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• PREFACE •

Perfect crystals are very well described by Bloch waves, but for real materials, even when highly regular, a variety of flaws exist, e.g. defects, such as substitutional and/or interstitial impurities, lattice vacancies, self-interstitials, dislocations, and complexes or aggregates of these entities. Many of these defects have been identified at the atomic level with the aid of EPR/ENDOR and IR measurements, coupled with uniaxial stress measurements, and of HRTEM studies. Even with such a detailed understanding of defects it is still not possible to treat the full complexity of the problems encountered experimentally. Fortunately, as described by P.W. Anderson [*Phys. Today*, 44, No. 7, 1991, pp. 9-11], the Science of Complexity has arisen as needed, with by his reckoning, broken symmetry, localization, fractals, and strange attractors coming to the fore. To these we would add: negative-U phenomena and a variety of metastabilities, motionally-averaged states, charge-state-sensitive properties, and ionization and defect-enhanced processes, e.g. athermal diffusion in the presence of ionization and the broad new understanding of nonlinear equations, such as govern defect processes, whose understanding falls under the rubric of Catastrophe Theory and Chaos. Several aspects of Complexity Theory are beginning to have a major impact on the understanding of diffusion, etching and damage processes. This book initiates the task of bringing some aspects of Complexity Theory to bear on the fascinating, multifaceted phenomena of amorphization-crystallization of semiconductors during ion implantation.

Studies of radiation damage, disorder and amorphization in semiconductors are almost forty years old and are extensive. There are excellent books on radiation defects, ion implantation and the amorphous state of semiconductors, in which different sides of these problems are examined. However, there seemed to be no work that developed enough of the intimate relationships between processes in irradiated semiconductors and non-equilibrium kinetics and non-equilibrium phase transitions to enable researchers to understand exactly how much new details of radiation processes in semiconductors can be found from the *synergetics* approach and to understand what are the limitations of the old theories and approaches in radiation physics of semiconductors.

In the last fifteen years it has become more and more evident that there exist numerous examples in physical, chemical, biological and engineering systems where spatial, temporal, or spatial-temporal structures arise out of chaotic states. These phenomena occur in systems in which there is an exchange of energy and matter with the an environment, and these structures develop spontaneously and are self-organizing. In addition to thermodynamic instabilities, in such systems one can expect so-called *kinetic phase transitions* that is the subject of study in the interdisciplinary, new science named *synergetics* first introduced by Herman Haken. It was shown in synergetics that numerous systems display striking similarities in their behavior when passing from the disordered to the ordered state and *visa versa.* This fact indicates that the functioning of these systems obey the same general principles.

During the processes of irradiation of semiconductors one can observe a number of analogies with phase transitions under thermodynamic equilibrium: from coagulation processes to the formation of different phases with different physical properties and with a well-defined sharp boundary. On the other hand, some features have been observed that are associated with systems far from equilibrium, e.g. phase transitions stimulated by an external beam of energy and matter, such as ion-beam-induced amorphization and crystallization, formation of quasi-periodical distributions of defects and impurity atoms, jump-similar processes, etc. A review of some experimental results in radiation physics of semiconductors shows that the processes of disordering, defects evolution, transformations of defect-impurity subsystem of irradiated semiconductors, transitions to a new states, for example amorphization, have a similar nature as other non-equilibrium systems in biology, chemistry, electronics, etc. Accordingly, we believe that the application of the scientific ideology, approaches, methods and mathematical tools, which are now widely used for the analysis of phenomena in open systems, will be useful in the field of study of disorder in the irradiation of semiconductors. The study of the evolution of radiation damage from the synergetics point of view is a new branch of radiation physics of semiconductors.

In this book we have tried to introduce a new scientific ideology for known phenomena, and we have attempted to show, in brief form, how some results of radiation physics of semiconductors, for example processes of disordering and amorphization, can be consider from the synergetics point of view and how we can apply these concepts and mathematical tools to derive something new, that we never would have expected using traditional methods. This book is not just a review publication nor is it a purely research work. It is something in between. We have not tried to include a catalogue of all phenomena in irradiated semiconductors which can be consider as a subject of analysis from the synergetics position, but we have selected some typical and important examples. We feel that it is unnecessary in this book to present all the details of the mathematics and analytical methods (for example, the theory of fractals or the theory of nonlinear differential equations and stability analysis), that scientists are now using for the study of non-equilibrium objects, because it is readily available in the cited literature, that presents these mathematical methods more systematically than it is possible and necessary here. We do not introduced the whole picture of non-equilibrium phenomena in irradiated semiconductors, because we do not yet have the complete picture. But, in our view, the requisite tools are available to achieve it. This book attempts to show the directions of this new field and was written for scientists who would like to become involved and familiar with present ideas and who realize that much remains to be done in understanding the disorder and transformations of defect subsystems of irradiated semiconductors, i.e. semiconductors under conditions far from equilibrium.

