Mechanical Engineering Doctoral Defense

Multiscale Modeling of Heterogeneous Material Systems

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abstract

Damage detection, accurate material modeling and structural health monitoring are essential to multidisciplinary investigations. A significant amount of research has been conducted in this field to enhance the fidelity of damage assessment models, particularly in heterogeneous materials including metallic materials and composites. Multiscale modeling which can track damage initiation at the microscale and providing damage information at the macroscale is used in substitution for physical sensors, and provide data for damage estimation and detection. In this research, effort has been dedicated to develop multiscale modeling approaches and associated damage criteria for the estimation of damage evolution which is essential to damage detection. Important issues regarding different length and time scales, statistical material properties and mechanical behavior are addressed. Two different materials, metallic alloy and epoxy polymer are studied.

For metallic material (Al 2024-T351), the methodology initiates at the microscale where extensive material characterization is conducted to capture the microstructural variability. A statistical volume element (SVE) model is constructed to represent the material properties. Geometric and crystallographic features including grain orientation, misorientation, size, shape, principal axis direction and aspect ratio are captured. This SVE model provides a computationally efficient alternative to traditional techniques using representative volume element (RVE) models while maintaining statistical accuracy. A physics based multiscale damage criterion is developed to simulate the fatigue crack initiation. The crack growth rate and probable directions can be estimated simultaneously.

For the smart polymer material, a spring-bead based network model is developed using molecular dynamics (MD) simulation results, configuration evaluation and mechanical equivalence optimization. The multiscale approach bridges the high accuracy MD model at the nanoscale and high efficiency finite element (FE) model at the macroscale. Statistical distribution of cross-linking degree of the polymer is captured in the network model to represent the heterogeneous material properties at the microscale. Parametric study using the network model is implemented to investigate the influence of the cross-linking degree on the material behavior. The molecular dynamics simulation and network model based simulation are implemented to evaluate the damage evolution of the smart polymer.

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