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Special Issue

New materials for micro-, nano-, and optoelectronics: properties, structure, and growth mechanisms

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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.

Currently, the majority of electronic devices are based on silicon. Silicon remains a fundamental material in the electronics industry. However, modern life requires an ever-increasing variety of devices that cannot be produced using only silicon for several reasons. First, silicon, as a semiconductor material, does not exhibit the desired physical properties. Second, it is only suitable for a certain range of devices, for example, silicon has an indirect bandgap, so it cannot be used to produce LEDs, lasers, etc. Moreover, silicon is not resistant to radioactive radiation, therefore, devices based on it cannot operate stably in high-radiation environments, such as outer space and nuclear power plants. In addition, devices produced using silicon cannot operate at high temperatures, and therefore require cooling. Silicon has also several other unavoidable disadvantages.

Modern life and the market require the creation of LEDs, semiconductor lasers, high electron mobility transistors (HEMT), gas control sensors and transmitters, microwave devices, next-generation pyro- and piezo sensors, optical switches, devices that emit and receive terahertz radiation, etc. Nowadays, there is also an urgent need for LEDs that emit hard ultraviolet radiation as well as ultraviolet radiation sensors.

For this reason we are currently focusing on the search for materials that can at least partially replace silicon. Such semiconductor materials include wide bandgap semiconductors: silicon carbide (SiC), gallium nitride (GaN), aluminium nitride (AlN), gallium oxide (Ga_2O_3), their solid solutions, and a number of other materials. These semiconductors have excellent electrical characteristics and can ensure the operation of electronic and optoelectronic devices at elevated temperatures and under high radiation. Semiconductor materials, such as SiC, AlN, GaN, and Ga_2O_3 , have wide bandgap. For example, gallium oxide is a new promising wide bandgap semiconductor with a bandgap $E_g \approx 4.9$ eV. This material has several physical properties that make it competitive with silicon carbide and III-nitrides. First of all, it is transparent in the UV spectrum and has a high breakdown voltage (8 MV/cm). In addition, Ga_2O_3 can be doped quite easily, which makes it possible to obtain highly conductive layers of this material. Zinc oxide (ZnO) is also a promising semiconductor owing to its potential use in thin-film transistors, LEDs, lasers, and photodetectors. It is a direct-bandgap semiconductor with a bandgap of 3.4 eV.

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Ferroelectric materials are also of particular interest to researchers. They are widely used in high-speed elements for static and dynamic memory, microelectromechanical systems (MEMS), infrared technology (IR), microwave electronics, piezoelectronics, and other modern high-tech devices. The main ferroelectric materials used in most chips and devices are solid solutions of lead zirconium titanate $\text{Pb}(\text{Ti},\text{Zr})\text{O}_3$.

In recent years, progress has been made in research on the growth and application of nanowhiskers of various compounds. Such structures have cross-sectional dimensions of 10–100 nm, and their length exceeds their diameter by an order of magnitude or more. Semiconductor nanowhiskers are promising for applications in microelectronics and optoelectronics, as well as in many other fields, such as cantilevers for probe microscopes, gas analyzers, etc. These nanowhiskers can be used to design field-effect transistors, photovoltaic cells, light-emitting elements, and other functional nanodevices.

Undoubtedly, diamond is one of the most promising materials for electronic devices, as it has a combination of the most important physical parameters. The electron mobility in diamond is about $2200 \text{ cm}^2/\text{V}\cdot\text{s}$, and the breakdown field reaches 107 V/cm . Diamond is chemically stable and insoluble in hydrofluoric, hydrochloric, sulfuric, and nitric acids. Diamond has the highest thermal conductivity of all known materials, about $22 \text{ W/cm}\cdot\text{K}$ at room temperature. Therefore, diamond can be a “perfect” heat-dissipating dielectric substrate. It is transparent over a wide spectral range (from ultraviolet to radio waves), has high hardness (81–100 GPa), and high sound velocity (18 km/s). Owing to these unique properties, diamond is promising for use as a heat sink in electronic devices. Diamond could also be widely used in the manufacture of high-power gyrotron and laser windows, as well as in the manufacture of various types of surface acoustic wave filters operating in the GHz range, and ionizing radiation detectors.

