Theory Of Defects In Solids Electronic Structure Of Defects In Insulators And Semiconductors Oxford Classic Texts In The Physical Sciences

The history of applications of space group theory to solid state physics goes back more than five decades. The periodicity of the lattice and the definition of a k-space were the corner-stones of this application. Prof. Volker Heine in Vol. 35 of Solid State Physics (1980) noted that, even in perfect crystals, where k-space methods are appropriate, the local properties (such as the charge densi ty, bond order, etc.) are defined by the local environment of one atom. Natural ly, "k-space methods" are not appropriate for crystals with point defects, sur faces and interfaces, or for amorphous materials. In such cases the real-space approach favored by chemists to describe molecules has turned out to be very useful. To span the gulf between the k-space and real space methods it is helpful to recall that atoms in crystalline solids possess a site symmetry defined by the symmetry of the local environment of the atom occupying the site. The site symmetry concept is familiar to crystallographers and commonly used by them in the description of crystalline structures. However, in the application of group theory to solid state physics problems, the site symmetry approach has been used only for the last ten to fifteen years. In our book Methods oj Group Theory in the Quantum Chemistry oj Solids published in Russian in 1987 by Leningrad University Press we gave the first results of this application to the theory of electronic structure of crystals.

This special issue of ZAMP is published to honor Paul M. Naghdi for his contributions to mechanics over the last forty years and more. It is offered in celebration of his long, productive career in continuum mechan ics; a career which has been marked by a passion for the intrinsic beauty of the subject, an uncompromising adherence to academic standards, and an untiring devotion to our profession. Originally, this issue was planned in celebration of Naghdi's 70th birthday, which occurred on 29 March 1994. But, as the papers were being prepared for the press, it became evident that the illness from which Professor Naghdi had been suffering during recent months was extremely serious. On 26 May 1994, a reception took place in the Department of Mechanical Engineering at Berkeley, at which Naghdi received The Berkeley Citation (which is given in lieu of an honorary degree) and where he was also presented with the Table of Contents of the present collection. Subse quently, he had the opportunity to read the papers in manuscript form. He was very touched that his colleagues had chosen to honor him with their fine contributions. The knowledge that he was held in such high esteem by his fellow scientists brought a special pleasure and consolation to him in his last weeks. On Saturday evening, 9 July 1994, Paul Naghdi succumbed to the lung cancer which he had so courageously endured.

Annotation Describes the development and application of the quasiparticle method in the modern quantum theory of solids, and presents an original general nonlinear dynamics theory of the deformable solids with quasiparticle excitations. Acidic paper. Annotation copyrighted by Book News, Inc., Portland, OR.

This book surveys the theory of defects in solids, concentrating on the electronic structure of point defects in insulators and semiconductors. The relations between different approaches are described, and the predictions of the theory compared critically with experiment. The physicalassumptions and approximations are emphasized. Theory of Defects in Solids begins with the perfect solid, then reviews the main methods of calculating defect energy levels and wave functions. The calculation of observable defect properties is discussed, and finally, the theory is applied to a range of defects that are very different in nature.This book is intended for research workers and graduate students interested in solid-state physics.

This is the first volume to appear under the joint editorship of J.P. Hirth and F.R.N. Nabarro. While Volume 11 concentrated on the single topic of dislocations and work hardening, the present volume spreads over the whole range of the study of dislocations from the application by Kléman and his colleagues of homotopy theory to classifying the line and point defects of mesomorphic phases to Chaudhri's account of the experimental observations of dislocations formed around indentations. Chapter 64, by Cai, Bulatove, Chang, Li and Yip, discusses the influence of the structure of the core of a dislocation on its mobility. The power of modern computation allows this topic to be treated from the first principles of electron theory, and with empirical potentials for more complicated problems. Advances in electron microscopy allow these theoretical predictions to be tested. In Chapter 65, Xu analyzes the emission of dislocations from the tip of a crack and its influence on the brittle to ductile transition. Again, the treatment is predominantly theoretical, but it is consistently related to the very practical example of alpha iron. In a dazzling interplay of experiment and abstract mathematics, Kléman, Lavrentovich and Nastishin analyze the line and point structural defects of the many mesomorphic phases which have become known in recent years. Chapter 67, by Coupeau, Girard and Rabier, is essentially experimental. It shows how the various modern techniques of scanning probe microscopy can be used to study dislocations and their interaction with the free surface. Chapter 68, by Mitchell and Heuer, considers the complex dislocations that can form in ceramic crystals on the basis of observations by transmission electron microscopy and presents mechanistic models for the motion of the dislocations in various temperature regimes. While the underlying aim of the study of dislocations in energetic crystals by Armstrong and Elban in Chapter 69 is to understand the role of dislocations in the process of detonation, it has the wider interest of studying dislocations in molecular crystals which are ``elastically soft, plastically hard, and brittle''. Chaudhri in Chapter 70 discusses the role of dislocations in indentation processes, largely on the basis of the elastic analysis by E.H. Yoffe. The special case of nanoindentations is treated only briefly.

