Atomistic Modeling of Fracture Properties in Nano-Particle Reinforced Polymers

ABSTRACT
This presentation is directed towards understanding damage progression and failure in advanced nanostructured composite materials. The molecular dynamics method is a subset of computational chemistry codes which creates system trajectories consistent with thermo-dynamic ensembles. The molecular dynamics program LAMMPS, (Large-scale Atomic/Molecular Massively Parallel Simulator) is a versatile code with numerous functionalities which can be used to simulate polymer systems. Although, the results for molecular simulation models, in particular polymer models are system size dependent, the ease with which large molecular systems can be evaluated, especially with parallel molecular dynamics codes such as LAMMPS makes it a more attractive choice compared to other approaches such as ab-initio calculations, which are limited to the calculation of a few 100 atoms.

In the context of fracture behavior in polymers, the critical value of the J-integral (JI) at crack initiation is related to the fracture toughness of the material, where the subscript I denotes the fracture mode (I=1,2,3). Therefore, the J-integral could be used as a suitable metric for estimating the crack driving force as well as the fracture toughness of the material as the crack begins to initiate. However, for the conventional macroscale definition of the J-integral to be valid at the nanoscale in terms of the continuum stress and displacement fields and their spatial derivatives requires the construction of local continuum fields from discrete atomistic data, and using these data in the conventional contour integral expression for atomistic J-integral. One such methodology is proposed by Hardy that allows for the local averaging necessary to obtain the definition of free energy, deformation gradient, and Piola-Kirchoff stress as fields (and divergence of fields) and not just as total system averages. Further, the atomistic J-integral accounts for the effect of reduction in J from continuum estimates due to the fact that the free energy available for crack propagation is less than the internal energy at sufficiently high temperature when entropic contributions become significant.

As a case study, the feasibility of computing the dynamic atomistic J-integral over the MD domain at finite temperatures using Hardy estimates of continuum fields based on localization functions is evaluated for a graphene nano-platelet with an embedded central crack. For model verification, the values of atomistic J-integral are compared with results from linear elastic fracture mechanics (LEFM) for isothermal crack initiation at 0 K. The atomistic computational results are in very good agreement with LEFM data up to the point of onset of a nonlinear regime near the crack tip at increased strain levels. Computational results related to the path-independence of the atomistic J-Integral and the influence of computational box size are also presented. Further, a novel approach that circumvents the complexities of direct computation of entropic contributions for the finite temperature case is discussed.

BIO
Dr. Samit Roy primarily works in computational solid mechanics with an emphasis in composite materials and nanostructured materials. He has been working in the development of analytical and numerical models of various solid structural systems for almost 20 years. As the Jordan Chair, Roy provides leadership in the solid mechanics group and expand the research areas, particularly in composite materials.