PREDICTION OF FAILURE ONSET IN MULTILAYER GRAPHENE REINFORCED EPOXY COMPOSITES USING MOLECULAR DYNAMICS SIMULATIONS

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Abstract:

Carbon fiber reinforced polymer composites have become more and more popular in aircraft and aerospace industries because its advantages in light weight, high stiffness and high strength. For these composites, the fibre/matrix interface strength is an important parameter to determine such mechanical properties as fracture toughness and creep resistance. Understanding how the carbon fiber interacts with the polymer matrix is critical for evaluating the role of matrix adhesion to the overall composite performance. Experimental observations have found two distinguish failure mechanisms of fiber/polymer interface, i.e. adhesive failure and cohesive failure [1]. How to explain these failures at the atomistic level is very interesting and also helpful to better understand influential factors contributing onset of interface failure. This paper reports our recent studies on carbon fiber/epoxy composites by using Molecular Dynamics (MD) simulations.

The epoxy/amine formulations we considered is Diglycidyl ether of bisphenol A (DGEBA) known commercially as Epon 825 with 3,3’ Diamino-Diphenyl Sulfone (33DDS). We simulate the curing processes of polymer matrix in the presence of graphite reinforcement, which is assumed to be composed of layers of graphene bound together via van der Waals interactions. Two configurations with multilayer graphene slabs with planes oriented parallel with or normal to the polymer interface are considered. The layers simulate the composite fiber reinforcement and characterize the two extreme configurations that can occur in carbon fiber surface consists of graphene edges with a distribution of angles relative to the radial direction. All MD simulations of the DGEBA/33DDS system are carried out using LAMMPS and the general Dreiding force field with harmonic form of potentials is employed. The initial configurations are equilibrated with constant stress, isothermal MD simulations at 600K and under atmospheric pressure. We use a recently developed procedure [2, 3] to simulate the curing of thermoset polymers based on MD simulations where chemical reactions are performed in a stepwise manner using a distance-based criterion. New bonds are turned on slowly using a 50 ps long multi-step relaxation procedure to avoid large atomic
forces. After the new bonds are fully relaxed an NPT simulation for an additional 50 ps is performed before a new set of bond creations is attempted. The curing process is simulated at a temperature of 600K and terminated if 85% conversion degree is reached and then the model systems are cooled down to room temperature.

Figure 1 Composite failure mechanism: (a) Cohesive failure; (b) Adhesive failure

In this study, we focus on the tensile failure of graphene/polymer composite in the direction normal to the interface. We characterize the mechanical response of the resulting samples via non-equilibrium molecular dynamics (MD) simulations focusing on yield stress and post yield behavior. The onset of failure and evolution are tracked. We found the strength of the composites under uniaxial tension are higher that the corresponding value for the bulk polymer regardless of the relative orientation of the MLG and the composite interface. However, the parallel MLG exhibits a stronger interface (higher interfacial energy) leading to cohesive failure in the bulk polymer. On the contrary, the normal MLG case exhibits adhesive failure at the interface leading to a more brittle behavior and steeper post yield softening due to its ability to localize deformation at the interface.

To understand the reason behind these two failure mechanisms, we investigate four factors: interfacial energy, reactive sites distributions, strain level and cooling rate. We find that interfacial energy play an critical role in failure modes. But the strain levels for these two failure modes are roughly the same. Cooling rate and reactive sites distributions have an effect on onset location of cohesive failure inside polymer.

REFERENCES