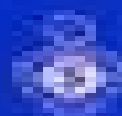


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Disordered Alloys Diffuse Scattering And Monte Carlo Simulations:

Disordered Alloys, 1998 Disordered Alloys Werner Schweika, 2014-04-17 The book reviews structural disorder in alloys and shows how detailed information can be found by applying thermal neutron and or x ray scattering Interactions among atoms of the alloy are modeled by Monte Carlo methods thus achieving a picture of the electronic structure of the system Precision Monte Carlo Simulations are also used for testing existing theories of wetting **Disordered Alloys** Werner Schweika, 1998 This monograph reviews the subject of structural disorder in alloys and describes how structural information can be exploited to build sound theoretical descriptions in terms of modified Ising models Scattering with thermal neutrons and x rays prove to be complementary approaches to measure the weak diffuse scattering which provides detailed information about the disorder The authors show how Monte Carlo methods are applied to determine the most realistic effective interactions among the alloying atoms These results can be used as a benchmark for modern electronic structure calculations Of more general interest the limitations of scattering experiments in a determination of an interaction model and thus also of the structure itself are discussed Finally simulations exhibit not only near surface disordering due to frustration effects but also new possible surface induced ordering phenomena Accurate Monte Carlo simulations are used to test existing theories of wetting **Diffuse Scattering and the Fundamental Properties of Materials** Rozaliya I. Barabash, Gene E. Ice, Patrice E. A. Turchi, 2009 Annotation Beginning with a concise review of the physics and chemistry of polymers and their structure and morphology this book goes on to describe and explain the common methods of characterizing polymers including optical microscopy scanning electron microscopy and transmission electron microscopy among others Also covered are the characterization and modification of such surface properties as adhesion wetting tribology and surface thermodynamics **Local Structure from Diffraction** S.J.L. Billinge, M.F. Thorpe, 2006-02-04 This series of books which is published at the rate of about one per year addresses fundamental problems in materials science The contents cover a broad range of topics from small clusters of atoms to engineering materials and involve chemistry physics materials science and engineering with length scales ranging from nanostroms up to millimeters The emphasis is on basic science rather than on applications Each book focuses on a single area of current interest and brings together leading experts to give an up to date discussion of their work and the work of others Each article contains enough references that the interested reader can access the relevant literature Thanks are given to the Center for Fundamental Materials Research at Michigan State University for supporting this series M F Thorpe Series Editor E mail thorpe pa msu edu East Lansing Michigan PREFACE One of the most challenging problems in the study of structure is to characterize the atomic short range order in materials Long range order can be determined with a high degree of accuracy by analyzing Bragg peak positions and intensities in data from single crystals or powders However information about short range order is contained in the diffuse scattering intensity This is difficult to analyze because it is low in absolute intensity though the integrated intensity

may be significant and widely spread in reciprocal space *Moving Interfaces in Crystalline Solids* Franz D. Fischer, Erich Schmid, 2007-03-23 Moving Interfaces in Solids are typically phase boundaries and grain or subgrain boundaries Continuum thermodynamics and continuum mechanics are applied to explain the motion process Related numerical and experimental concepts are dealt with Experts from material physics and mechanics bridge the gap between these fields The reader is offered a common view of interface motion in a unique representation Examples are presented for various material systems

Properties of Complex Inorganic Solids 2 Annemarie Meike, A. Gonis, Patrice E.A. Turchi, Krishna Rajan, 2012-12-06 The triennial International Alloy Conferences IACs aim at the identification and promotion of the common elements developed in the study either experimental phenomenological or theoretical and computational of materials properties across materials types from metals to minerals To accomplish this goal the IACs bring together scientists from a wide spectrum of materials science including experiment theory modeling and computation incorporating a broad range of materials properties The first IAC IAC I took place in Athens Greece June 16 21 1996 The present volume of proceedings contains the papers presented at IAC 2 that took place in Davos Switzerland August 8 13 1999 The topics in this book fall into several themes which suggest a number of different classification schemes We have chosen a scheme that classifies the papers in the volume into the categories Microstructural Properties Ordering Kinetics and Diffusion Magnetic Properties and Elastic Properties We have juxtaposed apparently disparate of revealing the dynamic character approaches to similar physical processes in the hope of the processes under consideration We hope this will invigorate new kinds of discussion and reveal challenges and new avenues to the description and prediction of properties of materials in the solid state and the conditions that produce them

