Multiscale Modeling of Polymer Materials Using a Statistics-Based Micromechanics Approach

1Department of Mechanical Engineering-Engineering Mechanics, Michigan Technological University, Houghton, MI
2National Institutive of Aerospace, Hampton, VA
3NASA Langley Research Center, Hampton, VA
4College of Engineering, Michigan Technological University, Houghton, MI

Abstract
A large number of possible polymer chain conformations exist for a given volume of an amorphous polymer. The prediction of elastic properties of a polymer must therefore consider more than a single combination of chain conformations. A multiscale modeling approach is proposed to predict the bulk elastic properties of polymer materials using a series of molecular models of individual polymer microstates and a statistics-based micromechanical modeling method. The method is applied to polyimide and polycarbonate systems. It is shown that individual microstates can yield a wide range of predicted elastic properties, whereas the consideration of multiple microstates yield predicted properties that more-closely agree with experimentally-determined values of Young’s modulus. Additionally, the upper and lower limits of possible elastic constants are also established based on the consideration of multiple microstates.

Keywords: Molecular Dynamics, Mechanical Properties, Conformation Space, Multiscale Modeling

Introduction
Polymer-based nanocomposite materials have the potential to provide significant increases in specific stiffness and specific strength relative to current materials used for many engineering structural applications. The gains in mechanical properties are due to increases in the reinforcement surface area relative to conventional composite materials for a given reinforcement volume fraction. The increased reinforcement surface area results in significant increases in load transfer between the reinforcement and matrix phases. To facilitate the development of polymer nanocomposite materials, constitutive relationships must be established that predict the bulk mechanical properties of the materials as a function of the molecular structure and interactions.

Multiscale modeling techniques must be used to relate the molecular structure at the nanometer length-scale to mechanical behavior at the macro-length scale. Molecular Dynamics (MD) simulations can be used to predict the equilibrated molecular structures of polymer-based materials for a given thermodynamic state [1-8]. Also, the mechanical behavior of a molecular system can be studied when a representative volume element (RVE) of the molecular structure is subjected to applied deformations. While most multiscale modeling studies have focused on