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dislocations, mesoscale simulations and plastic flow

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Dislocations Mesoscale Simulations And Plastic Flow Oxford Series On Materials Modelling

A. H. Cottrell



Dislocations Mesoscale Simulations And Plastic Flow Oxford Series On Materials Modelling:

Dislocations, Mesoscale Simulations and Plastic Flow L. Kubin, 2013-04-18 In the past twenty years new experimental approaches improved models and progress in simulation techniques brought new insights into long standing issues concerning dislocation based plasticity in crystalline materials Dislocation dynamics simulations are becoming accessible to a wide range of users This book presents to students and researchers in materials science and mechanical engineering a comprehensive coverage of the physical body of knowledge on which they are based This includes classical studies which are too often ignored recent experimental and theoretical advances as well as a discussion of selected applications on various topics [Modeling High Temperature Materials Behavior for Structural Analysis](#) Konstantin Naumenko, Holm Altenbach, 2016-05-11 This monograph presents approaches to characterize inelastic behavior of materials and structures at high temperature Starting from experimental observations it discusses basic features of inelastic phenomena including creep plasticity relaxation low cycle and thermal fatigue The authors formulate constitutive equations to describe the inelastic response for the given states of stress and microstructure They introduce evolution equations to capture hardening recovery softening ageing and damage processes Principles of continuum mechanics and thermodynamics are presented to provide a framework for the modeling materials behavior with the aim of structural analysis of high temperature engineering components **Multiscale Materials Modeling for Nanomechanics** Christopher R. Weinberger, Garritt J. Tucker, 2016-08-30 This book presents a unique combination of chapters that together provide a practical introduction to multiscale modeling applied to nanoscale materials mechanics The goal of this book is to present a balanced treatment of both the theory of the methodology as well as some practical aspects of conducting the simulations and models The first half of the book covers some fundamental modeling and simulation techniques ranging from ab initio methods to the continuum scale Included in this set of methods are several different concurrent multiscale methods for bridging time and length scales applicable to mechanics at the nanoscale regime The second half of the book presents a range of case studies from a varied selection of research groups focusing either on the application of multiscale modeling to a specific nanomaterial or novel analysis techniques aimed at exploring nanomechanics Readers are also directed to helpful sites and other resources throughout the book where the simulation codes and methodologies discussed herein can be accessed Emphasis on the practicality of the detailed techniques is especially felt in the latter half of the book which is dedicated to specific examples to study nanomechanics and multiscale materials behavior An instructive avenue for learning how to effectively apply these simulation tools to solve nanomechanics problems is to study previous endeavors Therefore each chapter is written by a unique team of experts who have used multiscale materials modeling to solve a practical nanomechanics problem These chapters provide an extensive picture of the multiscale materials landscape from problem statement through the final results and outlook providing readers with a roadmap for incorporating these techniques into