Powder Diffraction R E Dinnebier, S J L Billinge, 2015-11-09 Powder diffraction is a widely used scientific technique in the characterization of materials with broad application in materials science chemistry physics geology pharmacology and archaeology Powder Diffraction Theory and Practice provides an advanced introductory text about modern methods and applications of powder diffraction in research and industry The authors begin with a brief overview of the basic theory of diffraction from crystals and powders Data collection strategies are described including x ray neutron and electron diffraction setups using modern day apparatus including synchrotron sources Data corrections essential for quantitative analysis are covered before the authors conclude with a discussion of the analysis methods themselves The information is presented in a way that facilitates understanding the information content of the data as well as best practices for collecting and analyzing data for quantitative analysis This long awaited book condenses the knowledge of renowned experts in the field into a single authoritative overview of the application of powder diffraction in modern materials research The book contains essential theory and introductory material for students and researchers wishing to learn how to apply the frontier methods of powder diffraction *Spontaneous Ordering in Semiconductor Alloys* Angelo Mascarenhas, 2012-12-06 The phenomenon of spontaneous ordering in semiconductor alloys which can be categorized as a self organized process is observed

to occur spontaneously during epitaxial growth of certain ternary alloy semiconductors and results in a modification of their structural electronic and optical properties. There has been a great deal of interest in learning how to control this phenomenon so that it may be used for tailoring desirable electronic and optical properties. There has been even greater interest in exploiting the phenomenon for its unique ability in providing an experimental environment of controlled alloy statistical fluctuations. As such, it impacts areas of semiconductor science and technology related to the materials science of epitaxial growth, statistical mechanics, and electronic structure of alloys and electronic and photonic devices. During the past two decades, significant progress has been made toward understanding the mechanisms that drive this phenomenon and the changes in physical properties that result from it. A variety of experimental techniques have been used to probe the phenomenon, and several attempts have been made at providing theoretical models both for the ordering mechanisms as well as electronic structure changes. The various chapters of this book provide a detailed account of these efforts during the past decade. The first chapter provides an elaborate account of the phenomenon with an excellent perspective of the structural and electronic modifications it induces.

Complex Inorganic Solids Patrice E. A. Turchi, Antonios Gonis, Krishna Rajan, Annemarie Meike, 2007-12-31

One of the key aspects of this volume is to cut across the traditional taxonomy of disciplines in the study of alloys. Hence, there has been a deliberate attempt to integrate the different approaches taken towards alloys as a class of materials in different fields ranging from geology to metallurgical engineering. The emphasis of this book is to highlight commonalities between different fields with respect to how alloys are studied. The topics in this book fall into several themes which suggest a number of different classification schemes. We have chosen a scheme that classifies the papers in the volume into the categories: Microstructural Considerations, Ordering Kinetics and Diffusion, Magnetic Considerations, and Elastic Considerations. The book has juxtaposed apparently disparate approaches to similar physical processes in the hope of revealing a more dynamic character of the processes under consideration. This monograph will invigorate new kinds of discussion and reveal challenges and new avenues to the description and prediction of properties of materials in the solid state and the conditions that produce them.

Physical Metallurgy David E. Laughlin, Kazuhiro Hono, 2014-07-24

This fifth edition of the highly regarded family of titles that first published in 1965 is now a three volume set and over 3 000 pages. All chapters have been revised and expanded either by the fourth edition authors alone or jointly with new co authors. Chapters have been added on the physical metallurgy of light alloys, the physical metallurgy of titanium alloys, atom probe field ion microscopy, computational metallurgy, and orientational imaging microscopy. The books incorporate the latest experimental research results and theoretical insights. Several thousand citations to the research and review literature are included. Exhaustively synthesizes the pertinent contemporary developments within physical metallurgy so scientists have authoritative information at their fingertips. Replaces existing articles and monographs with a single complete solution. Enables metallurgists to predict changes and create novel alloys and processes.

