

Modeling and Simulation of Microstructure Evolution in Solidifying Alloys

Laurentiu Nastac



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Modeling and Simulation of Microstructure Evolution in Solidifying Alloys Laurentiu Nastac, 2004 **Modeling and Simulation of Microstructure Evolution in Solidifying Alloys** Laurentiu Nastac, 2004-05-31 The aim of Modeling and Simulation of Microstructure Evolution in Solidifying Alloys is to describe in a clear mathematical language the physics of the solidification structure evolution of cast alloys The concepts and methodologies presented here for the net shaped casting and the ingot remelt processes can be applied with some modifications to model other solidification processes such as welding and deposition processes Another aim of the book is to provide simulation examples of the solidification structure modeling in some crucial commercial casting technologies as well as to provide practical techniques for controlling the structure formation during the solidification processes Modeling and Simulation of Microstructure Evolution and Deformation in an Irradiated Environment Stephanie Anne Pitts, 2019 The ability to predict the behavior of structural components in a nuclear power plant is critical to the nuclear industry Structural metals in the primary loop of nuclear power plants must endure challenges such as irradiation and mechanical and thermal loading and these structural metal components must continue to function in potential transient and accident conditions throughout the operational lifetime of the power plant This extreme operational environment changes the metal microstructure by creating additional defects The physical interactions of dislocations with these defects govern how the metal will respond to future conditions Therefore predicting the mechanical response of these metals requires a set of physically based and reliable models of dislocation and defect interactions These microstructure elements include glide mobile and immobile dislocations geometrically necessary dislocations twinning dislocations irradiation defects and thermal aging defects We present here a continuum dislocation dynamics crystal plasticity framework to capture the interaction mechanisms of these dislocations and defects verified with a combination of benchmark problems and comparisons with experimental data for two different types of structural metals iron and nickel based alloys In our simulations of iron we highlight the advantages of applying a Monte Carlo stochastic model of cross slip dislocation motion and show the importance of capturing the 3D nature of glide dislocation and self interstitial atom loop radiation defect interactions We demonstrate coupling of glide dislocations with geometrically necessary dislocations to capture the influence of lattice bending including the sensitivity of the geometrically necessary dislocations to changes in the grain boundary angle We further examine the interaction of glide dislocations with the twin dislocations and thermally aged defects which have been observed in a nickel based alloy with additional models Finally we assess the reliability of this crystal plasticity framework by comparing two dislocation glide velocity models across the range of normal operation temperatures In successfully applying our crystal plasticity framework to multiple metals we provide further evidence of the reliability of our approach The results of this mechanism based continuum dislocation dynamics crystal plasticity framework can be used to inform engineering scale models throughout the nuclear industry Proceedings of the

6th International Conference on Recrystallization and Grain Growth (ReX&GG 2016) Elizabeth Holm, Susan Farjami, Priyadarshan Manohar, Gregory Rohrer, Anthony Rollett, David Srolovitz, Hasso Weiland, 2016-11-22 This collection represents a cross section of the papers presented at the 6th International Conference on Recrystallization and Grain Growth The volume is divided into nine sections Grain growth theory and simulation Recrystallization theory and simulation Low carbon and IF steels High strength steels Electrical steels Stainless steels Aluminum and magnesium alloys Nickel and nickel based superalloys Unconventional and advanced materials **Multi-Physics and Multi-Scale Modeling and Simulation Methods for Nuclear Reactor Application** Xingjie Peng, Qingming He, Jingang Liang, Shichang Liu, Jiankai Yu, 2024-02-28 A nuclear reactor operates in an environment where complex multi physics and multi scale phenomena exist and it requires consideration of coupling among neutronics thermal hydraulics fuel performance chemical dynamics and coupling between the reactor core and first circuit Safe reliable and economical operation can be achieved by leveraging high fidelity numerical simulation and proper considerations for coupling among different physics and required to provide powerful numerical simulation tools In the past simplistic models for some of the physics phenomena are used with the recent development of advanced numerical methods software design and high performance computing power the appeal of multi physics and multi scale modeling and simulation has been broadened 2D and 3D Grain Growth Modeling and Simulation Luis Antonio Barrales-Mora, 2008 Springer Handbook of Additive Manufacturing Eujin Pei, Alain Bernard, Dongdong Gu, Christoph Klahn, Mario Monzón, Maren Petersen, Tao Sun, 2023-10-24 This Handbook is the ultimate definitive guide that covers key fundamentals and advanced applications for Additive Manufacturing The Handbook has been structured into seven sections comprising of a thorough Introduction to Additive Manufacturing Design and Data Processes Materials Post processing Testing and Inspection Education and Training and Applications and Case Study Examples The general principles and functional relationships are described in each chapter and supplemented with industry use cases The aim of this book is to help designers engineers and manufacturers understand the state of the art developments in the field of Additive Manufacturing Although this book is primarily aimed at students and educators it will appeal to researchers and industrial professionals working with technology users machine or component manufacturers to help them make better decisions in the implementation of Additive Manufacturing and its applications **Computational Methods for Microstructure-Property Relationships** Somnath Ghosh, Dennis Dimiduk, 2010-11-17 Computational Methods for Microstructure Property Relationships introduces state of the art advances in computational modeling approaches for materials structure property relations Written with an approach that recognizes the necessity of the engineering computational mechanics framework this volume provides balanced treatment of heterogeneous materials structures within the microstructural and component scales Encompassing both computational mechanics and computational materials science disciplines this volume offers an analysis of the current techniques and selected topics important to industry researchers such as deformation creep and fatigue of

