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SPECIAL ISSUE

MULTISCALE MODELING AND UNCERTAINTY QUANTIFICATION OF HETEROGENEOUS MATERIALS

Guest Editor

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PREFACE

The increasing research activity for micro- and nano-scales over the last decade has significantly shown the need to account for disparate levels of uncertainty from various sources and across scales. Even over-refined deterministic approaches cannot account for the issue; the integration of stochastic and multiscale methodologies is required to provide a rational framework for uncertainty quantification and reliability analysis of heterogeneous materials. Facing the emergence of new advanced engineered materials, accurate stochastic modeling across multiple length scales becomes imperative.

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.

Volume 9, Issue 3 for the special issue consists of five papers that are devoted to the *homogenization and computation of effective elastic properties of random composites*.

M. Kamiński presents a computational strategy for estimation of the homogenized elasticity tensor of fiber-reinforced random composites using the stochastic generalized perturbation technique and a response function approach. The uncertainty of the composite appears at the level of the components' material properties, while its geometry remains deterministic and perfectly periodic. The response function relating to the homogenized tensor and the input random parameter is determined numerically using several deterministic solutions and least squares approximation.

A. Jean, F. Willot, S. Cantournet, S. Forest, and D. Jeulin propose a powerful method for deriving both apparent and effective elastic moduli of rubber with carbon black fillers using finite element and fast Fourier transform methods. The complex two-phase microstructure of the material is generated numerically from a mathematical model of its morphology, which is identified by statistical moments from transmission electron microscopy (TEM) images.

The role of a non-uniform distribution of heterogeneities on the elastic as well as electrical properties of composites with "infinitely-contrasted" characteristics is studied numerically and compared with available theoretical results in the contribution by F. Willot and D. Jeulin. It is shown that the non-uniform dispersion of heterogeneities in multiscale microstructures can lead to substantially different effective properties as compared to the one-scale Boolean model, particularly at low volume fractions.

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S. Mariani, R. Martini, A. Ghisi, A. Corigliano, and M. Beghi investigate the effects of polycrystal morphology on the macroscopic elastic properties of polysilicon films. The authors propose a homogenization technique based on numerical simulations of different representative volume elements (RVEs) generated via Voronoi tessellations. In these geometries, the effect of morphology, targeted grain size and RVE size on the overall elastic properties is examined and a new criterion is proposed to determine whether the RVE is indeed representative based on the results compared with standard Voigt and Reuss bounds.

X.F. Xu and G. Stefanou formulated a variational upper bounds for the effective elastic moduli of randomly cracked solids by applying the stochastic Hashin-Shtrikman variational principle and a Green-function-based multi-scale method. The upper bound expressions are explicitly given for penny shaped and slit-like random cracks with parallel and random orientations. Unlike previous works, no special underlying morphology is assumed in the variational formulation and the bounds obtained are applicable to many realistic non-self-similar morphologies.

Volume 9, Issue 4 includes the following articles. For more detailed information on these articles please see Issue 4.

- Hybrid Computing Models for Large-Scale Heterogeneous 3D, K. Schrader and C. Könke
- Stochastic Analysis of One-Dimensional Heterogeneous Solids with Long-Range Interactions, M. Di Paola, A. Sofi, and M. Zingales
- Perturbation-Based Stochastic Microscopic Stress Analysis of a Particle-Reinforced Composite Material via Stochastic Homogenization Analysis Considering Uncertainty in Material Properties, S. Sakata, F. Ashida, and K. Enya
- Inverse Stochastic Homogenization Analysis for a Particle-Reinforced Composite Material with the Monte Carlo Simulation, S. Sakata, F. Ashida, and Y. Shimizu
- Stochastic Design and Control in Random Heterogeneous Materials, R. Sternfels and P.-S. Koutsourelakis
- Identification and Probabilistic Modeling of Mesocrack Initiations in 304L Stainless, Steel, J. Rupil, L. Vincent, F. Hild, and S. Roux
- Stochastic Processes of $\{1012\}$ Deformation Twinning in Hexagonal Close-Packed Polycrystalline Zirconium and Magnesium, I. J. Beyerlein, R. J. McCabe, and C. N. Tomé
- Coupled Cohesive Zone Representations from 3D Quasicontinuum Simulation on Brittle Grain Boundaries Fillers, T. Luther and C. Könke

In summary, this special issue is aimed at informing researchers and engineers of 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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