Underneath the Bragg

Peaks Takeshi Egami, Simon J.L. Billinge, 2012-12-31 Underneath the Bragg Peaks Structural Analysis of Complex Materials focuses on the structural determination of crystalline solids with extensive disorder Well established methods exist for characterizing the structure of fully crystalline solids or fully disordered materials such as liquids and glasses but there is a dearth of techniques for the cases in between crystalline solids with internal atomic and nanometer scale disorder Egami and Billinge discuss how to fill the gap using modern tools of structural characterization This problem is encountered in the structural characterization of a surprisingly wide range of complex materials of interest to modern technology and is becoming increasingly important Takeshi Egami received the 2003 Eugene Bertram Warren Diffraction Physics Award for the work described in the book The authors received 2010 J D Hanawalt Award from the International Union of Crystallography largely based on the success of this book Introduces a unique method to study the atomic structure of nanomaterials Lays out the basic theory and methods of this important emerging technique The first edition is considered the seminal text on the subject

Alloy Physics Wolfgang Pfeiler, 2008-01-08 Covering the latest research in alloy physics together with the underlying basic principles this comprehensive book provides a sound understanding of the structural changes in metals and alloys ranging from plastic deformation deformation dynamics and ordering kinetics right up to atom jump processes first principle calculations and simulation techniques Alongside fundamental topics such as crystal defects phase transformations and statistical thermodynamics the team of international authors treats such hot areas as nano size effects interfaces and spintronics as well as technical applications of modern alloys like data storage and recording and the possibilities offered by materials design

Quasicrystals Esther Belin-Ferré, 2000 This book focuses on current topics in quasicrystal science and research Various themes are addressed such as atomic structure growth of quasicrystals statistical physics and thermodynamics magnetism phasons propagation of waves surfaces and technological potential of quasicrystals Insight into basics in physics and chemistry is also given with examples from metallurgy the surface of alloys plasticity etc in order to point out the possible genuine aspects of quasicrystals and allow a better comparison with conventional alloys

Quasicrystals: Current Topics - Proceedings Of The Spring School On Quasicrystals Esther Belin-ferre, Claire Berger, Marianne Quiquandon, Anne Sadoc, 2000-07-31 This book focuses on current topics in quasicrystal science and research Various themes are addressed such as atomic structure growth of quasicrystals statistical physics and thermodynamics magnetism phasons propagation of waves surfaces and technological potential of quasicrystals Insight into basics in physics and chemistry is also given with examples from metallurgy the surface of alloys plasticity etc in order to point out the possible genuine aspects of quasicrystals and allow a better comparison with conventional alloys

International Tables for Crystallography, Volume B Uri Shmueli, 2008-08-27 International Tables for Crystallography are no longer available for purchase from Springer For further information please contact Wiley Inc follow the link on the right hand side of this page Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research

After an introductory chapter Part 1 presents the reader with an account of structure factor formalisms an extensive treatment of the theory algorithms and crystallographic applications of Fourier methods and fundamental as well as advanced treatments of symmetry in reciprocal space In Part 2 these general accounts are followed by detailed expositions of crystallographic statistics the theory of direct methods Patterson techniques isomorphous replacement and anomalous scattering and treatments of the role of electron microscopy and diffraction in crystal structure determination including applications of direct methods to electron crystallography Part 3 deals with applications of reciprocal space to molecular geometry and best plane calculations and contains a treatment of the principles of molecular graphics and modelling and their applications A convergence acceleration method of importance in the computation of approximate lattice sums is presented and the part concludes with a discussion of the Ewald method Part 4 contains treatments of various diffuse scattering phenomena arising from crystal dynamics disorder and low dimensionality liquid crystals and an exposition of the underlying theories and or experimental evidence Polymer crystallography and reciprocal space images of aperiodic crystals are also treated Part 5 of the volume contains introductory treatments of the theory of the interaction of radiation with matter dynamical theory as applied to X ray electron and neutron diffraction techniques The simplified trigonometric expressions for the structure factors in the 230 three dimensional space groups which appeared in Volume I of International Tables for X ray Crystallography are now given in Appendix 1 4 3 to Chapter 1 4 of this volume Volume B is a vital addition to the library of scientists engaged in crystal structure determination crystallographic computing crystal physics and other fields of crystallographic research Graduate students specializing in crystallography will find much material suitable for self study and a rich source of references to the relevant literature

