APPLICATION OF CONCURRENT ATOMISTIC-CONTINUUM COUPLING TO STUDY FRACTURE IN POLYMER NANOCOMPOSITES

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Abstract

Nanoparticles have been used to improve the fracture toughness of polymer composites. Understanding the nanoscale mechanisms that promote enhanced toughness is critical to tailoring such material properties, and Molecular Dynamics (MD) simulations have been extensively used for this purpose. However, our ability to model real-life macroscale cracks purely using MD simulations is limited by the large length and time scales involved. Therefore, concurrently coupling continuum models such as Finite Element Method (FEM) with MD can potentially circumvent the length-scale issue and help provide insight into these basic failure mechanisms. The objective of this paper is to use a state-of-the-art concurrent atomistic-continuum coupling technique to study the nanoscale crack-tip behavior of a macroscale crack in a thermosetting resin and demonstrate its potential to study macroscale fracture in nanocomposites materials.

1. Introduction

The overarching aim of our research is to achieve better understanding of the structure-property relationship for polymer nanocomposite materials in the presence of a macro-scale crack. While experiments at the nanoscale can be challenging if not impossible to conduct, MD simulations are providing a predictive pathway to study material properties at the nanoscale. However, MD is computationally intensive, thus limiting system sizes to sub-micron levels. As a result, work related to MD prediction of real-life fracture properties has been limited, where simulating the appropriate loading conditions and system size is essential to capturing the correct nature and mechanisms of failure or toughening. Such problems have spawned a class of multiscale methods that concurrently connect two or more spatial domains represented by different physical models. For instance, by connecting an MD domain in the region of interest (i.e., crack tip) with an FEM domain surrounding it, it is possible to achieve much larger and physically relevant system sizes. Concurrent coupling methods are still in their infancy, and research is ongoing in developing general methods for amorphous materials simulated at finite temperatures. In this work, we use a staggered adaptation of the Arlequin method with partitioned domains to couple MD with FEM and demonstrate its application in macro-scale fracture modelling while including material interactions at the nanoscale.

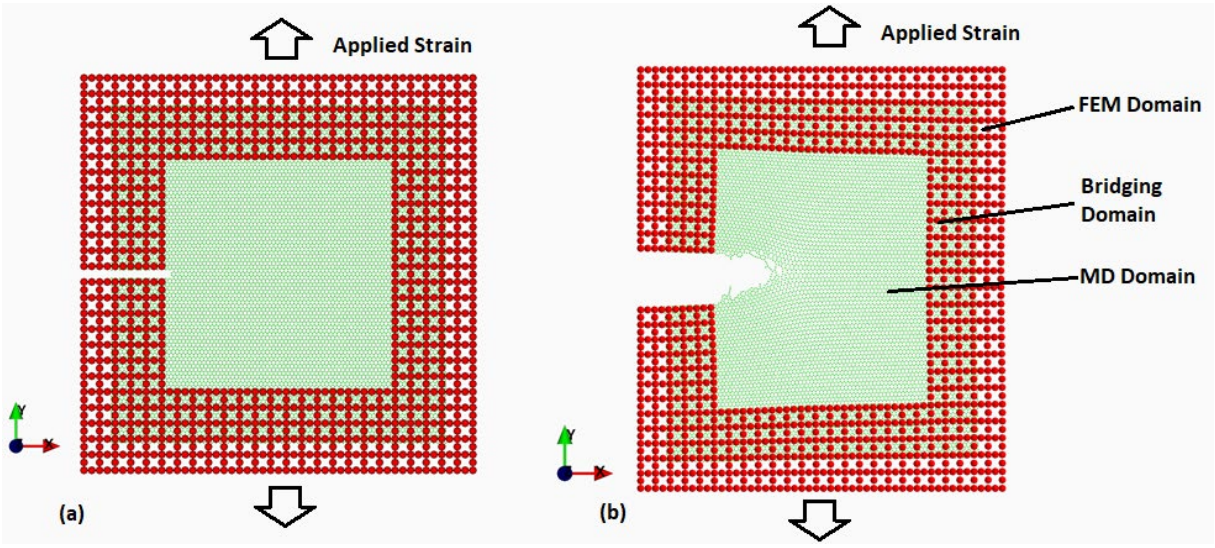

Fig.1 – (a) pre-cracked and (b) propagated graphene monolayer specimen with concurrent FEM-MD coupling.