It is a pleasure to thank our colleagues and friends for many fruitful discussions, for making valuable suggestions and for providing a stimulating environment. Especially, we would like to thank Professor Andrew J. Yencha for his enormous help in the reading and editing of this manuscript, Professor John C. Corelli for discussion of some chapters and Dr. Vladimir V. Tsukanov for his aid in discussing Chapter 6. We wish to thank Ms. Marlyn E. Thayer for her help with technical questions, Ms. Marilyn A. Peacock for assistance with the figures and Ms. Barbara M. Haws for her superior secretarial skills. And, of course, we thank our wives for their patience and support.

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INTRODUCTION

In this book we present and discuss in some detail the basic ideas and some experimental results in the physics of radiation damage, including results describing the accumulation and transformation of defects during ion implantation, amorphization, and ion-beam-induced crystallization of amorphized layers of semiconductors. All these phenomena are very interesting scientifically and practically. As we stressed in the Preface, the main goal of this book is to show that many processes in irradiated semiconductors, including amorphization, can be considered from the synergetics point of view, i.e. as processes similar in character to kinetic phase transitions observed in other non-equilibrium phenomena. We will show that the problem of stability is very closely related to the problem of ion-beam-induced transformations in disordered semiconductors. Whenever it is possible, and to preserve continuity, we shall illustrate this fact using experimental results from the physics of radiation damage, and we will apply the scientific ideology of synergetics to this field. Therefore, it will be useful if the reader is familiar with some of the basic concepts of synergetics and with some of the associated mathematical methods, such as analyses of stability of solutions for kinetic equations, and stochastic methods in physics before beginning this book. Very little attention will be given here to the basics of the theory of non-equilibrium phase transitions, but we will widely use the terms, concepts and methods from this field. Accordingly, we recommend that the reader obtain a primarily and an elementary knowledge of this subjects in the very interesting and easy-to-read book by Herman Haken: *Synergetics: An Introduction*.

When energetic particles, such as electrons, ions, etc., enter a semiconductors lattice, defects in that lattice may be created. We shall consider in this book those aspects of these defects that are related to chaos and pre-chaos, and to losses of stability, i.e. the nonlinear behavior of the defects, including the formation of new phases, for example the amorphous phase, which is of special interest to us. In the first Chapter we briefly review the different types of defects, their properties and interactions, and will discuss some of the properties of the amorphous state of semiconductors, focusing our attention on this last subject, which will be necessary in the following Chapters.

In Chapter 2 we give a brief overview of the experimental results for the process of amorphization of crystalline semiconductors under irradiation and the traditional (classical) theoretical approaches (both heterogeneous and homogeneous) used to describe such processes. Only on the basis of these models and theories and the experimental results is it possible to make new advances towards an understanding of the problem of amorphization in terms of stability and non-equilibrium phase transitions.

Ion implantation in semiconductors exhibits a rather unusual dichotomous behavior. On the one hand implantation results in disordering in crystalline semiconductors, up to complete amorphization, but on the other hand also to ordering of amorphized layers, which is ion-beam-induced crystallization. Chapter 3 deals with this latter phenomenon where we consider such transformations from the position of synergetics. It is shown that the processes of amorphization and ion-beam-induced crystallization, as a whole, can be describe in the terms of non-equilibrium phase transitions, and that analogies are deeper than just superficial likenesses.

Many results in the physics of radiation damage and their transformations may be termed "anomalous radiation effects", because they cannot be explained or describe in a traditional way by the application of conventional approaches to the radiation physics of semiconductors. Some of these "anomalies" are introduced and critically discussed in Chapter 4. We show that in the case of irradiated semiconductors we already have the basic features of open systems and that all processes characteristic of a whole class of non-equilibrium systems in chemistry, biology and physics, including the loss of stability and formation of dissipative structures, are possible in semiconductor system under irradiation.

