

# Preface

Design of and with materials plays an intrinsic role in today's challenging world of high performance structural components and applications. They constitute an integral part of comprehensive structural design, given the opportunity offered by optimal materials design for structural performance and life enhancement. These opportunities impose high demands on effective modeling and simulation methodologies to establish quantitative relations between the material microstructure and physical properties at different length scales. The rapid advances in computer and computational sciences enable sophisticated simulations that unravel the underpinnings of complex material microstructure on behavior. In concert with outstanding advances in experimental methods, these computational tools are increasingly able to enhance the fundamental understanding of microstructure–property relations, thus enabling materials and process design for improved performance and life.

The field of computational materials modeling transcends traditional disciplinary boundaries between mechanics, materials science, physics and chemistry, mathematics and computer science. In addition, it is creating a true synergy between experiments and modeling in terms of incorporation of physics, calibration, and validation. The results of these unified efforts at various scales are yielding unprecedented levels of rigor and accuracy in predictions of complicated phenomena that have previously eluded scientists and engineers. The role of microstructure on physical properties and performance is emerging as a quantitative discipline with broad and direct implications on material design.

This book “Computational Methods for Microstructure–Property Relationships” is an attempt to capture this rapid advancement at a period of time, with a glimpse of what is yet to come in this very dynamic emergent field of science and technology. It introduces state-of-the-art advances in computational modeling as well as experimental approaches for materials structure–property relations. Representing a body of collected works by well-known professionals in the field, it covers topics ranging from materials modeling principles with a multiscale perspective to materials design. It presents the current state of knowledge for a wide collection of research areas related to materials assessment in structures–materials interactions. The collection aims at establishing the necessity of a robust integrated computational mechanics and computational materials science framework,

together with an experimental validation protocol, that treats heterogeneous materials at microstructural and continuum scales. Selectively encompassing both computational mechanics and computational materials science disciplines, it offers an analysis of current techniques and selected topics important to industry researchers, such as deformation, creep, and fatigue of primarily metallic materials. It emphasizes modeling at continuum and heterogeneous microstructural scales, e.g. crystalline or grain scales, validated with experimental observations. This book is intended for researchers in academia, industry, and government laboratories to understand the issues and challenges involved in predicting performance and failure in materials, with a focus on the engineering structure–materials interaction. Researchers, engineers, and professionals involved with predicting the performance and failure of materials are expected to find this book a valuable reference.

This book is topically divided into four essential parts. The first part deals with 3D image-based materials structure data collection and representation and microstructure builders for mechanical response simulations.

Chapter “Serial Sectioning Methods for Generating 3D Characterization Data of Grain- and Precipitate-Scale Microstructures” introduces serial-sectioning methods for 3D characterization of grain- and precipitate-scale microstructures. It focuses on the use of serial-sectioning methods and associated instrumentation as a means for collecting microstructural, crystallographic, and chemical data. Chapter “Digital Representation of Materials Grain Structure” discusses the state-of-the-art methods in the field of microstructure representation with focus on the following: data collection, feature identification, mesh generation, quantitative descriptors, and synthetic structure generation. Chapter “Multi-Scale Characterization and Domain Partitioning for Multi-Scale Analysis of Heterogeneous Materials” discusses the development of a multiscale characterization methodology leading to a microstructural morphology-based domain partitioning method for materials having nonuniform heterogeneous microstructure. The set of methods is intended to provide a concurrent multiscale analysis model with the initial computational domain that delineates regions of statistical homogeneity and heterogeneity. The method is intended as a preprocessor to multiscale analysis of mechanical behavior and damage of heterogeneous materials. Chapter “Coupling Microstructure Characterization with Microstructure Evolution” discusses the synergistic coupling of quantitative microstructure characterization via experimental imaging techniques, with computer simulations of microstructural evolution using the phase-field method. Having experimental images as inputs, the chapter describes uses of the phase-field method at different length scales to explore mechanisms of microstructural evolution, extract material parameters, conduct physics-based repairs of experimentally reconstructed microstructures, and evolve the microstructure for different time, temperature, stress, etc. regimes.

