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PREDICTIVE SIMULATIONS OF AMORPHOUS COMPOSITES: THEIR ULTIMATE THERMO-MECHANICAL PROPERTIES

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Polymer-matrix composites are finding increase use as structural materials in fields from sports equipment to aircraft and aerospace. For example, the Boeing 787 has an essentially all-composite fuselage. Current optimization and certification of these materials is based on extensive experimentation leading to lengthy and costly cycles. A synergistic combination of predictive simulations with experiments via an uncertainty quantification framework for decision-making has the potential to change this status quo and contribute to a more effective approach to material design and certification.

This presentation will focus on the prediction of fundamental materials properties of the polymeric matrices and their interfaces with carbon fibers using atomistic simulations and the use of this information to predict processing and performance of polymer composites. We developed a procedure to mimic the chemical reactions during the curing process of thermoset polymers of interest in structural applications and used large-scale molecular dynamics simulations to predict their ultimate response. The characterization of density and stiffness evolution during curing and thermal cycles obtained from molecular simulations is used with continuum models to predict the internal stresses developed in the composite during processing. The predicted properties of the fully cured resin, including thermal and mechanical response, are in good agreement with available experimental data and show that atomistic simulations can capture non-trivial trends in polymer physics including the effect of temperature, thermal history and strain rate in yield and post-yield behavior. Molecular dynamics simulations of the ultimate response of polymer/graphite systems predict both cohesive failure of the bulk matrix with strain localization and nano-void formation and interface de-bonding depending on the orientation of graphite with respect to the interface. These two mechanisms lead to different post yield behavior and the molecular simulations provide key insight for the development models that capture yield and post-yield behavior in composites.