SPECIAL ISSUE

MULTISCALE MODELING AND UNCERTAINTY QUANTIFICATION OF HETEROGENEOUS MATERIALS

Guest Editor

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PREFACE

The papers for this special issue are included in Volume 9, Issues 3 and 4, 2011 of International Journal for Multiscale Computational Engineering and will focus on multiscale modeling and uncertainty quantification of heterogeneous materials. Particular emphasis is given to advanced computational methods which can greatly assist in tackling complex problems of multiscale stochastic material modeling. The papers can be grouped into several thematic topics that include homogenization and computation of effective elastic properties of random composites, development of computational models for large-scale heterogeneous microstructures, stochastic analysis and design of heterogeneous materials, and multiscale models for the simulation of fracture mechanisms in polycrystalline materials.

The first part which is published in Volume 9, Issue 3 includes the following articles.

- Homogenization of Fiber-Reinforced Composites with Random Properties Using the Least-Squares Response Function Approach, M. Kamiński

- Large-Scale Computations of Effective Elastic Properties of Rubber with Carbon Black, Fillers, A. Jean, F. Willot, S. Cantournet, S. Forest, and D. Jeulin

- Elastic and Electrical Behavior of Some Random Multiscale Highly-Contrasted Composites, F. Willot and D. Jeulin

- Overall Elastic Properties of Polysilicon Films: A Statistical Investigation of the Effects of Polycrystal Morphology, S. Mariani, R. Martini, A. Ghisi, A. Corigliano, and M. Beghi

- Variational Formulation on Effective Elastic Moduli of Randomly Cracked Solids, X. F. Xu and G. Stefanou

The second part of the special issue consists of eight papers dealing with the development of computational models for large-scale heterogeneous microstructures, the stochastic analysis and design of heterogeneous materials, and multiscale models for the simulation of fracture mechanisms in poly-crystalline materials.

The paper by K. Schrader and C. Könke is devoted to the *development of computational models for large-scale heterogeneous three-dimensionalmicrostructures*. The authors suggest a method to split a heterogeneous material model, consisting of a matrix material and embedded inclusions, into zones of elastic and inelastic behavior and to appropriately customize the discretization methods for these two zones.It is proposedto apply structured and unstructured meshes in a hybrid fashion and to solve the resulting equation systems with several millionsof degrees of freedom by iterative solver techniques.

The section on *stochastic analysis and design of heterogeneous materials* is represented by the following four papers.

The contribution by M. Di Paola, A. Sofi and M. Zingales deals with the stochastic analysis of non-local one-dimensional (1D) solids with random mass distribution. The random fluctuations of mass distribution involve a stochastic model of the non-local interactions and lead to a stochastic integro-differential equation governing the random displacement field of the 1D body. Some numerical results are presented to highlight the effects of mass fluctuations on the mechanical response of the 1D body with long-range interactions.

S. Sakata, F. Ashida, and K. Enya perform a perturbation-based stochastic microscopic stress analysis of a particle-reinforced composite material with uncertain properties via stochastic homogenization. A glass particle-reinforced composite material is used as an example. The obtained results are compared with those of the Monte Carlo simulation (MCS), and the validity and application limit of the first-order perturbation-based approach are investigated.

S. Sakata, F. Ashida, and Y. Shimizu deal with the identification of the microscopic random variation of elastic properties of the component materials in particle-reinforced composites. This inverse problem is solved within the framework of MCS and optimization techniques. The stochastic characteristics of the elastic properties of the microstructure are obtained based either on a set of homogenized elastic properties or on some probabilistic moments of these propertiesthrough a nonlinear (quadratic) mapping technique proposed in this paper.

The paper by R. Sternfels and P.S. Koutsourelakis treats the topic of design/optimization of heterogeneous materials in the presence of randomness. The design of random composites is performed in the framework of stochastic topology optimization by controlling the statistics of the probability distribution of the constitutive phases, while the resulting microstructure remains random.In addition, the optimization of the input (e.g. excitation) is addressed such that the expected response of the material is as close as possible to a desired output. Both problems are examined in the context of heat conduction.

The final section comprises three papers dealing with *multiscale models for the simulation of fracture mechanisms in polycrystalline materials.*

J. Rupil, L. Vincent, F. Hild, and S. Roux propose a probabilistic model to predict the initiation and growth of fatigue damage in an austenitic stainless steel at a mesoscopic scale. Fatigue mechanical tests are performed to detect and quantify mesocrack initiations for different loadings by using digital image correlation. The crack initiation is described by a Poisson point process,the intensity of whichis evaluated using a multiscale approach based on a probabilistic crack initiation law in a typical grain.

The paper by I.J. Beyerlein, R.J. McCabe, and C.N. Tomé reports on a multiscale modeling of twinning in hexagonal close packed (hcp) metals such as magnesium and zirconium based on micro-structural characterization. The proposed constitutive model is built upon the visco-plastic self-consistent (VPSC) polycrystal scheme. This framework includes a novel probabilistic model for predicting when, where, and which twins nucleate, a dislocation density model for crystallographic slip, and a micromechanical model for twin lamella thickening and twin reorientation.

T. Luther and C. Könke present a multiscale approach for computational intergranular fracture analysis on the atomistic scale and explain the transition to coupled cohesive zone representations of continuum models. The aim is to model the constitutive response of grain boundaries in polycrystalline materials, e.g. aluminum. The brittle intergranular fracture process on the atomistic scale is investigated in three dimensions by applying a parallelized nonlocal quasi-continuum method and size effects on extracted cohesive parameters are examined.

In summary, this special issue is aimed at informing researchers and engineersof the most recent advances in the field of multiscale modeling and uncertainty quantification in order to improve the safety and reliability of engineered materials. It is hoped that this special issue will contribute to further advancing the field and to defining directions of future research.

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