Abstract Title

Predictive Multiscale Theory for Design of Heterogeneous Materials

Symposium Track

Numerical Simulation in Nanomechanics

Authors' names

Wing Kam Liu, Cahal McVeigh, and Albert To

Authors' affiliations

Northwestern University

Abstract body

Nanotechnology, nanomechanics and nanomaterials have demonstrated the potential to improve the society, from national defense to homeland security to private industry. These fields can make our manufacturing processes more environmentally safe and energy efficient, our infrastructure last longer, and our daily lives more convenient. For example, microsystems such as micro-gyroscopes and micro-fluidic devices have found numerous applications in automobile industry and the medical industry. To ensure the long term performance and reliability of the products, predictive-science based modeling is necessary in the engineering design and analysis of the materials involved.

Engineering materials are composed of complicated microstructures which determine the material's processing behavior, mechanical and physical properties and product performance. Mechanical models involving direct numerical simulation of the heterogeneous microstructure through quantum mechanics, molecular dynamics or even continuum based methods remains prohibitively expensive due to the vast scale difference between the component and the underlying microstructure in most engineering applications. It is estimated that it will be 80 years before the atomistic simulation of fracture of a 1 cm cube of copper is feasible, according to the current rate of growth of computational power.

A general predictive multiscale theory for the design of heterogeneous materials is outlined. The theory begins with a simple virtual power domain decomposition which is extended to multiple scales of microstructure. Deformation is solved in terms of the constitutive behavior arising from the dominant microstructural features at each scale. Solution field resolution is also increased with each successive scale of analysis, achieving a multiresolution, multiphysics set of governing equations which can be solved numerically. The theory can be used to couple a homogenized continuum to a nested series of progressively more refined superimposed microscale domains. These microscale domain simulations can be continuum based direct numerical simulation of the underlying microstructure, discrete atomic regions or statistically based gradient enhanced continua. Three variations on the general theory are outlined: a coupled concurrent multiscale approach, a hierarchical approach and a power equivalence approach. Each offers an efficient manner for overcoming the inherent problems with traditional homogenization theory.

Keywords

Nanomechanics, nano-structured materials, multiscale theory, predictive modeling

References

W.K. Liu, E G. Karpov, H S. Park. Nano Mechanics and Materials: Theory, Multiscale Methods and Applications. Wiley, New York, 2005.

W.K. Liu, E.G. Karpov, S. Zhang, H.S. Park. An Introduction to Computational Nano Mechanics and Materials Computer Method in Applied Mechanics and Engineering 193, 1529-1578, 2004.

C. McVeigh, F. Vernerey, W.K. Liu, L. Cate Brinson. Multiresolution analysis for material design. Computer Methods in Applied Mechanics and Engineering, 195, 5053-5076, 2006.

G.J. Wagner, W.K. Liu. Coupling of Atomistic and Continuum Simulations using a Bridging Scale Decomposition. Journal of Computational Physics, 190, 249–274, 2003.

Corresponding author contact information

Wing Kam Liu, w-liu@northwestern.edu