Study of Crack Propagation of Graphene Using Atomic-scale Finite Element Method

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ABSTRACT

Graphene has attracted significant attention due to its unique electronic and mechanical properties. Several computational approaches such as molecular dynamics methods and modified continuum methods have been used to study the mechanical behavior of graphene including studies dealing with fracture mechanics.

Our preliminary studies show that the atomic-scale finite element method [1] (AFEM) [1] can be effectively used to model graphene [2]. Atomic-scale finite element method is an atom based finite element method, where the stiffness of the atoms is derived from a molecular mechanics force field. AFEM is much more superior compared to commonly used bond based finite element method for nanostructures. Figure 1 shows the basic AFEM element, which we use in this study. The central atom of the element interacts with three nearest neighboring atoms (No. 2 to No. 4) and with six second nearest neighbors (No. 5 to No. 10).

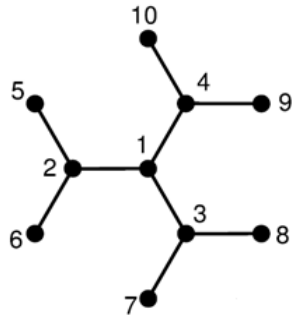

Figure 1. Basic AFEM element

In this work, an approach based on the virtual crack closure technique and the atomic-scale finite element method was employed to obtain the atomistic formulation of strain energy release rates for graphene sheets under mode I fracture. The proposed model is numerically less intensive in comparison to other numerical techniques, such as molecular dynamics simulations. It is shown that the proposed approach yields results that are quite accurate compared to more refined schemes such as molecular dynamics analysis.

REFERENCES

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