their own research **Advances in Applied Mechanics** ,2014-11-21 Advances in Applied Mechanics draws together recent significant advances in various topics in applied mechanics Published since 1948 Advances in Applied Mechanics aims to provide authoritative review articles on topics in the mechanical sciences primarily of interest to scientists and engineers working in the various branches of mechanics but also of interest to the many who use the results of investigations in mechanics in various application areas such as aerospace chemical civil environmental mechanical and nuclear engineering Covers all fields of the mechanical sciences Highlights classical and modern areas of mechanics that are ready for review Provides comprehensive coverage of the field in question **Theory and Application of Quantum-Based Interatomic Potentials in Metals and Alloys** John A. Moriarty,2023 The book spans the entire QBIP process from foundation in fundamental theory to development and machine learning optimization of accurate potentials for real materials to the application of the potentials to materials modeling and simulation of structural thermodynamic defect and mechanical properties of important metals and alloys Nickel Base Single Crystals Across Length Scales Loeiz Nazé,Vincent Maurel,Gunther Eggeler,Jonathan Cormier,Georges Cailletaud,2021-09-28 Nickel Base Single Crystals Across Length Scales is addresses the most advanced knowledge in metallurgy and computational mechanics and how they are applied to superalloys used as bare materials or with a thermal barrier coating system Joining both aspects the book helps readers understand the mechanisms driving properties and their evolution from fundamental to application level These guidelines are helpful for students and researchers who wish to understand issues and solutions optimize materials and model them in a cross check analysis from the atomistic to component scale The book is useful for students and engineers as it explores processing characterization and design Provides an up to date overview on the field of superalloys Covers the relationship between microstructural evolution and mechanical behavior at high temperatures Discusses both basic and advanced modeling and characterization techniques Includes case studies that illustrate the application of techniques presented in the book **From Creep Damage Mechanics to Homogenization Methods** Holm Altenbach,Tetsuya Matsuda,Dai Okumura,2015-06-03 This volume presents a collection of contributions on materials modeling which were written to celebrate the 65th birthday of Prof Nobutada Ohno The book follows Prof Ohno s scientific topics starting with creep damage problems and ending with homogenization methods Handbook of Software Solutions for ICME Georg J. Schmitz,Ulrich Prahl,2016-12-19 As one of the results of an ambitious project this handbook provides a well structured directory of globally available software tools in the area of Integrated Computational Materials Engineering ICME The compilation covers models software tools and numerical methods allowing describing electronic atomistic and mesoscopic phenomena which in their combination determine the microstructure and the properties of materials It reaches out to simulations of component manufacture comprising primary shaping forming joining coating heat treatment and machining processes Models and tools addressing the in service behavior like fatigue corrosion and eventually recycling complete the compilation An introductory

overview is provided for each of these different modelling areas highlighting the relevant phenomena and also discussing the current state for the different simulation approaches A must have for researchers application engineers and simulation software providers seeking a holistic overview about the current state of the art in a huge variety of modelling topics This handbook equally serves as a reference manual for academic and commercial software developers and providers for industrial users of simulation software and for decision makers seeking to optimize their production by simulations In view of its sound introductions into the different fields of materials physics materials chemistry materials engineering and materials processing it also serves as a tutorial for students in the emerging discipline of ICME which requires a broad view on things and at least a basic education in adjacent fields

Comprehensive Nuclear Materials ,2020-07-22 Materials in a nuclear environment are exposed to extreme conditions of radiation temperature and or corrosion and in many cases the combination of these makes the material behavior very different from conventional materials This is evident for the four major technological challenges the nuclear technology domain is facing currently i long term operation of existing Generation II nuclear power plants ii the design of the next generation reactors Generation IV iii the construction of the ITER fusion reactor in Cadarache France iv and the intermediate and final disposal of nuclear waste In order to address these challenges engineers and designers need to know the properties of a wide variety of materials under these conditions and to understand the underlying processes affecting changes in their behavior in order to assess their performance and to determine the limits of operation Comprehensive Nuclear Materials Second Edition Seven Volume Set provides broad ranging validated summaries of all the major topics in the field of nuclear material research for fission as well as fusion reactor systems Attention is given to the fundamental scientific aspects of nuclear materials fuel and structural materials for fission reactors waste materials and materials for fusion reactors The articles are written at a level that allows undergraduate students to understand the material while providing active researchers with a ready reference resource of information Most of the chapters from the first Edition have been revised and updated and a significant number of new topics are covered in completely new material During the ten years between the two editions the challenge for applications of nuclear materials has been significantly impacted by world events public awareness and technological innovation Materials play a key role as enablers of new technologies and we trust that this new edition of Comprehensive Nuclear Materials has captured the key recent developments Critically reviews the major classes and functions of materials supporting the selection assessment validation and engineering of materials in extreme nuclear environments Comprehensive resource for up to date and authoritative information which is not always available elsewhere even in journals Provides an in depth treatment of materials modeling and simulation with a specific focus on nuclear issues Serves as an excellent entry point for students and researchers new to the field

