Electronic Structure and the Properties of Solids

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E. Doni,R. Girlanda,G. Pastori Parravicini,A. Quattropani

Electronic Structure And The Properties Of Solids Harrison:

Electronic Structure and the Properties of Solids Walter A. Harrison,1989-07-01 Should be widely read by practicing physicists chemists and materials scientists Philosophical Magazine In this comprehensive and innovative text Professor Harrison Stanford University offers a basic understanding of the electronic structure of covalent and ionic solids simple metals transition metals and their compounds The book illuminates the relationships of the electronic structures of these materials and shows how to calculate dielectric conducting and bonding properties for each Also described are various methods of approximating electronic structure providing insight and even quantitative results from the comparisons Dr Harrison has also included an especially helpful Solid State Table of the Elements that provides all the parameters needed to estimate almost any property of any solid with a hand held calculator using the techniques developed in the book Designed for graduate or advanced undergraduate students who have completed an undergraduate course in quantum mechanics or atomic and modern physics the text treats the relation between structure and properties comprehensively for all solids rather than for small classes of solids This makes it an indispensable reference for all who make use of approximative methods for electronic structure engineering semiconductor development and materials science The problems at the ends of the chapters are an important aspect of the book They clearly show that the calculations for systems and properties of genuine and current interest are actually quite elementary Prefaces Problems Tables Appendixes Solid State Table of the Elements Bibliography Author and Subject Indexes Will doubtless exert a lasting influence on the solid state physics literature Physics Today Elementary Electronic Structure Walter Ashley Harrison,2004 This is a revised edition of the 1999 text on the electronic structure and properties of solids similar in spirit to the well known 1980 text Electronic Structure and the Properties of Solids The revisions include an added chapter on glasses and rewritten sections on spin orbit coupling magnetic alloys and actinides The text covers covalent semiconductors ionic insulators simple metals and transition metal and f shell metal systems It focuses on the most important aspects of each system making what approximations are necessary in order to proceed analytically and obtain formulae for the properties Such back of the envelope formulae which display the dependence of any property on the parameters of the system are characteristic of Harrison s approach to electronic structure as is his simple presentation and his provision of all the needed parameters In spite of the diversity of systems and materials the approach is systematic and coherent combining the tight binding or atomic picture with the pseudopotential or free electron picture This provides parameters the empty core radii as well as the covalent energies and conceptual bases for estimating the various properties of all these systems Extensive tables of parameters and properties are included The book has been written as a text with problems at the end of each chapter and others can readily be generated by asking for estimates of different properties or different materials than those treated in the text In fact the ease of generating interesting problems reflects the extraordinary utility and simplicity of the methods introduced Developments since the 1980 publication

have made the theory simpler and much more accurate besides allowing much wider application **Electronic Structure and the Properties of Solids** Walter Ashley Harrison,1989 *Structure and Bonding in Crystalline Materials* Gregory S. Rohrer,2001-07-19 One of the motivating questions in materials research today is how can elements be combined to produce a solid with specified properties This book is intended to acquaint the reader with established principles of crystallography and cohesive forces that are needed to address the fundamental relationship between the composition structure and bonding Starting with an introduction to periodic trends the book discusses crystal structures and the various primary and secondary bonding types and finishes by describing a number of models for predicting phase stability and structure Containing a large number of worked examples exercises and detailed descriptions of numerous crystal structures this book is primarily intended as an advanced undergraduate or graduate level textbook for students of materials science It will also be useful to scientists and engineers who work with solid materials **Physical Metallurgy** R.W. Cahn,P. Haasen,1996-02-09 This is the fourth edition of a work which first appeared in 1965 The first edition had approximately one thousand pages in a single volume This latest volume has almost three thousand pages in 3 volumes which is a fair measure of the pace at which the discipline of physical metallurgy has grown in the intervening 30 years Almost all the topics previously treated are still in evidence in this version which is approximately 50% bigger than the previous edition All the chapters have been either totally rewritten by new authors or thoroughly revised and expanded either by the third edition authors alone or jointly with new co authors Three chapters on new topics have been added dealing with dry corrosion oxidation and protection of metal surfaces the dislocation theory of the mechanical behavior of intermetallic compounds and most novel a chapter on polymer science for metallurgists which analyses the conceptual mismatch between metallurgists and polymer scientists way of looking at materials Special care has been taken throughout all chapters to incorporate the latest experimental research results and theoretical insights Several thousand citations to the research and review literature are included in this edition There is a very detailed subject index as well as a comprehensive author index The original version of this book has long been regarded as the standard text in physical metallurgy and this thoroughly rewritten and updated version will retain this status

