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# About This Book

This monograph consists of an introduction, 5 chapters and the list of reference. Chapter 1 is devoted to a review of experimental and theoretical works on defect formation in wide-band gap crystals, where ionizing effects at the surface–solid interface, surface defects in ionic crystals when exposed to electrons and ions, surface defects in wide-band oxide materials, luminescence bands in silicon dioxide, surface defects in zinc oxide crystal are given. Chapter 2 is devoted to the Measurement Methodology and experimental setup, which provides: TC spectroscopy, the design of the measuring device and its operating modes, the vacuum system and elements of the experimental setup, as well as additional methods for defect formation. Chapter 3 is devoted to the formation of defects and clusters on the surface of LiF crystals when irradiated with electrons and ions, where the following are given: the formation of defects and clusters on the surface of LiF crystals when irradiated with electrons; the formation of defects and clusters on the surface of LiF during ion irradiation; the effect of the bombarding ion mass on the formation of vacancies, interstitial and substitutional defects on the LiF surface. Chapter 4 presents the formation of defects and clusters on the surface of Si(111) and $SiO_x$ crystals when sputtered with electrons and ions, where the following are given: the TC spectra of the surface of Si(111) and $SiO_x$ crystals when irradiated with electrons and ions; the formation of defects and clusters on the surface of Si(111) crystals when sputtered with ions; annealing of defects and clusters on the surface of $SiO_x$ crystals. Chapter 5 presents: formation of defects and clusters on the surface of ZnO crystals under electron irradiation; TC spectra of poly—and monocrystals of zinc oxide; charging on the surface of poly and single crystals of zinc oxide under electron irradiation.

The monograph uses the results of scientific research conducted by the author jointly with the Physical—Technical Institute, Academy of Sciences of the Republic of Uzbekistan.

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# Introduction

## Unveiling the Future of High-Tech Materials

In a world where the boundaries of technology are ever-expanding, the quest for high-tech materials with unparalleled surface properties has taken center stage. These materials, critical for the advancement of microelectronics, optoelectronics, and even space science, possess unique surface characteristics that set them apart from their bulk counterparts. This narrative embarks on an exploration of the cutting-edge domain of defect formation in wide-gap materials when exposed to atomic particles—a journey fueled by the global demand for innovation in key technological sectors.

The spotlight shines on the intricate dance of atoms and electrons, revealing how their interactions at the surface level can significantly influence material performance. This discourse delves into the heart of nanoepitaxy and the quest to understand the mechanisms behind material irradiation effects, where the formation and migration of defects under the influence of low-energy particles become pivotal. Such insights are not just academic; they are the bedrock upon which the next generation of micro- and optoelectronic devices, from waveguides to photodetectors, will be built.

Venturing further, we discover how the world's scientific community is making significant strides in this arena, studying the transformative effects of defects throughout a material's structure. Their work underscores the importance of mastering defect engineering to tailor surface properties for specific technological applications. It's a testament to the global collaboration and innovation driving forward the study of wide-gap crystals—a key element in the development of new microelectronic devices.

This introduction is not merely a prelude but an invitation to embark on a fascinating journey through the world of materials science. It promises to unravel the mysteries of defect formation and its implications for the future of technology, setting the stage for a deep dive into a realm where science meets innovation.

Join us as we venture into the detailed exploration of how surface defects in wide-gap crystals are shaping the future of technology, guided by groundbreaking research and international collaboration. This is the threshold of a new era in materials science, where the manipulation of microscopic defects opens up a universe of possibilities for technological advancement.

On a global scale, high-tech materials are subject to requirements that imply the presence of special surface properties with special performance characteristics, in contrast to bulk ones. Interest in inelastic processes of defect formation in the near-surface region of wide-gap materials exposed to atomic particles is constantly growing due to the wide use of these materials in micro and optoelectronics, space materials science, and other fields of science and technology. Therefore, investigations aimed at establishing the nature of the processes of modification of the surface properties of materials upon bombardment with electrons and ions are important.