Addressing both theoretical and practical aspects of phase transformation in alloys, this text formulates significant aspects of the quantitative metallurgy of phase transformations. It further applies solid-state theoretical concepts to structure problems arising in experimental studies of real alloys. Author Armen G. Khachaturyan, Professor of Materials Science at Rutgers University, ranks among the foremost authorities on this subject. In this volume, he takes a creative approach to examining change in atomic structure and morphology caused by ordering, strain-induced ordering, strain-controlled decomposition, and strain-induced coarsening. Unifying relationships among various fields of solid-state physics are stressed throughout the book. Topics include structure changes in two-phase alloys controlled by the phase transformation elastic strain, in addition to important results in the area of microscopic elasticity regarding problems of elastic interaction in impurity atoms, and strain-induced ordering and decomposition in interstitial solutions. An excellent text for advanced undergraduate and graduate courses in physical metallurgy, solid state physics, solid state chemistry, and materials science, this volume is also a valuable reference for professionals conducting research in phase transformations

Solid State Physics

This volume brings together some of the presently available theoretical techniques which will be useful in the design of solid-state materials. At present, it is impossible to specify the atomic composition of a material and its macroscopic physical properties. However, the future possibilities for such a science are being laid today. This is coming about due to the development of fast, cheap computers which will be able to undertake the calculations which are necessary. Since this field of science is fairly new, it is not yet quite clear which direction of analysis will eventually prove to be the most successful. In this respect the author has included the most relevant promising subject areas, based on seven years of research experience in the field. An extensive literature already exists for most of the areas covered here, thus when more detailed analysis can be found elsewhere, the assumptions made are discussed, and only an outline of the method involved is presented. Comprehensive indexes are provided to assist the reader in further studies. This is a potentially

important field which is slowly getting underway and only needs a significant development to attract a broader scientific interest. The work will be of considerable interest to program managers needing to assess this new field.

The Advanced Study Institute of which this volume is the proceedings was held at the University of Exeter during 24 August to 6 September 1975. There were seventy participants of whom eighteen were lecturers and members of the advisory committee. All NATO countries except Holland, Iceland and Portugal were re presented. In addition a small number of participants came from non-NATO countries Japan, Ireland and Switzerland. An aim of the organising committee was to bring together scientists of wide interests and expertise in the defect structure of insulators and semiconductors. Thus major emphases in the pro gramme concerned the use of spectroscopy and microscopy in revealing the structure of point defects and their aggregates, line defects as well as planar and volume defects. The lectures revealed that in general little is known of the fate of the interstitial in most irradiated solids. Nor are the dynamic properties of defects under stood in sufficient detail that one can state how point defects cluster and eventually become macroscopic defects. Although this book faithfully reproduces the material covered by the invited speakers, it does not really follow the flow of the lectures. This is because it seemed advisable for each lecturer to provide a single self-contained and authoritative manuscript, rather than a series of short articles corresponding to the lectures.