Graphene is expected to be a serious competitor to silicon for use in electronics in the future. It is most likely that graphene will be used in transistors to replace current metal electrodes, as the contact layer thickness in graphene is only 0.34 nm. However, to date, graphene-based

devices are still a distant prospect. Indeed, it is not yet possible to grow graphene wafers of a large size, and it is very difficult to control the conductivity of the graphene layers. In particular, the methods for producing semiconductors from graphene are still underdeveloped. Graphene is primarily used only as a conductor or insulator.

Boron nitride (BN) is another new, little-studied material. Thin, one-atom-thick layers of BN could be used in flexible electronics together with graphene. BN is an insulator with an energy bandgap of about 6 eV, whereas graphene exhibits metalloid properties. However, research on this material is still in its infancy.

For spintronic applications, various composite structures based on semiconductor and magnetic materials are of interest.

The issue includes fifteen articles focusing on the main development areas of modern materials science. Presented below is a brief overview of these articles.

The first article in this issue [1] reviews the theoretical approaches to the calculation of interfacial and surface energies of nanoparticles of various geometries depending on the particle size. It is well-known that the kinetics of the formation of nanoparticles largely depends on their interfacial energies. This is especially evident in nanoparticles, the radii of which are in the single digits of nanometers. The article [1] focuses on this problem.

Of particular interest is also the second article [2]. It presents a new unusual approach to the description of the structures of solids and their properties. The authors suggest a new approach to the foundation of thermodynamics and statistical mechanics. They argue that classical statistical mechanics does not take into account the finiteness of the speed of interaction between particles (atoms, molecules, etc.), i.e. classical statistical mechanics is essentially a non-relativistic theory. The authors of the article [2] suggest a new theory of interaction between particle ensembles and fields based on a relativistic approach. With non-relativistic approximation, interactions between atoms are instantaneous. Therefore, an atom and the instantaneous field created by it are a single entity with a finite number of degrees of freedom. With relativistic theory, every motion of an atom

(the source of the field) leads to the evolution of its field, the propagation velocity of which does not exceed the speed of light. Therefore, the evolution of the system of interacting atoms includes both the dynamics of particles and the dynamics of the relativistic field created by the atoms.

The next article [3] studies the elastic interaction between overlap defects of dilatation and disclination types in the approximation of the linear isotropic medium. The authors calculated the dependence of the interaction energies of such defects on the angle between them. This article is of interest for researchers focusing on the synthesis of new materials due to the fact that a combination of defects, in particular point defects, can both increase and decrease the elastic energy in nanomaterials.

The rest of the articles in the issue present the results of experimental studies. They can be divided into three groups. Articles in the first group [4-7] consider the growth of thin films and nanostructures based on gallium nitride compounds. Article [4] reports the growth of semi-polar GaN (11-22) layers using epitaxy from metal organic compounds on a nanostructured NP-Si (113) substrate. Optoelectronics devices are currently produced based on gallium nitride structures grown in a direction parallel to the c-axis of a hexagonal GaN crystal (polar structures). However, the use of polar structures for the creation of quantum size (QW) III-nitride based optoelectronic devices result in the Stark effect. It is caused by strong piezoelectric polarization in polar structures. The fact that there is no piezoelectric polarization in semi-polar structures presents new opportunities for the creation of new generation devices based on semi-polar (Al, Ga, In)N structures. This explains the significance of the study presented in the article. Articles [5, 6] focus on the growth of filamentary nanostructures InGa_xN and GaN. Article [5] demonstrates for the first time that composition-graded In_xGa_{1-x}N nanowires with x from 40 to 60% can be grown using plasma-assisted molecular beam epitaxy. The authors determined that the samples demonstrate photoluminescence properties at room temperature with a maximum at about 890 nm. This means that the material can be used to

