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Applied Computational Materials Modeling

Theory, Simulation and
Experiment

 Springer

Applied Computational Materials Modeling Theory Simulation And Experiment

Francis Froes, Ma Qian



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Applied Computational Materials Modeling Guillermo Bozzolo, Ronald D. Noebe, Phillip B. Abel, 2007-12-19 While it is tempting to label computational materials modeling as an emerging field of research the truth is that both in nature and foundation it is just as much an established field as the concepts and techniques that define it It is the recent enormous growth in computing power and communications that has brought the activity to the forefront turning it into a possible component of any modern materials research program Together with its increased role and visibility there is also a dynamic change in the way computational modeling is perceived in such a vast field as materials science with its wide range of length and time scales As the pace of materials research accelerates and the need for often inaccessible information continues to grow the demands and expectations on existing modeling techniques have progressed that much faster Primarily because there is no one technique that can provide all the answers at every length and time scale in materials science excessive expectations of computational materials modeling should be avoided if possible While it is apparent that computational modeling is the most efficient method for dealing with complex systems it should not be seen as an alternative to traditional experimentation Instead there is another option which is perhaps the one that is most likely to become the defining characteristic of computational materials modeling

Applied Computational Materials Modeling Guillermo Bozzolo, Ronald D. Noebe, Phillip Benjamin Abel, 2007

Integrated Computational Materials Engineering (ICME) for Metals Mark F. Horstemeyer, 2018-03-01 Focuses entirely on demystifying the field and subject of ICME and provides step by step guidance on its industrial application via case studies This highly anticipated follow up to Mark F Horstemeyer's pedagogical book on Integrated Computational Materials Engineering ICME concepts includes engineering practice case studies related to the analysis design and use of structural metal alloys A welcome supplement to the first book which includes the theory and methods required for teaching the subject in the classroom Integrated Computational Materials Engineering ICME For Metals Concepts and Case Studies focuses on engineering applications that have occurred in industries demonstrating the ICME methodologies and aims to catalyze industrial diffusion of ICME technologies throughout the world The recent confluence of smaller desktop computers with enhanced computing power coupled with the emergence of physically based material models has created the clear trend for modeling and simulation in product design which helped create a need to integrate more knowledge into materials processing and product performance Integrated Computational Materials Engineering ICME For Metals Case Studies educates those seeking that knowledge with chapters covering Body Centered Cubic Materials Designing An Interatomic Potential For Fe C Alloys Phase Field Crystal Modeling Simulating Dislocation Plasticity in BCC Metals by Integrating Fundamental Concepts with Macroscale Models Steel Powder Metal Modeling Hexagonal Close Packed Materials Multiscale Modeling of Pure Nickel Predicting Constitutive Equations for Materials Design and more Presents case studies that connect modeling and simulation for different materials processing

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Computational Design of Engineering Materials Yong Du, Rainer Schmid-Fetzer, Jincheng Wang, Shuhong Liu, Jianchuan Wang, Zhanpeng Jin, 2023-06-29 Introducing state of the art computational methods this book combines detailed explanations with real world case studies to give a full grounding in the design of engineering materials This book presents a wide spectrum of key computational methods such as CALPHAD method first principles calculations phase field simulation and finite element analysis covering the atomic meso macro scale range The reader will see these methods applied to case studies for steel light alloys superalloys cemented carbides hard coating and energy materials demonstrating in detail how real world materials are designed Online ancillary material includes input files for computational design software providing the reader with hands on design experience Step by step instructions will allow you to perform and repeat the simulations discussed in the book Aimed at both graduate and undergraduate students as well as non specialist researchers in materials science and engineering including ceramics metallurgy and chemistry this is an ideal introductory and reference book

Models, Databases and Simulation Tools Needed for Realization of Integrated Computational Mat. Eng. (ICME 2010) Steven M. Arnold and Terry T. Wong, Editors, 2011 TMS 2018 147th Annual Meeting & Exhibition Supplemental Proceedings The Minerals, Metals & Materials Society, 2018-02-03 This collection features papers presented at the 147th Annual Meeting Exhibition of The Minerals Metals Materials Society