This new series Mechanics and Physics of Discrete Systems aims to provide a coherent picture of the modern development of discrete physical systems. Each volume will offer an orderly perspective of disciplines such as molecular dynamics, crystal mechanics and/or physics, dislocation, etc. Emphasized in particular are the fundamentals of mechanics and physics that play an essential role in engineering applications. Volume 1, Gauge Theory and Defects in Solids, presents a detailed development of a rational theory of the dynamics of defects and damage in solids. Solutions to field equations are used to determine stresses, dislocation densities and currents that arise from histories of loading of boundaries of bodies. Analysed in detail is a gauge theory with a gauge group that is not semi-simple, and whose action occurs at the classical macroscopic level. Yang-Mills theory is applied where the state variables are elastic displacements in solids, determination of mechanical and electromagnetic observables by choice of gauge conditions is demonstrated, and practices of classical dislocation theory are derived from first principles.

The author applies methods of nonlinear elasticity to investigate the defects in the crystal structure of solids such as dislocations and disclinations that characterize the plastic and strength properties of many materials. Contrary to the geometrically motivated nonlinear theory of dislocations continuously distributed over the body, nonlinear analysis of isolated dislocations and disclinations is less developed; it is given for the first time in this book, and in a form accessible to both students and researchers. The general theory of Volterra's dislocations in elastic media under large deformations is developed. A number of exact solutions are found. The nonlinear approach to investigating the isolated defects produces results that often differ qualitatively from those of the linear theory.

This book surveys the theory of defects in solids, concentrating on the electronic structure of point defects in insulators and semiconductors. The relations between different approaches are described, and the predictions of the theory compared critically with experiment. The physical assumptions and approximations are emphasized. The book begins with the perfect solid, then reviews the main methods of calculating defect energy levels and wave functions. The calculation and observable defect properties is discussed, and finally, the theory is applied to a range of defects that are very different in nature. This book is intended for research workers and graduate students interested in solid-state physics. From reviews of the hardback: 'It is unique and of great value to all interested in the basic aspects of defects in solids.' Physics Today 'This is a particularly worthy book, one which has long been needed by the theoretician and experimentalist alike.' Nature

This text surveys the theory of defects in solids, concentrating on the electronic structure of point defects in semiconductors and insulators. The relations between different approaches are described, and predictions of theory compared with experiments.

This extensive survey covers defects in nonmetals, emphasizing point defects and point-defect processes. It encompasses electronic, vibrational, and optical properties of defective solids, plus dislocations and grain boundaries. 1985 edition.

From its early beginning before the war, the field of semiconductors has developped as a classical example where the standard approximations of 'band theory' can be safely used to study its interesting electronic properties. Thus in these covalent crystals, the electronic structure is only weakly coupled with the atomic vibrations; one-electron Bloch functions can be used and their energy bands can be accurately computed in the neighborhood of the energy gap between the valence and conduction bands; nand p doping can be obtained by introducing substitutional impurities which only introduce shallow donors and acceptors and can be studied by an effective-mass weak-scattering description. Yet, even at the beginning, it was known from luminescence studies that these simple concepts failed to describe the various 'deep levels' introduced near the middle of the energy gap by strong localized imperfections. These imperfections not only include some interstitial and many substitutional atoms, but also 'broken bonds' associated with surfaces and interfaces, dis location cores and 'vacancies', i.e., vacant iattice sites in the crystal. In all these cases, the electronic structure can be strongly correlated with the details of the atomic structure and the atomic motion. Because these 'deep levels' are strongly localised, electron-electron correlations can also playa significant role, and any weak perturbation treatment from the perfect crystal structure obviously fails. Thus, approximate 'strong coupling' techniques must often be used, in line' with a more chemical de scription of bonding.

Provides a thorough understanding of the chemistry and physics of defects, enabling the reader to manipulate them in the engineering of materials. Reinforces theoretical concepts by placing emphasis on real world processes and applications. Includes two kinds of end-of-chapter problems: multiple choice (to test knowledge of terms and principles)

and more extensive exercises and calculations (to build skills and understanding). Supplementary material on crystallography and band structure are included in separate appendices.

