Aerospace Engineering Doctoral Defense

Physics-Based Modeling of Material Behavior and Damage Initiation in Nanoengineered Composites

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abstract

Materials with unprecedented properties are necessary to make dramatic changes in current and future aerospace platforms. Hybrid materials and composites are increasingly being used in aircraft and spacecraft frames; however, future platforms will require an optimal design of novel materials that enable operation in a variety of environments and produce known/predicted damage mechanisms. Nanocomposites and nanoengineered composites with CNTs have the potential to make significant improvements in strength, stiffness, fracture toughness, flame retardancy and resistance to corrosion. Therefore, these materials have generated tremendous scientific and technical interest over the past decade and various architectures are being explored for applications to light-weight airframe structures. However, the success of such materials with significantly improved performance metrics requires careful control of the parameters during synthesis and processing. Their implementation is also limited due to the lack of complete understanding of the effects the nanoparticles impart to the bulk properties of composites. It is common for computational methods to be applied to explain phenomena measured or observed experimentally. Frequently, a given phenomenon or material property is only considered to be fully understood when the associated physics has been identified through accompanying calculations or simulations.The computationally and experimentally integrated research presented in this dissertation provides improved understanding of the mechanical behavior and response including damage and failure in CNT nanocomposites, enhancing confidence in their applications. The computations at the atomistic level helps to understand the underlying mechanochemistry and allow a systematic investigation of the complex CNT architectures and the material performance across a wide range of parameters. Simulation of the bond breakage phenomena and interphase mechanisms to continuum scale damage capture the effects of applied loading and damage precursor, and provide insight into the safety of nanoengineered composites under service loads. The validated modeling methodology is expected to be a step in the direction of computationally-assisted design and certification of novel materials, thus liberating the pace of their implementation in future applications.

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