Today, interest in defect formation in the world is associated with solving problems of nanoepitaxy, obtaining information about the mechanism of interaction of irradiation with the surface of crystals and thin films. Wide-gap crystals and surface defects arising upon irradiation with low-energy electrons and ions are topical for surface physics. The most important task is to study the properties of thin films during their growth, adsorption, and coalescence, since the formation of defects and their migration over the surface during irradiation and annealing significantly affect the properties of the resulting surface. Also, the connection between surface defects and the processes of cluster sputtering of the surface of crystals is poorly understood and requires experimental and theoretical research. The volume and speed of information transmission is growing every day, which is determined by the need to create micro and optoelectronic devices and devices based on wide-gap crystals: waveguides, splitters, sensors for everyday use, modulators, and photodetectors. Until recently, the weakest point of microelectronics has been the lack of information and neglect of defects on the surface during ion implantation, diffusion, and other technological processes. The latter speaks of the use of defect engineering to create conditions for obtaining a surface with desired properties.

In the world, research work is underway on this topic, in particular, the study of defects in the structure of dielectrics throughout the volume, where the material is irreversibly amorphized, and the crystal structure changes significantly. When developing new microelectronic devices and devices based on wide-gap crystals, they face a fundamental problem: defects created in the near-surface region either stimulate the processes of obtaining p-n junctions or suppress them. In this regard, certain types of surface defects are of considerable interest, which were used in defect engineering—radiation-stimulated diffusion, planar epitaxial method and implantation, to obtain p-n junctions. Thus, the study of surface defects in wide-gap crystals is a priority and an urgent task in the field of modern materials science, which is engaged in the search and creation of materials for the element base of new generation microelectronic devices, the principle of operation of which is based on the manipulation of defects to change the surface and bulk properties of a material under the action of an electron beam and ion irradiation.

Review of foreign scientific research on the topic of the monograph. Scientific research in the field of defect formation and surface analysis of various substances, as well as studies of physicochemical processes occurring on the surface of a solid body, are carried out in leading centers, in higher educational institutions, including: St. Petersburg State University, laboratory of electronics of the surface of a solid body (Russia), Shanghai University, School of Materials Science and Engineering (China), in scientific laboratories of the Institute of Solid State Physics of the Latvian Academy of Sciences and the GSI Helmholtz Centre for Heavy Ion Research Materials Research Department and Technical University Darmstadt (Germany), the University of Copenhagen, Department of Physics (Denmark), and at the Institute of Nuclear Research of the Academy of Sciences of the Republic of Uzbekistan.

In the direction of research into defect formation on the surface, including in wide-gap crystals, a number of topical problems were solved at the world level and the following most important scientific results were obtained:

Based on radiation-resistant ZnO crystals, Schottky photodiodes were created for dosimetry of UV radiation. In particular, studies of laser generation in wide-gap heterojunctions were carried out by many scientists of the world, American (Schrier, A. P. Alivisatos), Russian (Zh. I. Alferov, P. V. Ivanov), Chinese (P. Chen, Y. Wang), Uzbek (E. M. Ibragimova, P. Kurbanov) and other specialists.

Currently, a huge amount of research is being carried out in the world on the development of devices and the development of methods for the formation, detection and analysis of defects on the surface of wide-gap crystals. Also, studies of the physicochemical parameters of the surface of wide-gap crystals are relevant in the following areas: the processes of purification and adsorption of atoms on the surface of a solid body; development and creation of certain types of surface defects that will be used in defect engineering—radiation-stimulated diffusion, planar epitaxial method and implantation, to obtain p-n junctions; revealing the physical and chemical properties of the surface during defect formation.

However, the following detailed studies have not been carried out: the state of the surface and electronic structure, the effect of various types of irradiations on the formation of defects on the surface, the relationship between charging and surface stoichiometry, oxygen concentration, the role of surface defects in the physicochemical processes of oxidation and purification of samples, the possibility of creating p-n transitions using radiation-stimulated diffusion of defects.

All over the world, in promising areas, in particular, in planar technology, in microelectronics, in optoelectronics, in modern materials science, in nanotechnology of low-dimensional systems, research work is being carried out to study defect formation in wide-gap crystals.

Most of the research related to defect formation was carried out by K. Schwartz, Popov A. I., Lushchik Ch. B., and Lushchik A. Ch. when irradiated with electrons and ions of high (MeV) energies. Therefore, an experimental study of defect formation on the surface of solids under irradiation with low-energy (sub-keV) electrons and ions is relevant for elucidating the mechanisms of the formation of point and aggregate defects with their subsequent coagulation into aggregate centers. An analysis of the works shows that almost the vast majority of works are devoted to the study of defect formation based on bulk crystals (Zakis Yu. R.), while several works are devoted to a comprehensive study of the conditions for the formation of point defects based on irradiated films of ionic crystals (Ch. Trautmann, Golek F., Sobolewski W. J.). Currently T. T. Basiev, L. N. Demyantsev determined that for the successful application of film lasers, it is necessary to increase the concentration and stability of aggregate defects by 2–3 times. Such a significant increase in efficiency requires new studies of the mechanism of formation of point defects and their aggregates, near-surface regions, in which the most important processes of excitation of the lattice of wide-gap crystals by slow electrons and ions occur.

