Aerospace Engineering Doctoral Defense

Novel Methodology for Atomistically Informed Multiscale

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abstract

With the maturity of advanced composites as feasible structural materials for various applications there is a critical need to solve the challenge of designing these material systems for optimal performance. However, determining superior design methods requires a deep understanding of the material-structure properties at various length scales. Due to the length-scale dependent behavior of advanced composites, multiscale modeling techniques may be used to describe the dominant mechanisms of damage and failure in these material systems. With polymer matrix fiber composites and nanocomposites it becomes essential to include even the atomic length scale, where the resin-hardener-nanofiller molecules interact, in the multiscale modeling framework. Additionally, sources of variability are also critical to be included in these models due to the important role of uncertainty in advance composite behavior. Such a methodology should be able to describe length scale dependent mechanisms in a computationally efficient manner for the analysis of practical composite structures. In the research presented in this dissertation, a comprehensive nano to macro multiscale framework is developed for the mechanical and multifunctional analysis of advanced composite materials and structures. An atomistically informed statistical multiscale model is developed for linear problems, to estimate and scale elastic properties of carbon fiber reinforced polymer composites (CFRPs) and carbon nanotube (CNT) enhanced CFRPs using information from molecular dynamics simulation of the resin-hardener-nanofiller nanoscale system. For modeling inelastic processes, an atomistically informed coupled damage-plasticity model is developed using the framework of continuum damage mechanics, where fundamental nanoscale covalent bond disassociation information is scaled up as a continuum scale damage identifying parameter. This damage model is coupled with a nanocomposite microstructure generation algorithm to study the sub-microscale damage mechanisms in CNT/CFRP microstructures. It is further integrated in a generalized method of cells (GMC) micromechanics model to create a low-fidelity computationally efficient nonlinear multiscale method with imperfect interfaces between the fiber and matrix, where the interface behavior is adopted from nanoscale MD simulations. This algorithm is used to understand damage mechanisms in adhesively bonded composite joints as a case study for the comprehensive nano to macroscale structural analysis of practical composites structures. At each length scale sources of variability are identified, characterized, and included in the multiscale modeling framework.

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