Computational Materials: Multi-Scale Modeling and Simulation of Nanostructured Materials

T.S. Gates\textsuperscript{a}, G.M. Odegard\textsuperscript{b}, S.J.V. Frankland\textsuperscript{c} and T.C. Clancy\textsuperscript{c}

\textsuperscript{a}NASA Langley Research Center, MS 188E, Hampton, VA 23681, USA
\textsuperscript{b}Michigan Technological University, 1400 Townsend Drive, Houghton, MI 49931, USA
\textsuperscript{c}National Institute of Aerospace, 100 Exploration Way, Hampton, VA 23666, USA

Abstract

The paper provides details on the current approach to multi-scale modeling and simulation of advanced materials for structural applications. Examples are given that illustrate the suggested approaches to predicting the behavior and influencing the design of nanostructured materials such as high-performance polymers, composites, and nanotube-reinforced polymers. Primary simulation and measurement methods applicable to multi-scale modeling are outlined. Key challenges including verification and validation are highlighted and discussed.

Keywords: Multi-scale modeling; Computational materials; Nanotechnology