primarily metallic materials Researchers engineers and professionals involved with predicting performance and failure of materials will find Computational Methods for Microstructure Property Relationships a valuable reference Computer Aided Innovation of New Materials J. Kihara,R. Yamamoto,M. Doyama,T. Suzuki,2012-12-02 This volume brings together the experience of specialists in the entire field of applications of Materials Science The volume contains 196 of the excellent papers presented at the conference This multidisciplinary meeting was held to bring together workers in a wide range of materials science and engineering activities who employ common analytical and experimental methods in their day to day work The results of the meeting are of worldwide interest and will help to stimulate future research and analysis in this area

Advances in Heterogeneous Material Mechanics 2011 Jinghong Fan,2011 *Proceedings of the 8th International Symposium on Superalloy 718 and Derivatives* The Minerals, Metals & Materials Society (TMS),2014-12-02

Computational Design of Engineering Materials Yong Du,Rainer Schmid-Fetzer,Jincheng Wang,Shuhong Liu,Jianchuan Wang,Zhanpeng Jin,2023-06-29 Presenting the fundamentals key multiscale methods and case studies for computational design of engineering materials Thermo-Mechanical Modeling of Additive Manufacturing Michael Gouge,Pan Michaleris,2017-08-03 Thermo mechanical Modeling of Additive Manufacturing provides the background methodology and description of modeling techniques to enable the reader to perform their own accurate and reliable simulations of any additive process Part I provides an in depth introduction to the fundamentals of additive manufacturing modeling a description of adaptive mesh strategies a thorough description of thermal losses and a discussion of residual stress and distortion Part II applies the engineering fundamentals to direct energy deposition processes including laser cladding LENS builds large electron beam parts and an exploration of residual stress and deformation mitigation strategies Part III concerns the thermo mechanical modeling of powder bed processes with a description of the heat input model classical thermo mechanical modeling and part scale modeling The book serves as an essential reference for engineers and technicians in both industry and academia performing both research and full scale production Additive manufacturing processes are revolutionizing production throughout industry These technologies enable the cost effective manufacture of small lot parts rapid repair of damaged components and construction of previously impossible to produce geometries However the large thermal gradients inherent in these processes incur large residual stresses and mechanical distortion which can push the finished component out of engineering tolerance Costly trial and error methods are commonly used for failure mitigation Finite element modeling provides a compelling alternative allowing for the prediction of residual stresses and distortion and thus a tool to investigate methods of failure mitigation prior to building Provides understanding of important components in the finite element modeling of additive manufacturing processes necessary to obtain accurate results Offers a deeper understanding of how the thermal gradients inherent in additive manufacturing induce distortion and residual stresses and how to mitigate these undesirable phenomena Includes a set of strategies for the modeler to improve