Theory of Defects in SolidsElectronic Structure of Defects in Insulators and SemiconductorsOxford University Press

The last quarter-century has been marked by the extremely rapid growth of the solid-state sciences. They include what is now the largest subfield of physics, and the materials engineering sciences have likewise flourished. And, playing an active role throughout this vast area of science and engineer ing have been very large numbers of chemists. Yet, even though the role of chemistry in the solid-state sciences has been a vital one and the solid-state sciences have, in turn, made enormous contributions to chemical thought, solid-state chemistry has not been recognized by the general body of chemists as a major subfield of chemistry. Solid-state chemistry is not even well defined as to content. Some, for example, would have it include only the quantum chemistry of solids and would reject thermodynamics and phase equilibria; this is nonsense. Solid-state chemistry has many facets, and one of the purposes of this Treatise is to help define the field. Perhaps the most general characteristic of solid-state chemistry, and one which helps differentiate it from solid-state physics, is its focus on the chemical composition and atomic configuration of real solids and on the relationship of composition and structure to the chemical and physical properties of the solid. Real solids are usually extremely complex and exhibit almost infinite variety in their compositional and structural features.

This book sterns from a course on Micromechanics that I started about fifteen years ago at Northwestern University. At that time, micro mechanics was a rather unfamiliar subject. Although I repeated the course every year, I was ne ver convinced that my notes have quite developed into a final manuscript because new topics emerged con stantly requiring revisions, and additions. I finally came to realize that if this is continued, then I will never complete the book to my total satisfaction. Meanwhile, T. Mori and I had coauthored a book in Micromechanics, published by Baifu-kan, Tokyo, in Japanese, entitled 1975. It received an extremely favorable response from students and researchers in Japan. This encouraged me to go ahead and publish my course notes in their latest version, as this book, which contains further development of the subject and is more comprehensive than the one published in Japanese. Micromechanics encompasses mechanics related to microstructures of materials. The method employed is a continuum theory of elasticity yet its applications cover a broad area relating to the mechanical behavior of materials: plasticity, fracture and fatigue, constitutive equa tions, composite materials, polycrystals, etc. These subjects are treated in this book by means of a powerful and unified method which is called the 'eigenstrain method. ' In particular, problems relating to inclusions and dislocations are most effectively analyzed by this method, and therefore, special emphasis is placed on these topics.

In this report we describe progress in developing and implementing a general theoretical approach to describing the properties of defects and impurities of a general nature in nonmetallic solid systems. This approach combines fully correlated, fully self-consistent electronic structure determination of the electrical and mechanical properties associated with neutral or charged defects/impurities in or on a non-metal. The system remote from the defect is described by the shell model which incorporates self-consistently, host polarization and distortion. This results in our being able to obtain absolute energies of the impurity ions in the host and their interaction. The model is free of adjustable or undefined parameters. This project is of non-trivial magnitude and the current computer implementation, which is functional in our laboratory, consists of a program, ICECAP, which is about 100,000 statements long. Originator supplied keywords include: Energetic solids, Molecular solids, Clusters, Defects, Impurities, and ICECAP.

The principal objective of this book is to stimulate interest in research that will extend available theory towards a greater understanding of the steps involved in solid-state decompositions and the properties of solids that control reactivities. Much of the activity in this field has been directed towards increasing the range of reactants for which decomposition kinetic data is available, rather than extending insights into the fundamental chemistry of the reactions being studied. The first part of the book (Chapters 1-6) is concerned with theoretical aspects of the subject. The second part (Chapters 7-17) surveys groups of reactions classified by similarities of chemical composition. The final Chapter (18) reviews the subject by unifying features identified as significant and proposes possible directions for future progress. Studies of thermal reactions of ionic compounds have contributed considerably to the theory of solid-state chemistry. Furthermore, many of these rate processes have substantial technological importance, for example, in the manufacture of cement, the exploitation of ores and in the stability testing of drugs, explosives and oxidizing agents. Despite the prolonged and continuing research effort concerned with these reactions, there is no recent overall review. This book is intended to contribute towards correcting this omission. The essential unity of the subject is recognized by the systematic treatment of reactions, carefully selected to be instructive and representative of the subject as a whole. The authors have contributed more than 200 original research articles to the literature, many during their 25 years of collaboration. Features of this book: • Gives a comprehensive in-depth survey of a rarely-reviewed subject. • Reviews methods used in studies of thermal decompositions of solids. • Discusses patterns of subject development perceived from an extensive literature survey. This book is expected to be of greatest value and interest to scientists concerned with the chemical properties and reactions of solids, including chemists, physicists, pharmacists, material scientists, crystallographers, metallurgists and others. This wide coverage of the literature dealing with thermal reactions of solids will be of value to both academic and industrial researchers by reviewing the current status of the theory of the subject. It could also provide a useful starting point for the exploitation of crystalline materials in practical and industrial applications. The contents will also be relevant to a wide variety of researchers, including, for example, those concerned with the stabilities of polymers and composite materials, the processing of minerals, the shelf-lives of pharmaceuticals, etc.

