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Computational Material Modeling: A Current Perspective

S. Ghosh [1]

1 Foreword

The recent times have seen a surge in the efforts on computational modeling of materials in academia as well as in industry. This is triggered by enhanced developments of advanced and more complex materials with a wide range of applications at various length and time scales. The challenges posed by the demands of successful development have made this field one of the most active and exciting areas of research in science and engineering. Robust modeling can yield better product control in manufacturing processes, improve performance and reliability of advanced materials, improve design of defense and space exploration systems, innovate new biomedical devices and processes, among many other applications. The rapid progress in computer technology has made possible, the incorporation of a high level of sophistication in the computational methods that is necessary to address more challenging problems.

In postulating the spatial or temporal variation in physical, thermal and mechanical properties of complex material systems, isolated testing of single idealized units outside of their microstructural context is not sufficient to capture the totality of a material's behavior. Challenging studies that reflect the details of the underlying microstructures and mechanisms are being conducted to understand structure-property relationships. However, very often, data extracted from experiments are impaired with respect to their comprehensiveness and in their ability to visualize material events. Advanced methods of computational modeling, using micromechanics and other methods, are useful in overcoming these limitations. With increasing computing power, creating large models reflecting the complex interaction between multitudes of objects to predict overall material response is now a reality. Assimilation of methods in computational science and engineering is being used to provide a unifying basis for modeling multidisciplinary problems in materials modeling and fill critical voids in experimental practice.

Materials modeling is multifaceted. It spans a range of aspects from materials characterization, to multi-scale modeling for response and reliability, and materials processing. A vision of materials research consciously fosters the interplay between these elements to design and fabricate more functionally effective materials. Computational Mechanics plays a major role in this development. To provide a forum for discussing the challenges and issues in computational mechanics associated with this vision, a symposium entitled 'Computational Modeling of Materials' was held at International Conference on Computational Engineering & Sciences at Puerto Vallarta, Mexico in August 2001. This special issue of Computational is an outcome of some of the papers presented at that conference. A total of 12 papers are published in this special issue of Computer Modeling in Engineering & Sciences (CMES) on 'Computational Modeling of Materials'. The papers may be broadly classified into five different categories, namely: *(i) Microstructural Characterization, (ii) Micromechanics Modeling, (iii) Microstructural Failure Modeling, (iv) Multi-scale Modeling and (v) Material Processing*.

The first paper [Yotte, Riss, Breysse and Ghosh (2004)] is on the development of effective computational tools for microstructural characterization of particle reinforced metal matrix composites or PRMMC's by Yotte, Riss, Breysse and Ghosh. Such characterization is necessary to quantitatively parameterize relevant features of complex heterogeneous microstrictructures. This study introduces methods of image analysis and statistical methods to identify clusters in the microstructure. Three papers represent the area of meso- and micromechanical analysis of heterogeneous materials. The paper on unit cell studies of discontinuously reinforced ductile matrix composites by Böhm, Han and Eckschlager

[1] Professor, Department of Mechanical Engineering, The Ohio State University, Columbus, Ohio, USA

(2004) develops a detailed finite element mesh for three-dimensional regions containing randomly distributed particles of different shapes and sizes. Predictions of macroscopic and microscopic stresses under uniaxial tensile loading are done with this model and the effects of the microstructural morphology is discussed. In their paper on unit-cell model of woven fabric composites, Kwon and Roach (2004) discuss a micromechanical model for compute effective material properties of a 2/2-twill composite and evaluate the tow stresses. Finally, Chen, Lee and Eskandarian (2004) develop thermo-visco-elastic models based on the micropolar theory and apply it to meso/microscopic problems.

Three papers in this issue explicitly discuss failure in heterogeneous microstructures. Li and Siegmund (2004) use the cohesive zone model or CZM to model indentation delamination of a bonded film system consisting of a ductile film on an elastic substrate. Chandra and Shet (2004) discuss mechanistic and computational issues in the application of CZM to model failure and fracture in real materials They closely examine the necessary distribution of total dissipation energy and other energy consuming mechanisms within the fracture process zone. A meso-scale model for analyzing dynamic fracture of granular ceramic materials is presented by Maiti and Geubelle (2004). An explicit grain-based cohesive/volumetric finite element scheme is explored in their work for modeling crack propagation along grain boundaries.