create sources of near IR radiation. Article [6] is devoted to the confirmation of spontaneous doping of GaN nanowires grown on vicinal SiC/Si hybrid substrates. Singular Si facets did not demonstrate the same effect. Article [7] presents a detailed experimental analysis of the formation and growth of ordered arrays of nanocolumns of GaN microcrystals by means of plasma-assisted molecular beam epitaxy on profiled sapphire substrates. The authors demonstrated that there is a significant difference between the growth mechanisms of nanocolumns of GaN microcrystals under nitrogen enriched conditions and metal (Ga) enriched conditions. The article presents a detailed analysis of the processes which determine the kinetics of the growth of III-N nanocolumns by means of plasma-assisted molecular beam epitaxy on profiled sapphire substrates.

The next three articles [8–10] are dedicated to the growth of single crystals and films of a semiconductor compound Ga₂O₃. Gallium oxide is a wide bandgap semiconductor with a bandgap of $E_g \approx 4.9$ eV. This material has a number of physical properties which make it quite competitive with III-nitrides. First of all, it is transparent in the UV spectrum and has a high breakdown voltage (8 MV/cm). The articles included in the issue demonstrate that the area is of current importance and is actively developing. Thus, article [8] demonstrates the possibility to produce the heterostructure based on Ga₂O₃. Article [9] presents the results of the study of the mechanical properties and defect structure of single crystals of the Ga₂O₃, β -phase grown from a melt using the Stepanov technique. Article [10] presents a new technique for obtaining the three main crystalline phases of Ga₂O₃, namely the α -phase, the ε -phase, and the β -phase by means of chloride-hydride epitaxy. The experimental study described in the article determined the conditions for phase transformations from one Ga₂O₃ polytype to another.

It is well-known that ferroelectric materials are of great importance for modern technologies. Thus, thin films of lead zirconate titanate (Pb(Zr,Ti)O₃ or PZT), the composition of which corresponds to the morphotropic phase boundary region, are characterized by abnormally high electromechanical and piezoelectric coefficients

and are currently the most common materials used in microelectronics, electro-optics, and microelectromechanics (MEMS). PZT films are used in IR detectors and microwave electronics, as well as static and dynamic memory elements. The issue of the journal includes two articles which focus on the crystallization features of the thin-film heterostructure PZT-PbO_{1+x} [11, 12]. Article [11] shows that the annealing of amorphous PZT 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, which results in the formation of the perovskite phase. Article [12] describes a new phenomenon occurring in thin PZT films, anomalous electron channeling. This means that the electrons from a scanning electron microscope can penetrate along the planes of the crystal. The phenomenon is explained by the structural features of the crystallographic structure of PZT films.

Out of the last three articles in the issue [13–15] two articles are brief reviews [13, 15]. Article [13] reviews the use of cast glass-coated amorphous micro- and nanowires for the reinforcement of glass aimed at enhancing its mechanical strength. The article presents approaches to the creation of protection screens that can resist mechanical load as well as electromagnetic pulses of various nature. The article proposes ideas related to the technology of production of cast glass-coated amorphous micro- and nanowires.

Article [14] presents a theoretical study of the electronic structure of the tetragonal crystalline modification of germanium dioxide by means of a linearized augmented plane wave method. Germanium dioxide is a wide bandgap semiconductor used in optoelectronics, solar energy, and catalysis. Normally, germanium dioxide exists in two stable crystalline modifications: a hexagonal (quartz structure) and a tetragonal (rutile structure). The results obtained in [14] can be used to analyze experimentally studied specimens of the Ge–O system.

The last article [15] reviews several issues related to the growth of transition metal silicides on a silicon substrate. The review presents a classification of solid phases of metal silicides formed on a silicon substrate. Particular

attention is paid to the formation of wetting layers stabilized by a Si substrate. Some of their optical, electrical, and magnetic properties are described. The article points out that wetting layers play an important role in the formation of bulk phases, epitaxial nanofilms, and multilayer nanostructures.

A brief review of the articles demonstrates that the current issue of the journal covers practically all the main areas of modern semiconductor materials studies.

The editorial board is grateful to the authors for the submitted articles and their eagerness to share their latest advances in the field with the scientific community.

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