Modeling of the Mechanical Properties of Nanoparticle/Polymer Composites

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Abstract

A continuum-based elastic micromechanics model is developed for silica nanoparticle/polyimide composites with various nanoparticle/polyimide interfacial treatments. The model incorporates the molecular structures of the nanoparticle, polyimide, and interfacial regions, which are determined using a molecular modeling method that involves coarse-grained and reverse-mapping techniques. The micromechanics model includes an effective interface between the polyimide and nanoparticle with properties and dimensions that are determined using the results of molecular dynamics simulations. It is shown that the model can be used to predict the elastic properties of silica nanoparticle/polyimide composites for a large range of nanoparticle radii, 10 Å to 10,000 Å. For silica nanoparticle radii above 1,000 Å, the predicted properties are equal to those predicted using the standard Mori-Tanaka micromechanical approach, which does not incorporate the molecular structure. It is also shown that the specific silica nanoparticle/polyimide interface conditions have a significant effect on the composite mechanical properties for nanoparticle radii below 1,000 Å.