Recent Advances in Computational Materials Science and Multiscale Materials Modeling

Guest Editors

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Preface

Material characterization and material analysis tools have played an important role in understanding the behavior of advanced heterogeneous materials and helped in discovering tailored materials with unprecedented properties. Inherently multiscale response of such systems has led researchers from many scientific communities to pay significant attention to the development of multiscale methods and models that can capture physical processes and phenomena across several spatial scales. In response to this increasing demand, the editors of this special issue have been organizing a series of symposia on the *Recent Advances in Computational Materials Science and Multiscale Materials Modeling*. These symposia provide a venue for researchers and engineers to identify the pressing challenges and exchange ideas in the area of multiscale computational modeling of materials. This special issue contains selected papers presented in the first of these symposia that was held in Boston, Massachusetts, as a part of the *2008 ASME International Mechanical Engineering Congress & Exposition*. The event was organized by the American Society of Mechanical Engineers (ASME) and sponsored by the Committee on Computing in Applied

Mechanics (CONCAM).

The manuscripts in this special issue address a range of problems concerning the fundamental understanding of the properties and response characteristics of heterogeneous materials at scales from the atomistic to macroscopic levels. The effect of nanoscale computational investigations on the understanding and modeling of material response has been addressed by Tomar *et al*., and Srivastava and Ghosh. The former manuscript addresses the effects of clustered nano-particles and the effect of particle size on the strength of nano-composites. The latter manuscript presents molecular dynamics simulations, employed to observe the glass transition temperatures of bulk polystrene. Many contributions concentrate on the development of computational methodologies for transferring information across the disparate spatial scales. Lee and Sundararaghavan employ molecular dynamics simulations of metallic nanocrystals to characterize and calibrate a meso-scale decohesion model for the tilt grain boundaries. Crouch and Oskay present a computational modeling framework to efficiently and accurately bridge the meso-scale, associated with a unit cell, and the macro-scales. In this work, a novel model reduction methodology, which is based on eigendeformation homogenization technique, is proposed to efficiently evaluate the nonlinear mechanical response at the mesoscopic scales. Collins *et al*. propose an alternative paradigm for model order reduction at the meso-scale. In this manuscript, the authors identify the geometrically smallest representative unit cell of random particulate heterogeneous materials, such as heterogeneous solid propellants, that maintains the statistical correspondence to the actual material structure as it is characterized by, for example, micro-computer tomography. Jackson and Stafford discuss a computational algorithm for packing of random particulate composites with spherical and non-spherical inclusion shapes. The proposed packing algorithm is later employed to study the convective burning of a porous medium. Gallier studies the dielectric breakdown of heterogeneous solid propellants using a finite difference technique for steady Maxwell equations and a breakdown dynamics model for a quasi-steady succession of local breakdowns between particles. This work tests the scaling theory, which explains the reduction in the dielectric breakdown strength in aluminized solid propellants, by simulating the breakdown in particulate composites in a three-dimensional setting.

Despite significant research activity in the past few years, multiscale computational materials modeling remains to be a relatively young field. This special issue addresses some important questions surrounding characterization, modeling, and simulation of heterogeneous material systems. The editors would like to thank all reviewers for their assessments of the manuscripts and the CONCAM and ASME for facilitating this symposium. Finally, the editors would like to thank Professor Jacob Fish for allowing the publication of this special issue in the *International Journal for Multiscale Computational Engineering*.