This volume presents recent developments in the theory of defects and the mechanics of material forces. The book constitutes a selection of the contributions presented at the International Symposium on Defect and Material Mechanics (ISDMM2011), held inSeville,Spain, June 2011. The ISDMM series of symposia provides a rare and much needed forum

for bringing together a diverse group of researchers from various areas ranging from theoretical, experimental and computational modeling of the mechanics of materials. The present volume constitutes a valuable snapshot of the field of the mechanics of materials and their defects, and a window to its many accomplishments, challenges and opportunities, and open questions. The volume is intended to motivate the young research community interested in the field. Reprinted from International Journal of Fracture, Vol. 174:1 (2012)

Volume 1 of Point Defects in Solids has as its major emphasis defects in ionic solids. Volume 2 now extends this emphasis to semiconductors. The first four chapters treat in some detail the creation, kinetic behavior, inter actions, and physical properties of both simple and composite defects in a variety of semiconducting systems. Also included, as in Vol. 1, are chapters on special topics, namely phonon-defect interactions and defects in organic crystals. Defect behavior in semiconductors has been a subject of considerable interest since the discovery some twenty-five years ago that fast neutron irradiation profoundly affected the electrical characteristics of germanium and silicon. Present-day interest has been stimulated by such semiconductor applications as solar cell power plants for space stations and satellites and semiconductor particle and y-ray detectors, since in both radiation damage can cause serious deterioration. Of even greater practical concern is the need to understand particle damage in order to capitalize upon the develop ing technique of ion implantation as a means of device fabrication. Although the periodic international conferences on radiation effects in semiconductors have served the valuable function of summarizing the extensive work being done in this field, these proceedings are much too detailed and lack the background discussion needed to make them useful to the novice.

Modern fracture mechanics considers phenomena at many levels, macro and micro; it is therefore inextricably linked to methods of theoretical and mathematical physics. This book introduces these sophisticated methods in a straightforward manner. The methods are applied to several important phenomena of solid state physics which impinge on fracture mechanics: adhesion, defect nucleation and growth, dislocation emission, sintering, the electron beam effect and fractal cracks. The book shows how the mathematical models for such processes may be set up, and how the equations so formulated may be solved and interpreted. The many open problems which are encountered will provide topics for MSc and PhD theses in fracture mechanics, and in theoretical and experimental physics. As a supplementary text, the book can be used in graduate level courses on fracture mechanics, solid matter physics, and mechanics of solids, or in a special course on the application of fracture mechanics methods in solid matter physics.

This volume on materials engineering comprises a collection of abstracts of recent scholarly papers and articles concerning a wide variety of topics related to the effects of structural defects and diffusion in many material areas, including thin-film manufacturing and facing metals.

This book stems from a course on Micromechanics that I started about fifteen years ago at Northwestern University. At that time, micromechanics was a rather unfamiliar subject. Although I repeated the course every year, I was never convinced that my notes have quite developed into a final manuscript because new topics emerged constantly requiring revisions, and additions. I finally came to realize that if this is continued, then I will never complete the book to my total satisfaction. Meanwhile, T. Mori and I had coauthored a book in Japanese, entitled Micromechanics, published by Baifu-kan, Tokyo, in 1975. It received an extremely favorable response from students and re searchers in Japan. This encouraged me to go ahead and publish my course notes in their latest version, as this book, which contains further development of the subject and is more comprehensive than the one published in Japanese. Micromechanics encompasses mechanics related to microstructures of materials. The method employed is a continuum theory of elasticity yet its applications cover a broad area relating to the mechanical behavior of materi als: plasticity, fracture and fatigue, constitutive equations, composite materi als, polycrystals, etc. These subjects are treated in this book by means of a powerful and unified method which is called the 'eigenstrain method. ' In particular, problems relating to inclusions and dislocations are most effectively analyzed by this method, and therefore, special emphasis is placed on these topics.

