Fracture Prediction of Epoxy Resin using Morse Bond Potential Embedded in GAFF using Molecular Dynamics Simulations

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ABSTRACT

A generic method is developed to investigate the fracture behavior of an epoxy resin using atomistic molecular (MD) dynamics simulations. The epoxy system consisted of the stoichiometric mixture of tetra-/tri-functional epoxies and di-functional hardener molecules and was cured with a step-growth crosslinking algorithm. A hybrid force field (hFF) in which Morse bond function were added in second generation-general Amber Force Field (GAFF2) was used to capture bond breaking of the crosslinked epoxy system under uniaxial deformation. The Morse bond parameters for covalent bonds in the crosslinked backbone were fit to dissociation curves computed by CASPT2/6-311+G**. After the systems in various crosslink densities were obtained and equilibrated, the full length of stress-strain (σ-ε) curve was produced including initial elastic regime, yielding, plastic flow, strain hardening, and progressive failure. We found that the hFF was effective in studying the dissociation of crosslinked polymers and understanding the failure mechanism. In the results, the hFF delivered the same elastic property obtained from the unmodified force field GAFF. The stress-strain curve, however, began to be distinct in the plastic regime due to broken covalent bonds capable of altering the tensile behavior. Once the stress reached maximum, it progressively decreased until the ultimate failure (σ=0). Since hFF employed the existing GAFF functions with including a minimal change of its bond potential, this approach is easier to perform and computationally more efficient for unveiling the fracture behavior of

polymer materials at the molecular level than other approaches with reactive force fields. We expect this approach will be utilized to accelerate the material-by-design process for thermosets by incorporate data from molecular models.