The system of radiation defects exhibits a feature common to other non-equilibrium objects in that its analysis requires a specific time-dependent model. In the former, this model must be established after a careful examination of the defect formation process and defect-impurity interactions on a case-by-case basis for each combination of "implanted ion + semiconductors target". In many cases, as we show in Chapters 2-4, the effects of defect transformations can be consider as a loss of stability and the evolution of the instabilities can be the reason (i) for the formation of new regimes of relaxation of defects, (ii) for the formation of new distributions of defects and impurities, and (iii) for the formation of new states - the amorphous state, in particular. Accordingly, in Chapter 5 we discuss ways to study the evolution of radiation defects in terms of stability. We introduce some methods by which it is possible to find some combinations of external and internal parameters that result in the loss of stability and the formation of a new state dramatically different from the initial state. Chapter 5 also develops further the ideas of the role of diffusion, in combination with the local quasi-chemical interactions between defects, in the of evolution of radiation damage. In addition, in Chapter 5 we briefly discuss the question of dimensionality related to the defect-transformation phenomena and introduce several schemes of interactions between defects for which instability regimes can arise under some conditions of critical combinations of a kinetic parameters.

Based on those ideas and on analyses of the previously discussed material, in Chapter 6 we introduce the main steps for modeling of processes of ion-beam-assisted amorphization-crystallization of semiconductors from the point of view of the theory of non-equilibrium phase transitions and stochastic processes. We show, using the ideas of synergetics, how we can construct some approach that can be a basis for a complete qualitative and quantitative description of amorphization and related phenomena in radiation physics of semiconductors.

In our Closing Remarks we briefly introduce some systems for which the new concepts put forth in this work can be applied.

CHAPTER 1

RADIATION DAMAGE, DEFECTS AND THE AMORPHOUS STATE IN IRRADIATED SEMICONDUCTORS

1.1. Introduction

When energetic particles enter a semiconductor lattice, defects in that lattice may be created, which may be electronic (e.g. non-equilibrium electrons and holes), or structural (e.g. lattice vacancies and interstitials, their complexes, dislocation loops, etc.), and atoms of chemical impurities which may be introduced in the case of ion implantation. We shall consider in this book the aspects of these defects which relate to chaos and pre-chaos, i.e. the non-linear behavior of the equations describing these defects, including the formation of new phases. There have been a number of conferences, reviews, and books about properties of single defects produced in semiconductors by an external beam of electrons, X-rays, neutrons, and ions since the microscopic study of defects began [1-27]. We will briefly review these defects, their properties and interactions in Section 1.4; we will focus on defects in silicon, which are more fully documented than are defects in other systems. First, however, in Section 1.2 we will briefly review how energy is lost by energetic particles impinging on a semiconductor, and, then in Section 1.3, we will describe how defects are produced by an external beam of energetic particles. In Section 1.5 we will review some properties of the amorphous state of semiconductors concentrating our attention on the subjects which will be necessary for the following chapters (in particular, for an understanding of the model of amorphization presented in Chapter 6). In Section 1.6 we will summarize the conclusions of this Chapter.

1.2. Mechanisms of Energy Loss

In general, when high-energy ions penetrate a solid they lose energy in two ways:

1. Ionization, which is the dominant energy loss mechanism, and
2. Energetic nuclear (Rutherford) scattering events, which give rise to displacement damage.

For an ion incident on a solid in a random direction, the rate of energy loss is given by [28]:

$$-\frac{dE}{dx} = 2\pi \cdot e^4 \cdot Z_1^{\,2} \cdot Z_2 \cdot N \cdot \frac{M_2}{m} \cdot \frac{1}{E} \cdot \ln \frac{4 \cdot E}{I}, \qquad (1.1)$$

where Z_1 and Z_2 are the atomic charges of incident and lattice atoms, respectively, N is the atomic density of the lattice, M_2 is the mass of lattice atoms, m is the mass of the electron, E is the energy of the incident ion and I is the mean ionization potential of the lattice atoms, which is approximately equal to $8.8 \cdot Z_2$ for all elements except the lightest. The value of I, in the general case, should be energy dependent in that it is an average over the electrons of each atom in the solid. By dividing the energy loss by the approximate mean ionization potential and by the atomic density we can express these results in terms of a cross section per atom, which will facilitate comparison to other cross sections; typical ionization cross-sections are atomic in size ~ 10^{-16} cm^2.

We note that this ionization energy loss is not correct for low-energies, because the moving ions begin to capture and lose electrons from the solid, and its effective charge fluctuates. There has been extensive work calculating the energy loss in the low-energy region. Robinson [29] has critically reviewed the main theories in this area: the Lindhard theory [30] and Firsov theory [31]. Both theories give a good approximation to the low-energy results, but in detail there remain some difficulties concerning the dependencies of electronic stopping power on velocity and on Z_1 and on Z_2. The results of investigations on these subjects have been surveyed [32-34] in detail.