Physics of Disordered Materials

Institute for Amorphous Studies Series

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PHYSICAL PROPERTIES OF AMORPHOUS MATERIALS

Edited by David Adler, Brian B. Schwartz, and Martin C. Steele

PHYSICS OF DISORDERED MATERIALS

Edited by David Adler, Hellmut Fritzsche, and Stanford R. Ovshinsky

TETRAHEDRALLY-BONDED AMORPHOUS SEMICONDUCTORS

Edited by David Adler and Hellmut Fritzsche

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Physics of Disordered Materials

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To
Sir Nevill Mott
with respect and affection on the occasion
of his eightieth birthday

PREFACE

This volume and its two companion volumes, entitled Tetrahedrally-Bonded Amorphous Semiconductors and Localization and Metal-Insulator Transitions, are our way of paying special tribute to Sir Nevill Mott and to express our heartfelt wishes to him on the occasion of his eightieth birthday. Sir Nevill has set the highest standards as a physicist, teacher, and scientific leader. Our feelings for him include not only the respect and admiration due a great scientist, but also a deep affection for a great human being, who possesses a rare combination of outstanding personal qualities. We thank him for enriching our lives, and we shall forever carry cherished memories of this noble man.

Scientists best express their thanks by contributing their thoughts and observations to a Festschrift. This one honoring Sir Nevill fills three volumes, with literally hundreds of authors meeting a strict deadline. The fact that contributions poured in from all parts of the world attests to the international cohesion of our scientific community. It is a tribute to Sir Nevill's stand for peace and understanding, transcending national borders.

The editors wish to express their gratitude to Ghazaleh Koefod for her diligence and expertise in deciphering and typing many of the papers, as well as helping in numerous other ways. The blame for the errors that remain belongs to the editors.

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INTRODUCTION

David Adler, Hellmut Fritzsche, and
Stanford R. Ovshinsky

This volume, one of three in this series presented as a Festschrift in honor of the eightieth birthday of Sir Nevill Mott, is devoted to the physics of disordered systems. The effects of disorder on the physical properties of materials has long been an interest of Sir Nevill, and his contributions permeate the field. We now speak of the Mott 8-N Rule, Mott variable-range hopping, Mott excitons, and the Mott minimum metallic conductivity, among many, many others. The present volume consists of 65 papers by 116 authors from 18 countries throughout the world. It is divided into six parts.

Part One is concerned with general overviews of the nature of disordered systems. It begins a contribution by Weaire and Wooten dealing with the origin of random networks, one by Zallen discussing current models in which glass structure is analyzed by projecting from a higher dimensional space, and one by Joannopoulos reviewing the progress being made in an area once considered to be beyond the scope of our analytic ability, viz. predicting the lowest-energy structure of a given collection of atoms. Next, Ovshinsky provides further insight into the structure of amorphous solids by analyzing the degrees of freedom available to an atom upon deposition as well as the interplay of chemistry and processing conditions. In addition, Thorpe discusses glass structure from the point of view of percolation of flexible units until a rigid network forms, and Edwards and Vilgis present a model in which the glass transition marks the point at which the diffusion constant vanishes. Taken together, these six papers provide great insights into the philosophy as well as the physics of disorder.

Part Two consists of 17 papers relating to the structure, both global and local, of disordered systems. It begins with a general discussion by J.C. Phillips of quasi-phase-transitions in glasses, followed by a simple, elegant explanation of the heretofore mysterious first diffraction peak observed in glassy solids by Moss and Price. Then, Plischke et al. theoretically analyze the structure of a heterogeneous fluid, Sadoc provides an elementary introduction to the curved-space models of disordered systems, and Popescu demonstrates how computer simulations have increased our understanding not only of the

structure of amorphous solids but also of the photostructural changes that often characterize them. Stern discusses how the extended X-ray absorption fine structure (EXAFS) technique can be and has been used to determine the structure of disordered materials, while Bienenstock et al. review the progress attained from synchrotron radiation studies in general. Galeener and Lannin both analyze the advances that have emerged from recent Raman-spectroscopy studies, the former developing a model predicting the observed regular ring structures in amorphous SiO_2 and related glasses, the latter considering the effects of annealing from the viewpoint of variable order. Next, Greaves et al. describe the effects of Fe modification of a chalcogenide glass, Feltz looks at disordered systems as resulting from disproportionation, Chopra and Malhotra review the unusual light and particle induced densifications of up to 40% that characterize certain obliquely deposited chalcogenide alloys, and de Gennes analyzes the state of water in a partially filled porous structure such as rock from a modern point of view, making use of fractal dimensions over particular length scales. The free energies of defect structures in nonstoichiometric oxides are estimated by Stoneham et al. using a combination of both new methods and the technique pioneered by Mott and Littleton almost a half-century ago, while Vardeny et al. describe the new understanding of disorder in polyacetylene that has been obtained from Raman studies. Finally, Pantelides et al. investigate the thermal creation of localized amorphous regions in crystalline silicon, and Regel and Glazov calculate the electronic entropy changes upon the melting of a crystal. These papers together constitute an up-to-date review of the immense progress in understanding the structure of disordered materials that has occurred over the past few years.

