Predicting Fracture Toughness in Polymers using Capriccio-Based Atomistic-Continuum Concurrent Coupling Technique

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**Abstract**

Prediction of fracture properties in brittle materials using computer simulations is the primary objective of this seminar. One of the main challenges to achieving this goal for brittle thermoset polymers is that the crack size and fracture process zone (FPZ) size needs to be in the micron scale in order for linear elastic fracture mechanics (LEFM) to be valid, thereby enabling toughness prediction and comparison with macro-scale experimental data. However, due to the high computational cost of performing purely atomistic simulations with millions of atoams, the range of crack lengths and FPZs simulated have been severely limited to nanometer scale, resulting in highly incorrect toughness estimates. In this paper, a state-of-the-art multiscale modeling technique is employed to allow atomistic simulations to run with much larger crack lengths and process zone sizes to truly replicate conditions necessary for brittle fracture in a polymer. A thermosetting epoxy polymer system of EPON862/DETDA is modelled using the OPLS molecular dynamics (MD) force field available in LAMMPS, coupled with Morse potential which allows for bond breakage. The MD system is concurrently coupled with a much larger finite element model (FEM) using the Capriccio algorittm.

The atomistic-continuum coupling is performed using a novel anchor-point based statistical method incorporating internal volume cells (IVCs), with displacement and strain continuity enforced in the handshake region using Lagrange multipliers. Atomistic J-integral , developed by the authors, is used to compute the fracture energy near the crack tip using contour integrals. The critical strain energy release rate (SERR) is computed using the atomistic J-integral specifically developed by the authors for simulating fracture in amorphous polymers. The applied mode 1 stress intensity factor (K1 ) is increased and its effect on the size of FPZ and critical SERR is studied. The in-house FEM code NOVA-3D is integrated into concurrent coupling code, which iteratively executes the coupled MD simulations. Our preliminary results indicate a monotonic increase in notch-sensitivity and FPZ with the increasing size of a subcritical crack, with the predicted SERR from atomistic J-integral tending towards macro-scale GC for epoxy as the FPZ becomes fully developed.