Electronic Structure and Optical Properties of Semiconductors Marvin L. Cohen,James R. Chelikowsky,2012-12-06 We began planning and writing this book in the late 1970s at the suggestion of Manuel Cardona and Helmut Lotsch We also received considerable en couragement and stimulation from colleagues Some said there was a need for instructional material in this area while others emphasized the utility of a research text We tried to strike a compromise The figures tables and references are included to enable researchers to obtain quickly essential information in this area of semiconductor research For instructors and stu dents we attempt to cover some basic ideas about electronic structure and semiconductor physics with applications to real rather than model solids We wish to thank our colleagues and collaborators whose research re sults and ideas are presented here Special thanks are due to Jim Phillips who influenced us both during our formative years and

afterwards We are grateful to Sari Yamagishi for her patience and skill with the typing and production of the manuscript Finally we acknowledge the great patience of Helmut Lotsch and Manuel Cardona Berkeley CA M L Cohen Minneapolis MN J R Chelikowsky March 1988 VII Contents 1 Introduction 1 2 Theoretical Concepts and Methods 4 2 1 The One Electron Model and Band Structure 7 2 2 Properties of En k 11 3 Pseudopotentials 16 3 1 The Empirical Pseudopotential Method 20 3 2 Self Consistent and Ab Initio Pseudopotentials 25 4 Response Functions and Density of States 30 4 1 Charge Density and Bonding 38 **Electronic Structure, Correlation Effects and Physical Properties of D- and F-metals and Their Compounds** Valentin Yu Irkhin,Yu. P. Irkhin,2007 The book includes all main physical properties of d and f transition metal systems and corresponding theoretical concepts Special attention is paid to the theory of magnetism and transport phenomena Some examples of non traditional questions which are treated in detail in the book the influence of density of states singularities on electron properties many electron description of strong itinerant magnetism mechanisms of magnetic anisotropy microscopic theory of anomalous transport phenomena in ferromagnets Besides considering classical problems of solid state physics as applied to transition metals modern developments in the theory of correlation effects in d and f compounds are considered within many electron models The book contains where possible a simple physical discussion More difficult questions are considered in Appendices *Electronic Properties of Semiconductor Interfaces* Winfried Mönch,2013-04-17 Almost all semiconductor devices contain metal semiconductor insulator semiconductor insulator metal and or semiconductor semiconductor interfaces and their electronic properties determine the device characteristics This is the first monograph that treats the electronic properties of all different types of semiconductor interfaces Using the continuum of interface induced gap states IFIGS as a unifying theme M nch explains the band structure lineup at all types of semiconductor interfaces These intrinsic IFIGS are the wave function tails of electron states which overlap a semiconductor band gap exactly at the interface so they originate from the quantum mechanical tunnel effect He shows that a more chemical view relates the IFIGS to the partial ionic character of the covalent interface bonds and that the charge transfer across the interface may be modeled by generalizing Pauling s electronegativity concept The IFIGS and electronegativity theory is used to quantitatively explain the barrier heights and band offsets of well characterized Schottky contacts and semiconductor heterostructures respectively

Electronic Structure of Materials Rajendra Prasad,2013-07-23 Most textbooks in the field are either too advanced for students or don t adequately cover current research topics Bridging this gap Electronic Structure of Materials helps advanced undergraduate and graduate students understand electronic structure methods and enables them to use these techniques in their work Developed from the author s lecture notes this classroom tested book takes a microscopic view of materials as composed of interacting electrons and nuclei It explains all the properties of materials in terms of basic quantities of electrons and nuclei such as electronic charge mass and atomic number Based on quantum mechanics this first principles approach does not have any adjustable parameters The first half of the text presents the fundamentals and

methods of electronic structure Using numerous examples the second half illustrates applications of the methods to various materials including crystalline solids disordered substitutional alloys amorphous solids nanoclusters nanowires graphene topological insulators battery materials spintronic materials and materials under extreme conditions Every chapter starts at a basic level and gradually moves to more complex topics preparing students for more advanced work in the field End of chapter exercises also help students get a sense of numbers and visualize the physical picture associated with the problem Students are encouraged to practice with the electronic structure calculations via user friendly software packages