A Quantum Approach to Alloy Design Masahiko Morinaga, 2018-11-16 A Quantum Approach to Alloy Design An Exploration of Material Design and Development Based Upon Alloy Design Theory and Atomization Energy Method presents a molecular orbital approach to alloy design that is based on electronic structure calculations using the DV X alpha cluster method and new alloying parameters obtained from these calculations Topics discussed include alloy properties such as corrosion resistance shape memory effect and super elasticity that are treated by using alloying parameters in biomedical titanium alloys This book covers various topics of not only metals and alloys but also metal oxides hydrides and even hydrocarbons In addition important alloy properties such as strength corrosion resistance hydrogen storage and catalysis are treated in view of electron theory Presents alloy design theory and the atomization energy method and its use for the fundamental understanding of materials and materials design and development Discusses for the first time the atomization energy analysis of the local lattice strains introduced around alloying elements in metals Illustrates a simplified approach to predict the structure and phases stability of new alloys materials

Titanium in Medical and Dental Applications Francis Froes, Ma Qian, 2018-05-09 Titanium in Medical and Dental Applications is an essential reference book for those involved in

biomedical materials and advanced metals Written by well known experts in the field it covers a broad array of titanium uses including implants instruments devices the manufacturing processes used to create them their properties corrosion resistance and various fabrication approaches Biomedical titanium materials are a critically important part of biomaterials especially in cases where non metallic biomedical materials are not suited to applications such as the case of load bearing implants The book also covers the use of titanium for implants in the medical and dental fields and reviews the use of titanium for medical instruments and devices Provides an understanding of the essential and broad applications of Titanium in both the medical and dental industries Discusses the pathways to manufacturing titanium into critical biomedical and dental devices Includes insights into further applications within the industry

Physico-Chemical Properties of Nanomaterials Richard C. Pleus, Vladimir Murashov, 2018-07-17 Throughout human history we have long encountered the combination of promise risk and uncertainty that accompanies emerging technologies Nanotechnology is a recent example of an emerging technology that promises to drastically improve existing products as well as allow for creative development of new goods and services This new technology also has its potential downsides Industry academia and regulatory agencies are all working overtime to assess risks accurately while keeping up with the pace of development Subtle changes in the physicochemical properties of engineered nanomaterials ENMs can influence their toxicity and behavior in the environment and so can be used to help control potential ENM risks This book attempts to encompass the state of the science regarding physicochemical characterization of ENMs It illuminates the effort to understand these properties and how they may be used to ensure safe ENM deployment in existing or future materials and products

Computational Modelling of Nanomaterials Panagiotis Grammatikopoulos, 2020-09-30 Due to their small size and their dependence on very fast phenomena nanomaterials are ideal systems for computational modelling This book provides an overview of various nanosystems classified by their dimensions 0D nanoparticles QDs etc 1D nanowires nanotubes 2D thin films graphene etc 3D nanostructured bulk materials devices Fractal dimensions such as nanoparticle agglomerates percolating films and combinations of materials of different dimensionalities are also covered e g epitaxial decoration of nanowires by nanoparticles i e 0D 1D nanomaterials For each class the focus will be on growth structure and physical chemical properties The book presents a broad range of techniques including density functional theory molecular dynamics non equilibrium molecular dynamics finite element modelling FEM numerical modelling and meso scale modelling The focus is on each method s relevance and suitability for the study of materials and phenomena in the nanoscale This book is an important resource for understanding the mechanisms behind basic properties of nanomaterials and the major techniques for computational modelling of nanomaterials Explores the major modelling techniques used for different classes of nanomaterials Assesses the best modelling technique to use for each different type of nanomaterials Discusses the challenges of using certain modelling techniques with specific nanomaterials

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