The processes of defect formation on the surface of semiconductor samples of zinc and silicon oxide are little studied. This is due to the difficulty of obtaining point defects on the surface of single-crystal semiconductor substrates. It is also necessary to develop surface-sensitive methods for detecting point defects in single-crystal semiconductor substrates. The processes of defect formation on the surface of wide-gap crystals under irradiation with low-energy electrons and ions are at the stage of preliminary study. Therefore, a comprehensive study of the conditions for the formation of point defects and their aggregates based on wide-gap crystals is an urgent scientific and practical problem.

At the same time, many aspects of the mechanisms of defect formation on the surface remain unclear to this day. The potential sputtering in dielectrics, which was studied independently by Sh. P. Radjabov and F. Avmaur, what "stimulates the sputtering" "Coulomb explosion" or "Sputtering stimulated by defects"?

There are a number of scientific and technological problems, such as the effect of surface defects on sputtering, cleaning, charging, oxidation, etc., which can contribute to changing ideas about the processes of surface defect formation, theoretical models, and mechanisms.

These as well as a number of problems that have not been solved to date, the influence of temperature, kinetics, mass and charge of primary ions concerning the formation of defects on the surface of wide-gap crystals under electron and ion irradiation, served as an incentive for research, the results of which formed the basis of this monograph.

In this monograph considering is to determine the patterns of formation of surface defects in wide-gap crystals under electron and ion irradiation, as well as to establish the relationship between defects and surface states and other physical processes occurring on the surface. The motivation behind research work is rooted in the critical role of surface defects in determining the material properties of wide-gap crystals, which are pivotal in applications ranging from optoelectronics to photovoltaics. The monograph attempts to bridge theoretical understanding and practical applications, illustrating how surface defect manipulation can enhance material performance in relevant technological fields.

## Research Objectives

- $SiO_x$ and LiF crystals by the method of TC spectroscopy under electron and ion bombardment;
- study of the formation of surface defects in the LiF/Si(111) system during electron bombardment;
- study of the formation of surface defects in the LiF/Si(111) system and their effect on sputtering during ion bombardment;
- to study the formation of defects and their clusters on the surface of $SiO_x$ crystals during bombardment with electrons and ions;
- study of the influence of the formation of defects on the surface of $SiO_x$ crystals on the processes of purification and oxidation during bombardment with electrons and ions;
- perform experimental studies and determine the thresholds for the formation of surface defects in ZnO during electron bombardment;
- study of the influence of the formed negative charge during electron bombardment and the formed defects on the surface states in ZnO.

**The objects of study** are samples of wide-gap crystals of lithium fluoride, silicon, and zinc oxides.

**The subject of the study** is the stimulation of surface states by electron and ion bombardment, which makes it possible to obtain a defective and modified surface of the samples under study, as well as patterns of defect formation, and physical mechanisms, analytical relationships and mathematical models that reflect the process of influencing surface states, device parameters, operating modes and indicators, and the laws of their change.

**Research methods.** The TC electron spectroscopy method makes it possible to obtain quantitative information about radiation defects. To clarify the role of defects and the state of the surface in the sputtering processes, comparative studies were carried out by the method of SIMS, and the simulation of the processes of ion bombardment of crystals was carried out using the SRIM software package. The methods of mathematical statistical analysis, DFT, determination of the degree of error, planning of experiments, as well as the methods specified in the current regulatory documents were also used.

**Practical study results** are as follows:

- The technique for determining defects in a secondary cluster by mass spectra, which undoubtedly play an important role in the field of physical electronics, makes it possible to detect defects during crystal sputtering.
- The proposed method of ion etching followed by annealing at a temperature of 650 °C makes it possible to obtain an atomically clean silicon surface.
- A certain kinetics of silicon surface oxidation due to ODCs makes it possible to effectively monitor the thickness of the MIS structure in sample preparation processes, which undoubtedly play an important role in the field of microelectronics.