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Multiscale Process Modeling Analysis for the Prediction of Composite Strength Allowables

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Abstract : During the processing of high-performance thermoset polymer matrix composites, chemical reactions occur during elevated pressure and temperature cycles, causing the constituent monomers to crosslink and form a molecular network that gradually can sustain stress. As the crosslinking process progresses, the material naturally experiences a gradual shrinkage due to the increase in covalent bonds in the network. Once the cured composite completes the cure cycle and is brought to room temperature, the thermal expansion mismatch of the fibers and matrix cause additional residual stresses to form. These compounded residual stresses can compromise the reliability of the composite material and affect the composite strength. Composite process modeling is greatly complicated by the multiscale nature of the composite architecture. At the molecular level, the degree of cure controls the local shrinkage and thermal-mechanical properties of the thermoset. At the microscopic level, the local fiber architecture and packing affect the magnitudes and locations of residual stress concentrations. At the macroscopic level, the layup sequence controls the nature of crack initiation and propagation due to residual stresses. The goal of this research is use molecular dynamics (MD) and finite element analysis (FEA) to predict the residual stresses in composite laminates and the corresponding effect on composite failure. MD is used to predict the polymer shrinkage and thermomechanical properties as a function of degree of cure. This information is used as input into FEA to predict the residual stresses on the microscopic level resulting from the complete cure process. Virtual testing is subsequently conducted to predict strength allowables. Experimental characterization is used to validate the modeling.

Keywords : molecular dynamics, finite element analysis, processing modeling, multiscale modeling
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