Mechanical Engineering Doctoral Defense

Fundamental Investigations into the Properties and Performance of Advanced Materials

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Abstract

Intelligent engineering designs require an accurate understanding of material behavior, since any uncertainties or gaps in knowledge must be counterbalanced with heightened factors of safety, leading to overdesign. Therefore, building better structures and pushing the performance of new components requires an improved understanding of the thermomechanical response of advanced materials under service conditions. This dissertation prospectus provides fundamental investigations of several advanced materials: thermoset polymers, a common matrix material for fiber-reinforced composites and nanocomposites; aluminum alloy 7075-T6 (AA7075-T6), a high-performance aerospace material; and ceramic matrix composites (CMCs), an extreme-temperature material for high-efficiency turbine blades.To understand matrix interactions with various interfaces and nanoinclusions at their fundamental scale, the properties of thermoset polymers are studied at the atomistic scale. An improved proximity-based molecular dynamics (MD) technique for modeling the crosslinking of thermoset polymers is carefully established, enabling realistic curing simulations through its ability to dynamically and probabilistically perform complex topology transformations. The proximity-based MD curing methodology is then used to explore damage initiation and the local anisotropic evolution of mechanical properties in thermoset polymers under uniaxial tension with an emphasis on changes in stiffness through a series of tensile loading, unloading, and reloading experiments. Aluminum alloys in aerospace applications often require a fatigue life of over 109 cycles, which is well over the number of cycles that can be practically tested using conventional fatigue testing equipment. In order to study these high-life regimes, a detailed ultrasonic cycle fatigue study is presented for AA7075-T6 under fully reversed tension-compression loading. The geometric sensitivity, frequency effects, size effects, surface roughness effects, and the corresponding failure mechanisms for ultrasonic fatigue across different fatigue regimes are investigated. Because CMCs are used in extreme temperature applications, temperature and oxidation play an important role in their degradation. A new finite element is developed to address the complex coupling between oxygen diffusion, oxidation reaction, anisotropic damage, and deformation in typical material architectures.

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