This textbook provides students with a complete working knowledge of the properties of imperfections in crystalline solids. Readers will learn how to apply the fundamental principles of mechanics and thermodynamics to defect properties in materials science, gaining all the knowledge and tools needed to put this into practice in their own research. Beginning with an introduction to defects and a brief review of basic elasticity theory and statistical thermodynamics, the authors go on to guide the reader in a step-by-step way through point, line, and planar defects, with an emphasis on their structural, thermodynamic, and kinetic properties. Numerous end-of-chapter exercises enable students to put their knowledge into practice, and with solutions for instructors and MATLAB® programs available online, this is an essential text for advanced undergraduate and introductory graduate courses in crystal defects, as well as being ideal for self-study.

Crystal defects can no longer be thought of as a scientific curiosity, but must be considered an important aspect of solid-state science. This is largely because many of the more interesting properties of crystalline solids are disproportionately dominated by effects due to a tiny concentration of imperfections in an otherwise perfect lattice. The physics of such lattice defects is not only of significance in a great variety of applications, but is also interesting in its own right. Thus, an extensive science of point defects and dislocations has been constructed during the past two and a half decades. Stimulated by the technological and scientific interest in plasticity, there have appeared in recent years rather a large number of books dealing with dislocations; in the case of point defects, however, only very few broad and extensive treatments have been published. Thus, there are few compre hensive, tutorial sources for the scientist or engineer whose research ac tivities are affected by point defect phenomena, or who might wish to enter the field. It is partially to fill this need that the present treatise aims.

Volume is indexed by Thomson Reuters BCI (WoS). This first volume, in a new series covering entirely general results in the fields of defects and diffusion, includes abstracts of papers which appeared between the beginning of 2008 and the end of October 2009 (journal availability permitting).

The book presents a unified and self-sufficient and reader-friendly introduction to the anisotropic elasticity theory necessary to model a wide range of point, line, planar and volume type crystal defects (e.g., vacancies, dislocations, interfaces, inhomogeneities and inclusions). The necessary elasticity theory is first developed along with basic methods for obtaining solutions. This is followed by a detailed treatment of each defect type. Included are analyses of their elastic fields and energies, their interactions with imposed stresses and image stresses, and the interactions that occur between them, all employing the basic methods introduced earlier. All results are derived in full with intermediate steps shown, and "it can be shown" is avoided. A particular effort is made to describe and compare different methods of solving important problems. Numerous exercises (with solutions) are provided to strengthen the reader's understanding and extend the immediate text. In the 2nd edition an additional chapter has been added which treats the important topic of the self-forces that are experienced by defects that are extended in more than one dimension. A considerable number of exercises have been added which expand the scope of the book and furnish further insights. Numerous sections of the book have been rewritten to provide additional clarity and scope. The major aim of the book is to provide, in one place, a unique and complete introduction to the anisotropic theory of elasticity for defects written in a manner suitable for both students and professionals.

We started our work on theoretical methods in the phys ics of high pressures (in connec tion with geophysical applications) in 1956, and we immediately encountered many problems. Naturally, we searched the published literature for solutions to these problems but whenever we failed to find a solution or when the solution did not satisfy us, we attempted to solve the problern ourselves. We realized that other investigators working in the physics of high pres sures would probably encounter the same problems and doubts. Therefore, we decided to write this book in order to save our colleagues time and effort. Apart from the descriptions of ex perimental methods, the book deals only with those problems which we encountered in our own work. Allproblems in high-pressure physics have, at present, only approximate solutions, which are very rough. Therefore, it is not surprising that different investigators approach the same problems in different ways. Our approach does not prejudge the issue and we are fully aware that there are other points of view. Our aim was always to solve a glven problern on a physical basis. For example, the concept of the Grüneisenparameter needs further develop ment but it is based on reliable physical ideas. On the other hand, Simon's equation for the melting curve has, in our opinion, no clear physical basis and is purely empirical. Equations of this type are useful in systematic presentation of the experimental material but they are un suitable for any major extrapolation.