AMORPHOUS SEMICONDUCTORS

Understanding the structural unit of crystalline solids is vital in determining their optical and electronic properties. However, the disordered nature of amorphous semiconductors, where no long-range order is retained, makes it difficult to determine their structure using traditional methods. This book shows how computer modeling can be used to overcome the difficulties that arise in the atomic-scale identification of amorphous semiconductors.

The book explains how to generate a random structure using computer modeling, providing readers with the techniques to construct realistic material structures. It shows how their optical and electronic properties are related to random structures. Readers will be able to understand the characteristic features of disordered semiconductors. The structural and electronic modifications by photon irradiation are also discussed in detail. This book is ideal for both physicists and engineers working in solid state physics, semiconductor engineering, and electrical engineering.

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To my wife, Szabina, and our children, Szilvia and Zsófia

SK

To my wife, Akiko, and our children, Tetsuro, Shoko, and Ryo

KS

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Preface

Understanding the structural unit of crystalline solids is vital in determining their optical and electronic properties. Determination of the structure of a condensed phase without periodicity is not an easy task. An important objective of the book is to provide an introduction to the reader of how to construct computer modeling of realistic random structures of amorphous IV- and VI-column-element semiconductors and their alloys. Both the merits and drawbacks of the techniques currently used to generate structures using powerful computers are discussed. Furthermore, the structural, electronic, and optical properties of mostly sigma-bonded amorphous semiconductors can be learned.

The basis of this monograph was a course given by Sándor Kugler (SK) during several years at Budapest University of Technology and Economics (and other universities in Europe and Japan), with an extension by Koichi Shimakawa (KS). Our common research experience with amorphous semiconductors extends back more than twenty years. The book is aimed at final-year university students and PhD students in physics, materials science, and chemistry who have already completed introductory courses on quantum mechanics and solid state physics. This book will be useful for both physicists and engineers working in solid state physics, semiconductor engineering, and electrical engineering. For most of the text, no high-level mathematics is needed. This book provides a much wider literature overview than is usual for most handbooks.

A historical overview and a detailed summary of applications are given in the first part of Chapter 1. Readers are informed how to develop further the current technology (photovoltaic cells, thin-film transistors, DVDs, and direct x-ray image detectors for medical use, etc.) using amorphous semiconductors. The rest of the chapter analyzes and answers one of the most exciting questions in the field: what are amorphous semiconductors?

This is followed by a discussion of preparation techniques in Chapter 2. As the glass-transition temperature determines most of the physical properties of glasses, it is briefly discussed, together with Phillip's constraint theory of glassy materials, at the end of the chapter.

The third and longest chapter begins with an important topic, namely how to determine experimentally whether a sample has an amorphous or crystalline phase. The chapter describes atomic-scale computer modeling, including atomic interactions, different simulation methods, and models obtained by structure simulation. The final part of Chapter 3 introduces readers to the most successful commercialized product of chalcogenide glasses, the phase-change materials.

Chapter 4 deals with the electronic behavior of covalently bonded amorphous semiconductors, including defect-free systems and deviation from the ideal networks, i.e. defects. Optical properties of amorphous semiconductors are also described in this chapter.

Chapter 5 presents experimental results of photoinduced changes. It is shown that the structural studies by means of atomic-scale computer simulations are very useful for understanding the experimental results. The photoinduced changes observed in both amorphous chalcogenides and hydrogenated amorphous silicon films are discussed.

We, SK and KS, would like to thank Kazuo Morigaki for introducing us to the physics of amorphous semiconductors. Thanks are also due to Jai Singh (University of Charles Darwin), S.O. Kasap (University of Saskatchewan), Keiji Tanaka (Hokkaido University), Ted Davis (University of Leicester), Stephen Elliott (University of Cambridge), and Takeshi Aoki (Tokyo Polytechnic University) for their powerful discussions. We must also thank Tokyo Polytechnic University (formerly the Tokyo Institute of Polytechnics) for allowing us to use their computing facilities for our large-scale computer simulations.

SK is indebted to many of his colleagues at the Budapest University of Technology and Economics, but he is especially grateful to his four PhD students, Krisztina Kádas (Uppsala University), Krisztián Koháry (University of Exeter), József Hegedüs (University of Helsinki), and Rozália Lukács (Norwegian University of Life Sciences). Furthermore, SK extends his thanks to István László and László Pusztai, with whom he has had the pleasure of working on diverse aspects of research on amorphous semiconductors. Special thanks are also due to Károly Härtlein (Budapest University of Technology and Economics) for his careful work in drawing some of the figures.

KS wishes to thank his colleagues at Gifu University, Shuichi Nonomura and Takashi Itoh, for discussions, and also his PhD student, Yutaka Ikeda (YM systems, Company Executive), who developed a precise measurement system for the photoinduced volume change observed in amorphous chalcogenides. Discussions with Alex Kolobov (Advanced Institute of Industrial Science, Tsukuba), Hiroyoshi Naito (Osaka Prefecture University), Hideo Hosono (Tokyo Institute of Technology), Takashi Uchino (Kobe University), Masaru Aniya (Kumamoto University), and Sergei Baranovskii (University of Marburg) were also very fruitful and enjoyable in promoting our subjects.

Tomas Wagner and Miloslav Frumar (University of Pardubice) provided KS with the opportunity to continue the research work at the Department of General and Inorganic Chemistry (University of Pardubice), after his retirement from Gifu University, supported by grant project CZ.1.07/2.3.00/20/0254 *ReAdMat* financed by the European Union. KS wishes to express his thanks for this opportunity.