Mechanical Engineering Doctoral Defense

A New Atomistic Simulation Framework for Mechanochemical Reaction Analysis of Mechanophore Embedded Nanocomposites

School for Engineering of Matter, Transport and Energy

Bonsung Koo

Advisor: Aditi Chattopadhyay

abstract

A hybrid molecular dynamics (MD) simulation framework is developed to emulate mechanochemical reaction of mechanophores in epoxy-based nanocomposites. Two different force fields, a classical force field and a bond order based force field are hybridized to mimic the experimental processes from specimen preparation to mechanical loading test. Ultra-violet photodimerization for mechanophore synthesis and epoxy curing for thermoset polymer generation are successfully simulated by developing a numerical covalent bond generation method using the classical force field within the framework. Mechanical loading tests to activate mechanophores are also virtually conducted by deforming the volume of a simulation unit cell. The unit cell deformation leads to covalent bond elongation and subsequent bond breakage, which is captured using the bond order based force field. The outcome of the virtual loading test is used for local work analysis, which enables a quantitative study of mechanophore activation. Through the local work analysis, the onset and evolution of mechanophore activation indicating damage initiation and propagation are estimated; ultimately, the mechanophore sensitivity to external stress is evaluated. The virtual loading tests also provide accurate estimations of mechanical properties such as elastic, shear, bulk modulus, yield strain/strength, and Poisson's ratio of the system. Experimental studies are performed in conjunction with the simulation work to validate the hybrid MD simulation framework. Less than 2% error in estimations of glass transition temperature (Tg) is observed with experimentally measured Tgs by use of differential scanning calorimetry. Virtual loading tests successfully reproduce the stress-strain curve capturing the effect of mechanophore inclusion on mechanical properties of epoxy polymer; comparable changes in Young's modulus and yield strength are observed in experiments and simulations. Early damage signal detection, which is identified in experiments by observing increased intensity before the yield strain, is captured in simulations by showing that the critical strain representing the onset of the mechanophore activation occurs before the estimated yield strain. It is anticipated that the experimentally validated hybrid MD framework presented in this dissertation will provide a low-cost alternative to additional experiments that are required for optimizing material design parameters to improve damage sensing capability and mechanical properties

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