International Tables for Crystallography, Volume B

U. Shmueli, 2008-08-25 International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science Volume B presents accounts of the numerous aspects of reciprocal space in crystallographic research This volume is a vital addition to the library of scientists engaged in crystal structure determination crystallographic computing crystal physics and other fields of crystallographic research Graduate students specializing in crystallography will find much material suitable for self study and a rich source of references to the relevant literature New to this edition A new chapter on modern extensions of the Ewald method for Coulomb interactions in crystals Three new sections on electron diffraction and electron microscopy in structure determination describing point group and space group determination by convergent beam electron diffraction three dimensional reconstruction and single particle reconstruction Substantial revisions to the chapters on space group representations in reciprocal space direct methods Patterson and molecular replacement techniques and disorder diffuse scattering More information on the series can be found at <http://it.iucr.org>

Metallic Alloys: Experimental and Theoretical Perspectives J.S. Faulkner, R.G. Jordan, 2012-12-06 The development of new materials is recognized as one of the major elements in the overall technological evolution that must go on in order to

sustain and even improve the quality of life for citizens of all nations There are many components to this development but one is to achieve a better understanding of the properties of materials using the most sophisticated scientific tools that are available As condensed matter physicists and materials scientists work toward this goal they find that it is useful to divide their efforts and focus on specific areas because certain analytical and theoretical techniques will be more useful for the study of one class of materials than another One such area is the study of metals and metallic alloys which are used in the manufacture of products as diverse as automobiles and space stations Progress in this area has been very rapid in recent years and the new developments come from many different countries For these reasons the Advanced Research Workshop Programme in the NATO Scientific Affairs Division has seen fit to sponsor several meetings to bring together the researchers and students working in this field from the NATO countries and elsewhere There have been a series of NATO ASI s that have dealt with the results of research on the electronic structure of materials and the properties of metals alloys and interfaces They are Electrons in finite and infinite structures P Phariseau and L Statics and Dynamics of Alloy Phase Transformations Patrice E.A. Turchi,A. Gonis,2012-12-06 The study of phase transformations in substitutional alloys including order disorder phenomena and structural transformations plays a crucial role in understanding the physical and mechanical properties of materials and in designing alloys with desired technologically important characteristics Indeed most of the physical properties including equilibrium properties transport magnetic vibrational as well as mechanical properties of alloys are often controlled by and are highly sensitive to the existence of ordered compounds and to the occurrence of structural transformations Correspondingly the alloy designer facing the task of processing new high performance materials with properties that meet specific industrial applications must answer the following question What is the crystalline structure and the atomic configuration that an alloy may exhibit at given temperature and concentration Usually the answer is sought in the phase diagram of a relevant system that is often determined experimentally and does not provide insight to the underlying mechanisms driving phase stability Because of the rather tedious and highly risky nature of developing new materials through conventional metallurgical techniques a great deal of effort has been expended in devising methods for understanding the mechanisms controlling phase transformations at the microscopic level These efforts have been bolstered through the development of fully ab initio accurate theoretical models coupled with the advent of new experimental methods and of powerful supercomputer capabilities

Compton Scattering Frank Wissmann,2003-12-03 A comprehensive summary of experiments on Compton scattering from the proton and neutron performed at the electron accelerator MAMI The experiments cover a photon energy range from 30 MeV to 500 MeV The reader is introduced to the theoretical concepts of Compton scattering followed by a description of the experiments on the proton their analysis and results

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