

THE ATOMISTIC STUDIES OF MECHANICAL BEHAVIOR OF GRAPHENE SHEET USING TERSOFF POTENTIAL

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ABSTRACT

In this work the atomic-scale finite element method (AFEM), proposed by Liu et al. (2004), is used to describe the mechanical behaviour of graphene sheet having armchair edges. Nanomaterials as graphene sheet, carbon nanotubes (CNT) (Iijima, 1991), require many-body potential formulations. In this work the Tersoff potential is considered. Initially, in order to validate the AFEM implementation, the force-strain curve of perfect graphene sheet will be compared with molecular dynamics (MD) LAMMPS code. Additionally, the influence of the presence of crack on the ultimate tensile strength of graphene will be studied considering four different sized meshes.

Keywords: AFEM, graphene, Tersoff, armchair edges.

INTRODUCTION

Graphene as carbon nanotubes (CNT), are found to possess superior mechanical, electronic, thermal and optical properties [The Royal Society and The Royal Academy of Engineering, 2004]. AFEM, proposed by Liu et al. (2004) has been used to model the mechanical behaviour of graphene sheet. AFEM uses both first and second derivatives of system energy in the energy minimization computation.

Tersoff potential, proposed by Tersoff (1987), is used to study the mechanical behaviour of graphene sheet, as well as the effects of vacancy defects on the mechanical behaviour. In this potential, the internal force between two atoms depends on their separation distance, r_{ij} and it's based on the relative position of second nearest-neighbor atoms. The energy stored on the bond between atoms i and j is given by,

$$V_{ij} = f_c(r_{ij}) \left[V_{ij}^R(r_{ij}) + B_{ij} V_{ij}^A(r_{ij}) \right] \quad (1)$$

RESULTS AND CONCLUSIONS

In order to validate the AFEM implementation, the force-strain curve of perfect graphene sheet, as shown in Figure 1(a), will be compared with molecular dynamics (MD) LAMMPS code. The curve obtained from AFEM shows good agreement with the curve obtained from MD, as shown in Figure 1(b).

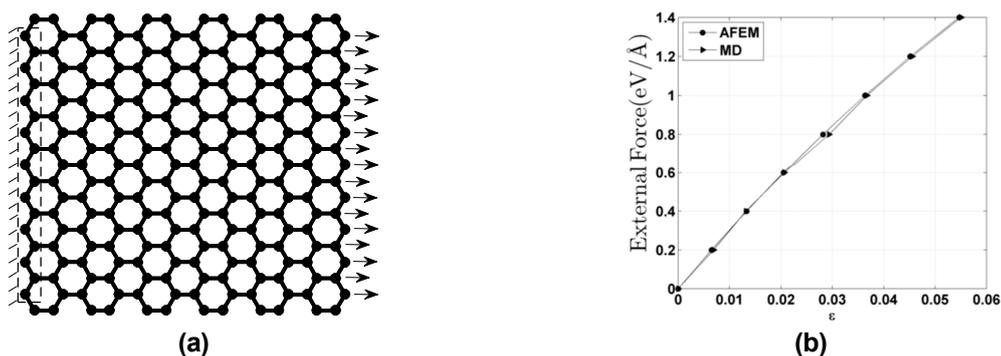


Fig. 1 - (a) Graphene sheet, (b) force-strain curves obtained from AFEM and MD

Figure 2 shows the stress-strain curves of the graphene sheets obtained from AFEM under uniaxial tensile loading. The crack of length is set as 1.4 nm, and the size of graphene sheet is increased from 5 nm x 5 nm to 14.5 nm x 14.5 nm.

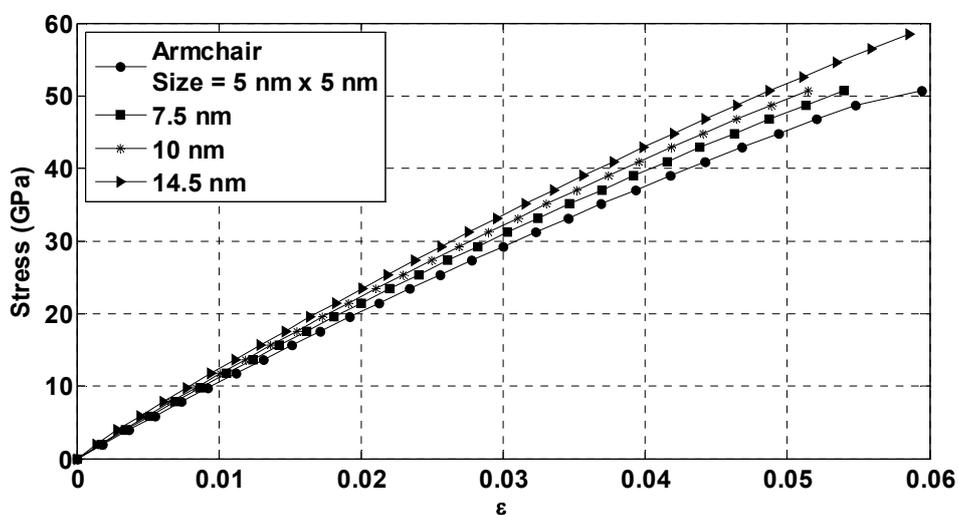


Fig. 2 - Stress-strain curves obtained from AFEM

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