Part Three contains 15 papers relating to electronic structure and transport. In the first two contributions, Adler reviews the current understanding of these subjects in amorphous semiconductors in general and in hydrogenated amorphous silicon in particular, paying particular attention to the remaining unsolved problems, while Cohen et al. describe some recent progress in attaining a rigorous theoretical basis for resolving these problems. Next, Cody and Mattis both discuss optical absorption in amorphous semiconductors from somewhat different viewpoints, and Cyrot-Lackmann and Pavuna review the theory of electronic structure in liquid and glassy transition-metal alloys. Eagles then analyzes the temperature dependence of the effective mass in transition-metal oxides in which the carriers form both large and small polarons, while Schlenker reviews the evidence for bipolarons in the same class of materials. Several theoretical contributions follow. Rose presents a simple formalism for understanding electronic mobility in all solids, and Movaghar and Friedman each analyze the Hall effect in disordered materials, the often anomalous sign of which remains one of our most perplexing problems. The effect of long-range potential fluctuations on transport are then discussed by Pistoulet et al. and an analysis of magnetoresistance in materials for which Mott variable-range hopping transport predominates is carried out

by Kamimura and Kurobe. Finally, Hauser describes the problems in understanding the ac loss mechanisms in amorphous semiconductors, Tiedje presents a new approach for analyzing capacitance measurements in materials characterized by exponential band tails, based on the use of a frequency-dependent screening length, and Mackenzie and Nasu review the transport mechanisms in transition-metal oxide glasses. The message which permeates this section is the necessity for further work before we can consider the electronic structure of disordered systems to be well understood.

The 18 papers of Part Four are all concerned with the origin, structure, and effects of defects in disordered semiconductors and insulators. The initial one by Abkowitz presents evidence that defects in chalcogenide glasses are thermodynamically induced and frozen in at the glass transition temperature, T_g , a hypothesis initially suggested on theoretical grounds without experimental verification. Next, Balkanski analyzes the results of experiments in which an array of structural changes in these materials is induced by the absorption of light, and Taylor describes the information provided about defects in both chalcogenides and pnictide glasses by the nuclear quadrupole resonance technique. The papers by Pohl et al. and W.A. Phillips are both concerned with problems with the interpretation of the low-temperature vibrational properties of glasses, while that of Redfield points out the value of studying transport in the band tails of disordered crystalline semiconductors in which the Fermi level is controlled by compensation. Several contributions deal with the modern techniques of transient spectroscopy. In particular, Monroe and Kastner describe a surprising asymmetry between trapping cross-sections of band-tail and defect states in chalcogenide glasses, Marshall and Barclay suggest that these cross-sections have a strong energy dependence, Pai reviews the effects of geminate recombination in molecularly doped organic polymers, and Hughes and Sockal discuss the problem of transient photoconductivity in amorphous SiO_2 . Following these, Cavenett reviews the information attained from several elegant spin-dependent experimental techniques, Klinger presents a theoretical analysis of defects with a negative effective correlation energy, and Bonch-Bruевич discusses the behavior of a material with such defects under highly nonequilibrium conditions. The remaining papers in Part Four are all concerned with disordered chalcogenide alloys, a class of materials believed to be characterized by defects having a negatively effective correlation energy. The origin of the p-n transitions upon chemical modification is the subject of the contribution of Nagels et al., while Kolomiets and Averyanov discuss modifications in general, and Lyubin reviews the reversible photostructural changes often observed in these materials. Finally, Freitas et al. discuss light-induced unpaired spins in chalcogenide glasses and Welland et al. describe the evidence for the simultaneous presence of two distinct Te coordinations in liquid Te-Tl alloys. Despite the fact that defects control many aspects of transport in disordered semiconductors, it appears that we presently understand the electronic structure of defects but

must consider the details of most transport phenomena as still somewhat enigmatic.

The fascinating topic of disordered magnetic systems is the subject of the four papers in Part Five, which begins with Moorjani's review of the field in general. Babic et al. then present evidence for itinerant ferromagnetism in amorphous transition-metal alloys, and both Coey and Connell and Bloomberg review amorphous antiferromagnetism, the former from a theoretical viewpoint, the latter with an eye on its potential in magneto-optical recording devices.

The concluding section, Part Six, provides an introduction to some future subjects of interest. First, Kreidl presents an overview of the interplay between science and technology over the past 25 years, thereby providing some insight into the future by extrapolation, and Zarzycki describes the progress that might be expected from the recent development of the gel technique for glass formation. The volume concludes with analyses of some materials that promise to have major technological importance. Both Hensch et al. and Shaw review our current understanding of the switching phenomena which characterize thin films of many chalcogenide glasses, while Chain and Seraphin discuss the properties of certain disordered cermets that have great potential in solar thermal applications.

It should be clear even from the above capsule summary how comprehensive this volume actually is. Nevertheless, there is not one area discussed that has not been catapulted forward by a major contribution from Sir Nevill Mott, whom we honor explicitly this year and implicitly at all times.