2. Results

MD simulations were conducted using the open-source LAMMPS code. The material is represented in MD in all-atom resolution at finite temperature. A wrapper FEM code is used to implement the staggered approach, iterating between FE and MD steps until convergence is achieved for a given load state. Preliminary tests are conducted using a 2D monolayer of graphene as shown in Fig. 1. There is an outer FEM domain and an inner MD domain, coupled via a bridging region. All boundary conditions are applied to the FEM and displacements and forces are transmitted to the MD, resulting in mode I propagation of the crack as shown in Fig. 1. Strain energy release rates (SERR) are calculated at various load points before crack propagation. These data, as shown in Fig. 2, match well with those from an identical simulation modelled using purely FEM.

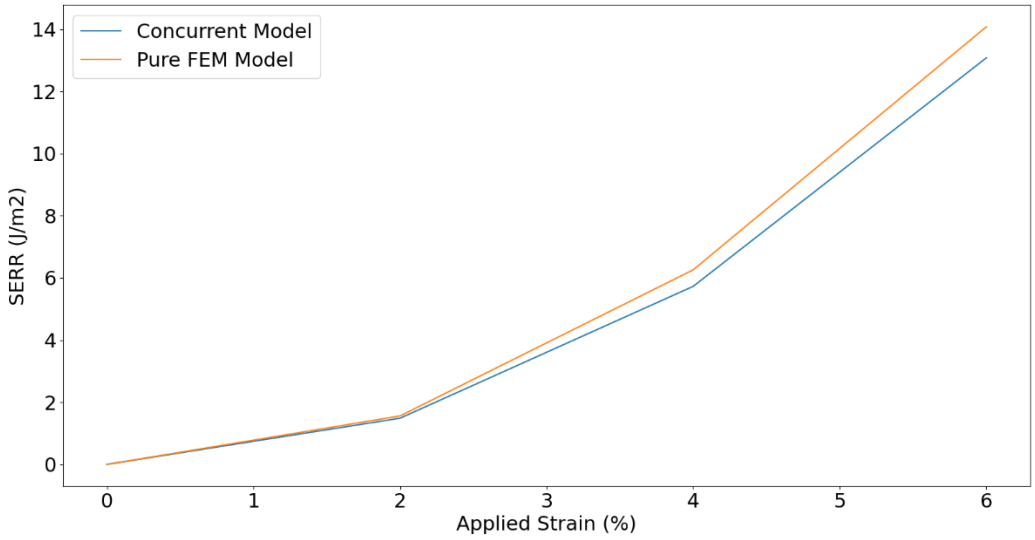

Fig.2 – Strain energy release rate (SERR) at various load levels in the concurrent model and an identical pure FEM model.

With the coupling methodology validated for monolayer crystalline graphene, work is currently underway to simulate fracture in amorphous thermosetting polymer resins and their nanocomposites.

3. Conclusions

Realistic macro-scale fracture modelling in polymer nanocomposite materials using MD simulations necessitates concurrent coupling with continuum models such as FEM to arrive at appropriate length scales. We use the state-of-the-art in concurrent atomistic-continuum coupling techniques for crystalline and amorphous materials to establish a proof-of-concept. Results are shown for concurrently coupled fracture modelling in monolayer graphene. The validated fracture model is currently being tested for amorphous thermosetting polymers and their nanocomposites, and the latest results will be included in the conference presentation.

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