Part of this volume is devoted to materials constitutive laws and kinematical approaches, together with their coupling of material structure to responses via simulation codes. These are presented in next six chapters. Chapter “Representation of Materials Constitutive Responses in Finite Element Based Design Codes” surveys

FEM-based tools for simulating materials behavior and reviews the material models available in commercial codes. Chapter “Accounting for Microstructure in Large Deformation Models of Polycrystalline Metallic Materials” analyzes the influence of microstructure on large-strain mechanical behavior for metallic polycrystalline materials. Results of a macroscale continuum internal state variable-based model for tantalum are compared with those from a multiscale polycrystalline plasticity approach having explicit representation of the polycrystalline aggregate. In Chapter “Dislocation Mediated Continuum Plasticity: Case Studies on Modeling Scale Dependence, Scale-Invariance, and Directionality of Sharp Yield-Point”, the authors discuss a field dislocation dynamics theory to account for the emergence of inhomogeneous dislocation distributions at mesoscopic length scales, as well as their coupling to initial and boundary conditions and consequences on mechanical behavior. Size effects and scale-invariant intermittency are interpreted through field dislocation dynamics. Anisotropy of strain hardening induced by the emergence of internal stress fields is also reviewed in this chapter. Chapter “Dislocation-Mediated Time-Dependent Deformation in Crystalline Solids” shows a methodology for incorporating the effects of slip gradients associated with intra-grain deformation heterogeneity in crystal-plasticity-based finite element simulation. The treatise quantifies the orientation dependence of the misorientation field in the polycrystalline microstructure and introduces a modification of the kinematic decomposition that accommodates distortions arising from the presence of a static dislocation distribution. Chapter “Modeling Heterogeneous Intra-Grain Deformations Using Finite Element Formulations” is a review of two crystal plasticity-based methodologies for the prediction of microstructure–property relations in polycrystalline aggregates. These include a mean-field, second-order viscoplastic self-consistent method and a Fast Fourier Transform-based full-field method. Numerical examples demonstrate that models like the FFT-based formulation can explicitly account for interaction between individual grains. Finally, chapter 11 discusses multiscale modeling of plastic deformation and strength in crystalline materials with emphasis on models and experiments below the grain level. Specifically, the chapter deals with experimental advances and theoretical models for characterizing dislocations at the subgrain level.

The third part introduces computational mechanics for time dependency of materials with links to fracture mechanics and multi-time scaling methods for fatigue in next three chapters. Chapter “Stochastic Upscaling for Inelastic Material Behavior from Limited Experimental Data” develops time-dependent plastic deformation and creep models for crystalline solids using dislocation-level mechanics. The theory uses microstructural information to develop broad quantitative mechanistic relationships that match the observed phenomenology. The discussion includes mobility-controlled systems, where dislocations move through the crystal under stress and interaction of dislocations with discrete obstacles for a range of alloys. Chapter “DDSim: Framework for Multiscale Structural Prognosis” introduces a prototype hierarchical computational simulation system called damage and durability simulator (DDSim) for prognosis of fatigue life of airframe components. While this prototype focuses on fatigue cracking, the framework can be extended to other

modes of damage. Chapter “Modeling Fatigue Crack Nucleation Using Crystal Plasticity Finite Element Simulations and Multi-Time Scaling” addresses two important aspects of predicting fatigue crack nucleation in polycrystalline alloys under dwell cyclic loading. The first is a microstructure-sensitive criterion for dwell fatigue crack initiation in polycrystalline titanium alloys, while the second part of this chapter discusses a wavelet transformation-based multi-time scaling (WATMUS) algorithm for accelerated crystal plasticity finite element simulations. The WATMUS algorithm significantly enhances the computational efficiency for fatigue life prediction.

Finally, the fourth part of this book deals with some additional emerging topics in the next three chapters. Chapter “Challenges Below the Grain Scale and Multiscale Models” examines selected experimental methods at different length scales that are important tools in building models for location specific design. While special experimental techniques are needed to probe the material at finer scales to assess the local behaviors, testing methods at all scales are discussed to demonstrate the breadth of experimental capability available at each scale of the material. A stochastic up-scaling approach for strain-hardening plastic materials from limited experimental data based on random matrix theory is introduced in chapter “Emerging Methods for Matching Simulation and Experimental Scales”. The uncertainty characterized by constitutive tangential matrices can be construed as a reflection, on the coarse scales, of fluctuations of the fine scale features from which constitutive matrices are constructed. Finally, chapter “Simulation-Assisted Design and Accelerated Insertion of Materials” introduces some emerging concepts for robust design of materials and challenges for the synthesis of modeling and simulation and materials design. The distinction between materials design and multiscale modeling is elucidated in this chapter with emphasis on top-down requirements on material structure and performance to meet product requirements.

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Columbus, Ohio  
Dayton, Ohio

*Somnath Ghosh*  
*Dennis M. Dimiduk*  
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Ghosh, S.; Dimiduk, D. (Eds.)

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