Progress in Electron Properties of Solids E. Doni,R. Girlanda,G. Pastori Parravicini,A. Quattropani,2012-12-06 This volume on the novelties in the electronic properties of solids appears in occasion of Franco Bassani sixtieth birthday and is dedicated to honour a scientific activity which has contributed so much of the development of this very active area of research It is re markable that this book can cover so large a part of the current research on electronic properties of solids by contributions from Bassani s former students collaborators at different stages of his scientific life and physicists from all over the world who have been in close scientific relationship with him A personal flavour therefore accompanies a number of the papers of this volume which are both up to date reports on present research and original recollections of the early events of modern solid state physics The volume begins with a few contributions dealing with theoretical procedures for electronic energy levels a primary step toward the interpretation of structural and optical properties of extended and confined systems Other papers concern the interacting state of electrons with light polaritons and the effect of the coupling of electrons with lattice vibrations with emphasis on the thermal behaviour of the electron levels and on such experimental procedures as piezospectroscopy Electron lattice interaction in external magnetic field and transport related properties due to high light excitation are also con sidered The impact of synchroton radiation on condensed matter spectroscopy is dis cussed in a topical contribution and optical measurements are presented for extended and impurity levels Solid State Physics ,1992-11-18 Solid State Physics *Properties of Impurity States in Superlattice Semiconductors* C.Y. Fong,Inder P. Batra,S. Ciraci,2012-12-06 A NATO workshop on The Properties of Impurity States in Semiconductor Superlattices was held at the University of Essex Colchester United Kingdom from September 7 to 11 1987 Doped semiconductor superlattices not only provide a unique opportunity for studying low dimensional electronic behavior they can also be custom designed to exhibit many other fascinating el ctronic properties The possibility of using these materials for new and novel devices has further induced many astonishing advances especially in recent years The purpose of this workshop was to review both advances in the state of the art and recent results in various areas of semiconductor superlattice research including i growth and characterization techniques ii deep and shallow im purity states iii quantum well states and iv two dimensional conduction and other novel electronic properties This volume consists of all the papers presented at the workshop Chapters 1 6 are concerned with growth and characterization techniques for superlattice semiconductors The question of a layer is also

discussed in this section Chapters 7 15 contain a discussion of various aspects of the impurity states Chapters 16 22 are devoted to quantum well states Finally two dimensional conduction and other electronic properties are described in chapters 23 26 **Molecular Approach to Solids** A.N. Lazarev,1998-07-09 The current volume in the series Vibrational Spectra and Structure is a single topic volume on the vibrational spectra of molecules containing silicon in the solid state Molecular Approaches to Solids has been treated by the workers in the Institute for Silicate Chemistry of the Russian Academy of Science in St Petersburg for the past two decades In the last 15 years a number of publications have originated from the laboratory where quantum mechanical computations for suitably selected molecules have been utilized to explain the origins of some structure bonding interrelationships and silicates and to evaluate their force constants Since most of the developments in this area have been published in the Russian literature they remain relatively inaccessible to the Western scientists This volume is a compilation of many of these publications and summarizes the essential conclusions of these studies Unfortunately Professor Lazarev passed away after he had submitted the volume for publication *Theoretical Geochemistry* John A. Tossell,David J. Vaughan,1992-03-19 This work is based on the observation that further major advances in geochemistry particularly in understanding the rules that govern the ways in which elements come together to form minerals and rocks will require the application of the theories of quantum mechanics The book therefore outlines this theoretical background and discusses the models used to describe bonding in geochemical systems It is the first book to describe and critically review the application of quantum mechanical theories to minerals and geochemical systems The book consolidates valuable findings from chemistry and materials science as well as mineralogy and geochemistry and the presentation has relevance to professionals in a wide range of disciplines Experimental techniques are surveyed but the emphasis is on applying theoretical tools to various groups of minerals the oxides silicates carbonates borates and sulfides Other topics dealt with in depth include structure stereochemistry bond strengths and stabilities of minerals various physical properties and the overall geochemical distribution of the elements Materials Science for Structural Geology Mervyn S. Paterson,2012-11-28 This book sets out the basic materials science needed for understanding the plastic deformation of rocks and minerals Although at atmospheric pressure or at relatively low environmental pressures these materials tend to be brittle that is to fracture with little prior plastic deformation when non hydrostatically stressed they can undergo substantial permanent strain when stressed under environmental conditions of high confining pressure and high temperature such as occur geologically in the Earth s crust and upper mantle Thus the plastic deformation of rocks and minerals is of fundamental interest in structural geology and geodynamics In mountain building processes and during convective stirring in the Earth s mantle rocks can undergo very large amounts of plastic flow accompanied by substantial changes in microstructure These changes in microstructure remain in the rocks as evidence of the past deformation history There are a number of types of physical processes whereby rock and minerals can undergo deformation under geological conditions The physics of these

processes is set out in this book **Introduction to Solid-State Theory** Otfried Madelung,2012-12-06 Introduction to Solid State Theory is a textbook for graduate students of physics and materials science It also provides the theoretical background needed by physicists doing research in pure solid state physics and its applications to electrical engineering The fundamentals of solid state theory are based on a description by delocalized and localized states and within the concept of delocalized states by elementary excitations The development of solid state theory within the last ten years has shown that by a systematic introduction of these concepts large parts of the theory can be described in a unified way This form of description gives a pictorial formulation of many elementary processes in solids which facilitates their understanding

