronic and atomic structure, Nanomaterials, metal, Silicon
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