Dislocations in Solids: without special title Frank Reginald Nunes Nabarro,1979 **Metals Abstracts** ,1999-04 *Computer Simulations of Dislocations* Vasily Bulatov,Wei Cai,2006-11-02 This book presents a broad

collection of models and computational methods from atomistic to continuum applied to crystal dislocations. Its purpose is to help students and researchers in computational materials sciences to acquire practical knowledge of relevant simulation methods. Because their behavior spans multiple length and time scales, crystal dislocations present a common ground for an in-depth discussion of a variety of computational approaches, including their relative strengths, weaknesses, and interconnections. The details of the covered methods are presented in the form of numerical recipes and illustrated by case studies. A suite of simulation codes and data files is made available on the book's website to help the reader to learn by doing through solving the exercise problems offered in the book.

The Application of Distributed Dislocations to the Modelling of Plane Plastic Flow P. M. Blomerus, 1998

Multiscale Modelling of Plasticity and Fracture by Means of Dislocation Mechanics Peter Gumbsch, Reinhard Pippan, 2011-01-30

The latest state of simulation techniques to model plasticity and fracture in crystalline materials on the nano and microscale is presented. Discrete dislocation mechanics and the neighbouring fields molecular dynamics and crystal plasticity are central parts. The physical phenomena, the theoretical basics, their mathematical description, and the simulation techniques are introduced, and important problems from the formation of dislocation structures to fatigue and fracture from the nano to microscale as well as its impact on the macro behaviour are considered.

Modeling the Deformation of Engineered Nano-Layered Structures by Computer Simulations, 2006

We developed here fundamental models of plasticity based on dislocation dynamics and atomistic computer simulation methods for the prediction of the strength and plastic deformation at the nano to micro length scales. The models are applied to the simulation of plastic flow in ultra strong nano laminates. The developed methods are:

1. An ab initio based hybrid approach based on an extension of the parametric dislocation dynamics (DD) to bi materials where the dislocation spreading over the interface is explicitly accounted.
2. A hybrid ab initio discrete dislocation dynamics model to study the core structure in straight and curved dislocations with application to single layers and across material interfaces.
3. Molecular dynamics (MD) modeling of dislocation motion and deformation in nano layered composite materials and twins.
4. Dislocation Dynamics (DD) modeling of dislocation motion and deformation modes of anisotropic nano layered composite materials.

Multiscale Modeling of Dislocation Processes in BCC Tantalum, 2001

Plastic deformation in bcc metals at low temperatures and high strain rates is controlled by the motion of a 2111 screw dislocations, and understanding the fundamental atomistic processes of this motion is essential to develop predictive multiscale models of crystal plasticity. The multiscale modeling approach presented here for bcc Ta is based on information passing where results of simulations at the atomic scale are used in simulations of plastic deformation at mesoscopic length scales via dislocation dynamics (DD). The relevant core properties of a 2111 screw dislocations in Ta have been obtained using quantum based interatomic potentials derived from model generalized pseudopotential theory and an ab initio data base together with an accurate Green's function simulation method that implements flexible boundary conditions. In particular, the stress dependent activation enthalpy for

the lowest energy kink pair mechanism has been calculated and fitted to a revealing analytic form This is the critical quantity determining dislocation mobility in the DD simulations and the present activation enthalpy is found to be in good agreement with the previous empirical form used to explain the temperature dependence of the yield stress

Dislocation Dynamics During Plastic Deformation Ulrich Messerschmidt, 2010-04-19 Along with numerous illustrative examples this text provides an overview of the dynamic behavior of dislocations and its relation to plastic deformation It introduces the general properties of dislocations and treats the dislocation dynamics in some detail

The Investigation of Plastic Behavior by Discrete Dislocation Dynamics for Single Crystal Pillar at Submicron Scale Yinan Cui, 2016-10-26 This thesis transports you to a wonderful and fascinating small scale world and tells you the origin of several new phenomena The investigative tool is the improved discrete dislocation based multi scale approaches bridging the continuum modeling and atomistic simulation Mechanism based theoretical models are put forward to conveniently predict the mechanical responses and defect evolution The findings presented in this thesis yield valuable new guidelines for microdevice design reliability analysis and defect tuning