Fundamentals of Semiconductors Peter YU,Manuel Cardona,2010-04-07 Excellent bridge between general solid state physics textbook and research articles packed with providing detailed explanations of the electronic vibrational transport and optical properties of semiconductors The most striking feature of the book is its modern outlook provides a wonderful foundation The most wonderful feature is its efficient style of exposition an excellent book Physics Today Presents the theoretical derivations carefully and in detail and gives thorough discussions of the experimental results it presents This makes it an excellent textbook both for learners and for more experienced researchers wishing to check facts I have enjoyed reading it and strongly recommend it as a text for anyone working with semiconductors I know of no better text I am sure most semiconductor physicists will find this book useful and I recommend it to them Contemporary Physics Offers much new material an extensive appendix about the important and by now well established deep center known as the DX center additional problems and the solutions to over fifty of the problems at the end of the various chapters World Scientific Reference Of Amorphous Materials, The: Structure, Properties, Modeling And Main Applications (In 3 Volumes) ,2020-12-28 Amorphous solids including glassy and non crystalline solids are ubiquitous since the vast majority of solids naturally occurring in our world are amorphous Although the field is diverse and complex this three volume set covers the vast majority of the important concepts needed to understand these materials and their principal practical applications One volume discusses the most important subset of amorphous insulators namely oxide glasses the other two volumes discuss the most important subsets of amorphous semiconductors namely tetrahedrally coordinated amorphous semiconductors and amorphous and glassy chalcogenides Together these three volumes provide a comprehensive set of theoretical concepts and practical information needed to become conversant in the field of amorphous materials They are suitable for advanced graduate students postdoctoral research associates and researchers wishing to change fields or sub fields The topics covered in these three volumes include 1 concepts for understanding the structures of amorphous materials 2 techniques to characterize the structural electronic and optical properties of amorphous materials 3 the roles of defects in affecting the electronic and optical properties of amorphous materials and 4 the concepts for understanding practical devices and other applications of amorphous materials Applications discussed in these volumes include transistors solar cells displays

bolometers fibers non volatile memories vidicons photoresists and optical disks *Electronic and Optoelectronic Properties of Semiconductor Structures* Jasprit Singh,2007-03-26 A graduate textbook presenting the underlying physics behind devices that drive today s technologies The book covers important details of structural properties bandstructure transport optical and magnetic properties of semiconductor structures Effects of low dimensional physics and strain two important driving forces in modern device technology are also discussed In addition to conventional semiconductor physics the book discusses self assembled structures mesoscopic structures and the developing field of spintronics The book utilizes carefully chosen solved examples to convey important concepts and has over 250 figures and 200 homework exercises Real world applications are highlighted throughout the book stressing the links between physical principles and actual devices Electronic and Optoelectronic Properties of Semiconductor Structures provides engineering and physics students and practitioners with complete and coherent coverage of key modern semiconductor concepts A solutions manual and set of viewgraphs for use in lectures are available for instructors from solutions cambridge org The Structures of Binary Compounds J. Hafner,F. Hulliger,W.B. Jensen,J.A. Majewski,K. Mathis,P. Villars,P. Vogl,2013-10-22 Up to date compilation of the experimental data on the structures of binary compounds by Villars and colleagues Coloured structure maps which order the compounds into their respective structural domains and present for the first time the local co ordination polyhedra for the 150 most frequently occurring structure types pedagogically very helpful and useful in the search for new materials with a required crystal structure Crystal co ordination formulas a flexible notation for the interpretation of solid state structures by chemist Bill Jensen Recent important advances in understanding the quantum mechanical origin of structural stability presented in two clearly written chapters by leading experts in the field Hafner Majewski and Vogl The Structures of Binary Compounds presents not only the most up to date compilation of the experimental data on the structures of binary compounds but also the recent important theoretical advances in understanding the quantum mechanical origin of structural stability In addition to this volume a large wall chart displaying the structure maps for the AB ABs and AB3 stoichiometries together with the corresponding co ordination polyhedra has been published The first half of the book details the successful ordering of the known experimental data in two or three dimensional coloured structure maps the 150 most frequently occurring structure types being characterized for the first time by their local co ordination polyhedra The second half of the book details the success of first principle theoretical calculations within the Local Density Functional Approximation in predicting the correct ground state structures of binary semiconductors insulators and metals The book concludes with a chapter on the cohesion and structure of solids from the more localized tight binding point of view

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