Various aspects of multi-scale modeling are addressed in three papers that incorporate a range of length scales. Micro/meso to macroscopic length scales are modeled in the papers by Okada, Fukui and Kumazawa (2004), and Raghavan and Ghosh (2004), while the atomistic length scale is dealt with in the paper by Chung, Raju and Henz (2004). In their paper, Okada et. al. (2004) combine the asymptotic homogenization method with microscopic RVE analysis by the boundary element method for two-scale analysis of particle reinforced composite materials. The paper of Raghavan and Ghosh (2004) presents an adaptive multi-level computational model that combines a macroscopic finite element model with a microstructural Voronoi cell finite element model for multi-scale analysis of composite structures with non-uniform microstructural heterogeneities. The model combines three levels of hierarchy, with different resolutions to overcome shortcomings posed by modeling and discretization errors in the analysis of heterogeneous structures. The paper of Chung, Namburu and Henz (2004) develops a novel hyper-elasticity based finite element model that is viable at the atomic length scale, in the context of lattice statics. The method is developed with a specific form of the Tersoff- Brenner potential for carbon and predicts the in-plane deformation behavior of a single graphite sheet. Finally, two papers in this issue address aspects of materials processing and fabrication. Ngo and Tamma (2004) discuss in details an integrated and comprehensive approach to the modeling of resin transfer molded (RTM) composite manufactured net-shaped parts. The paper includes a multi-scale methodology for predicting the effective constitutive thermo-physical properties like permeability, conductivity and elasticity tensors and also makes advances towards the prediction of induced residual stresses in the manufacturing process during post-cure cool down. The set ends with the paper by Larsson, Faleskog and Massih (2004) on the analysis of densification and swelling of granular material of granular materials using pressure and porosity dependent plasticity. While the scope of the topic selected is very large, the set of papers authored by a distinguished group of mechanics and materials researchers covers a significant thrust areas in this field of research.

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References

Böhm, H. J.; Han, W.; Eckschlager, A. (2004): Multi-inclusion Unit Cell Studies of Reinforcement Stresses and Particle Failure in Discontinuously Reinforced Ductile Matrix Composites, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 1, pp. 5-20.

Chandra, N.; Shet, C. (2004): A Micromechanistic Perspective of Cohesive Zone Approach in Modeling Fracture, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 1, pp. 21-33.

Chen, Y.; Lee, J. D.; Eskandarian, A. (2004): Micropolar Theory and its Applications to Mesoscopic and Microscopic Problems, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 1, pp. 35-43.

Chung, P. W.; Namburu, R. R.; Henz, B. J. (2004): A Lattice Statics-Based Finite Element Method, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 1, pp. 45-62.

Kwon, Y. W.; Roach, K. (2004): Unit-cell Model of 2/2-twill Woven Fabric Composites for Multi-scale Analysis, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 1, pp. 63-72.

Larsson, J.; Faleskog, J.; Massih, A. R. (2004): Analysis of Densification and Swelling of Solids Using Pressure Dependent Plasticity Criteria, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 1, pp. 73-80.

Li, W.; Siegmund, T. (2004): Numerical Study of Indentation Delamination of Strongly Bonded Films by Use of a Cohesive Zone Model, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 1, pp. 81-90.

Maiti, S.; Geubelle, P. H. (2004): Mesoscale Modeling of Dynamic Fracture of Ceramic Materials, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 2, pp. 91-101.

Ngo, N. D.; Tamma, K. K. (2004): An Integration Comprehensive Approach to the Modeling of Resin Transfer Molded Composite Manufactured Net-Shaped Parts, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 2, pp. 103-133.

Okada, H.; Fukui, Y.; Kumazawa, N. (2004): Homogenization Analysis for Particulate Composite Materials Using the Boundary Element Method, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 2, pp. 135-149.

Raghavan, P.; Ghosh, S. (2004): Adaptive Multiscale Computational Modeling of Composite Materials, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 2, pp. 151-170.

Yotte, S; Riss, J; Breysse, D; Ghosh, S. (2004): Cluster Analysis for Particle Reinforced Metal Matrix Composites, *CMES: Computer Modeling in Engineering & Sciences*, Vol. 5, No. 2, pp. 171-187.