Dislocations and Plastic Flow in Crystals A. H. Cottrell, 1953

Statistical Analysis and Constitutive Modeling of Crystal Plasticity Using Dislocation Dynamics Simulation Database Shamseddin

Akhondzadeh, 2021 Most metals are crystalline materials that can undergo significant plastic permanent deformation when subjected to applied loading Plastic deformation is usually accompanied by an increase in the flow stress of the material This phenomenon is called strain hardening and is of vital importance in many engineering applications including aerospace automotive and power generation industries Developing accurate material models to predict the plastic response and hardening behavior of metals during deformation is a prerequisite to the engineering design processes which requires a physical understanding of the underlying deformation mechanisms In single crystals plastic deformation of the crystal is governed by the evolution of dislocations line defects inside the crystalline materials which marks the boundary between the slipped and unslipped regions moving and interacting in response to the applied loading Dislocation dynamics DD simulations which track the time space trajectories of individual dislocation lines provide a promising tool to establish a physical link between the dislocation microstructure evolution and the strain hardening phenomenon However the high computational cost of DD simulations renders the accessible length and time scales to well below those which are relevant to most engineering applications Due to this challenge instead of directly using DD simulations for engineering applications we have utilized DD simulations to delineate how constitutive relations of crystal plasticity CP can be constructed for FCC copper based on coarse graining of high throughput DD simulations This thesis consists of three main components and we show how they fit together into a complete physical model like three pieces of a puzzle The first piece is a massive DD simulation database that we were able to generate thanks to recent computational advances in DD including the subcycling time integration algorithm and its implementation on Graphics Processing Units GPUs By systematically coarse graining the

database we present a strain hardening model which consists of two components 1 a dislocation multiplication model which accounts for slip free multiplication and 2 an exponential flow rule connecting slip system shear rate to the resolved shear stress through an exponential function These components can be thought of as the second and third puzzle pieces By analyzing the data it was discovered that dislocation multiplication frequently occurs on slip systems which experience zero applied shear stress i e zero Schmid factor and have a plastic strain rate of zero we termed such multiplication slip free multiplication and it serves as the second puzzle piece This finding questions the assumption of the existing phenomenological expression that multiplication is proportional to the shear rate We propose to add a correction term to the generalized Kocks Mecking expression to account for slip free multiplication whose mechanistic explanation is provided A major finding of this thesis is that DD results suggest an exponential flow rule in contrast to the commonly used power law flow rule even in the cases where thermal fluctuations are not present The exponential flow rule is the third piece in the puzzle of the presented strain hardening model We demonstrate that the observed exponential flow rule despite the common notion that thermal fluctuations are the responsible mechanism can be explained by statistical properties of the dislocation links Hence by statistically analyzing the number density and plastic activity of links in terms of their length we formulate a physically justified link length based flow rule which can numerically capture the exponential dependence of shear rate on shear stress The proposed link length based flow rule has two key components 1 the number density of links on each slip system which was observed to follow the sum of two exponentials distribution and 2 an average velocity of links as a function of resolved shear stress and link length whose fitting coefficients are independent of the loading orientation The exponential dependence of on resolved shear stress is traced to the spatial fluctuation of the internal stress field which can be approximated by a Laplace distribution The proposed average velocity function incorporates the Laplace distribution in its form This thesis shows that discrete dislocation dynamics simulations can be used to inform higher length scale models of non phenomenological constitutive relations The presented model captures the strain hardening as a result of slip system interactions in FCC single crystals It works as an example for developing similar coarse grained models based on DDD which includes additional strain hardening mechanisms such as cross slip or precipitate hardening We hope that the present thesis motivates more researchers to use DDD simulations for constructing constitutive relations

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