computational efficiency when simulating various additive manufacturing processes Serves as an essential reference for engineers and technicians in both industry and academia *Multiscale Materials Modelling* Z. X. Guo,2007-05-31 Multiscale materials modelling offers an integrated approach to modelling material behaviour across a range of scales from the electronic atomic and microstructural up to the component level As a result it provides valuable new insights into complex structures and their properties opening the way to develop new multi functional materials together with improved process and product designs Multiscale materials modelling summarises some of the key techniques and their applications The various chapters cover the spectrum of scales in modelling methodologies including electronic structure calculations mesoscale and continuum modelling The book covers such themes as dislocation behaviour and plasticity as well as the modelling of structural materials such as metals polymers and ceramics With its distinguished editor and international team of contributors Multiscale materials modelling is a valuable reference for both the modelling community and those in industry wanting to know more about how multiscale materials modelling can help optimise product and process design Reviews the principles and applications of mult scale materials modelling Covers themes such as dislocation behaviour and plasticity and the modelling of structural materials Examines the spectrum of scales in modelling methodologies including electronic structure calculations mesoscale and continuum modelling **Computational Materials Engineering** Koenraad George Frans Janssens,Dierk Raabe,Ernest Kozeschnik,Mark A Miodownik,Britta Nestler,2010-07-26 Computational Materials Engineering is an advanced introduction to the computer aided modeling of essential material properties and behavior including the physical thermal and chemical parameters as well as the mathematical tools used to perform simulations Its emphasis will be on crystalline materials which includes all metals The basis of Computational Materials Engineering allows scientists and engineers to create virtual simulations of material behavior and properties to better understand how a particular material works and performs and then use that knowledge to design improvements for particular material applications The text displays knowledge of software designers materials scientists and engineers and those involved in materials applications like mechanical engineers civil engineers electrical engineers and chemical engineers Readers from students to practicing engineers to materials research scientists will find in this book a single source of the major elements that make up contemporary computer modeling of materials characteristics and behavior The reader will gain an understanding of the underlying statistical and analytical tools that are the basis for modeling complex material interactions including an understanding of computational thermodynamics and molecular kinetics as well as various modeling systems Finally the book will offer the reader a variety of algorithms to use in solving typical modeling problems so that the theory presented herein can be put to real world use Balanced coverage of fundamentals of materials modeling as well as more advanced aspects of modeling such as modeling at all scales from the atomic to the molecular to the macro material Concise yet rigorous mathematical coverage of such analytical tools as the Potts type Monte Carlo method cellular

automata phase field dislocation dynamics and Finite Element Analysis in statistical and analytical modeling *Additive Manufacturing of High-performance Metals and Alloys* Igor Shishkovsky, 2018-07-11 Freedoms in material choice based on combinatorial design different directions of process optimization and computational tools are a significant advantage of additive manufacturing technology The combination of additive and information technologies enables rapid prototyping and rapid manufacturing models on the design stage thereby significantly accelerating the design cycle in mechanical engineering Modern and high demand powder bed fusion and directed energy deposition methods allow obtaining functional complex shapes and functionally graded structures Until now the experimental parametric analysis remains as the main method during AM optimization Therefore an additional goal of this book is to introduce readers to new modeling and material s optimization approaches in the rapidly changing world of additive manufacturing of high performance metals and alloys **Creep and Fracture in High Temperature Components** European Creep Collaborative Committee, 2005

Provides information from around the world on creep in multiple high temperature metals alloys and advanced materials

Handbook of Materials Modeling Sidney Yip, 2007-11-17 This Handbook contains a set of articles introducing the modeling and simulation of materials from the standpoint of basic methods and studies The intent is to provide a compendium that is foundational to an emerging eld of computational research a new discipline that may now be called Computational Materials This area has become suf ciently diverse that any attempt to cover all the pertinent topics would be futile Even with a limited scope the present undertaking has required the dedicated efforts of 13 Subject Editors to set the scope of nine chapters solicit authors and collect the manuscripts The contributors were asked to target students and non specialists as the primary audience to provide an accessible entry into the eld and to offer references for further reading With no precedents to follow the editors and authors were only guided by a common goal to produce a volume that would set a standard toward de ning the broad community and stimulating its growth The idea of a reference work on materials modeling surfaced in conver tions with Peter Bin eld then the Reference Works Editor at Kluwer Academic Publishers in the spring of 1999 The rationale at the time already seemed quite clear the eld of computational materials research was t ing off powerful computer capabilities were becoming increasingly available and many sectors of the scienti c community were getting involved in the enterprise *Nanostructures in Ferroelectric Films for Energy Applications* Jun Ouyang, 2019-06-07 Nanostructures in Ferroelectric Films for Energy Applications Grains Domains Interfaces and Engineering Methods presents methods of engineering nanostructures in ferroelectric films to improve their performance in energy harvesting and conversion and storage Ferroelectric films which have broad applications including the emerging energy technology usually consist of nanoscale inhomogeneities For polycrystalline films the size and distribution of nano grains determines the macroscopic properties especially the field induced polarization response For epitaxial films the energy of internal long range electric and elastic fields during their growth are minimized by formation of self assembled nano domains This book is an

accessible reference for both instructors in academia and R D professionals **Electromigration in Metals** Paul S. Ho,Chao-Kun Hu,Martin Gall,Valeriy Sukharev,2022-05-12 Learn to assess electromigration reliability and design more resilient chips in this comprehensive and practical resource Beginning with fundamental physics and building to advanced methodologies this book enables the reader to develop highly reliable on chip wiring stacks and power grids Through a detailed review on the role of microstructure interfaces and processing on electromigration reliability as well as characterisation testing and analysis the book follows the development of on chip interconnects from microscale to nanoscale Practical modeling methodologies for statistical analysis from simple 1D approximation to complex 3D description can be used for step by step development of reliable on chip wiring stacks and industrial grade power ground grids This is an ideal resource for materials scientists and reliability and chip design engineers

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