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Molecular Dynamics Analysis on Impact Behaviour of Carbon Nanotubes and Graphene Sheets

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***Abstract*—**Impact behavior of striker on graphene sheet and carbon nanotube is investigated based on molecular dynamics (MD) simulations. A MD simulation is conducted to obtain the maximum dynamic deflections of a square and rectangular single-layered graphene sheets (SLGSs) with various values of side-length and striker parameter. Effect of (i) chirality, (ii) graphene side-length and nanotube length, (iii) striker mass on the maximum dynamic deflections of graphene and nanotube are investigated. The effect of different types of boundary condition on the maximum dynamic deflections is studied for zigzag and armchair SWCNTs with various aspect ratios (Length/Diameter).

***Keywords*—**Impact, molecular dynamic, graphene, nanotube.

I. Introduction

THE immense stiffness, strength and enhanced electrical conductivity of the graphene sheet and nanotube may make them an ideal material to provide a new foundation to apply in different emerging fields of nanoscience and nanotechnology.

Jin-leen Tsai et al. [1] investigated the macroscopic fracture parameters from both atomistic simulation and the continuum model, the results show that the strain energy release rates obtained from the continuum model indicated excellent agreement with those derived from discrete atomistic model. Lee et al. [2] measured elasticity modulus and intrinsic breaking strength of free-standing monolayer graphene membranes by using an AFM in the nanoindentation experiment. Seifoori and Liaghat [3] formulated the impact of mass on nanotubes using nonlocal model of Timoshenko beam theory (TBT) and a 3D explicit finite element model. The increase of the nonlocal effect increases the magnitudes of dynamic deflections and decreases frequencies.

Mylvaganam and Zhang [4] discussed several important issues in a MD simulation for carbon nanotubes and mechanical properties. They found that the ultimate tensile strain of a carbon nanotube is around 40% before atomic bond breakage.

Seifoori [5] presented dynamic analysis of transverse impact of a mass on Euler–Bernoulli and Timoshenko nanobeams (nanotubes) based on the two degree of freedom model. MD simulations were carried out for a series of armchair and zigzag SWCNTs by varies striker velocity, striker mass and nanotubes boundary conditions. Seifoori and Hajabdollahi [6] performed the dynamic analysis of impact of striker on SLGS by using the two degree of freedom spring-mass model and the MD and finite element simulations.

Wang et al. [7] measured the elastic properties and mechanical behavior of some rectangular SLGS under various indentation depths, velocities, and radius of indenter using MD simulations.

In this article, the impact of striker on carbon nanostructure is investigated by MD simulation. MD simulations for estimating dynamic behavior are carried out to illustrate the nanostructure dynamic behavior. Based on these simulations, the maximum dynamic deflections of nanostructure with different geometries, as well as chiralities, are obtained and then compared with theory investigation.

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II. MD Simulation

MD simulation is considered a powerful and accurate method enabling the simulation of nanostructures by solving Newtonian equations of motion.

Using large-scale atomic/molecular massively parallel simulator (LAMMPS), MD simulations are performed to the modeling of impact behavior of nanostructure. The simulation was considered in an NVT ensemble at a constant room temperature of 300 K. The AIREBO potential and the time step of 0.001 ps are selected to simulate the impact response of the nanostructure.

To consider boundary conditions, one layer of atoms at the end of SWCNTs is fixed to simulate boundary conditions, as can be seen in Fig. 1.

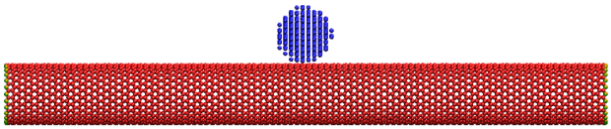

Fig. 1 The schematic of boundary conditions of SWCNT

For the MD simulations of the indenter and the graphene film, the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential are established. To consider boundary conditions, one layer of atoms at all sides of SLGSs is fixed in space to simulate conditions which is shown in Fig. 2.

In most simulations, striker is considered as a rigid body. For the target originally at rest, the striker is struck with an initial velocity 5 Angstroms/picosecond at the center of the graphene and nanotube. The striker is a spherical Au nanoparticle with radius 10 Angstroms.

The closest possible dimensions for the armchair (15, 15) and zigzag (26, 0) are considered so that they have nearly the

same diameters that make it possible to study the chirality effect on dynamic deflection.

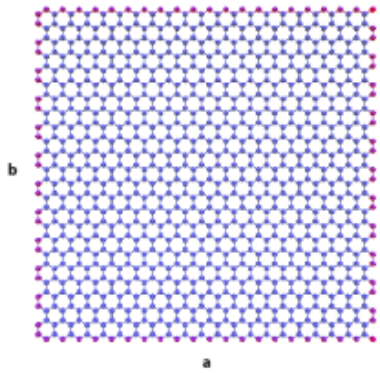

Fig. 2 The schematic of boundary conditions in MD simulation of graphene sheet

The deformation shapes at maximum deflections of the nanotubes and graphene are shown in Figs. 3 and 4 for simulations.

Fig. 3 The deformation shapes at maximum deflections on SWNTs in MD simulation

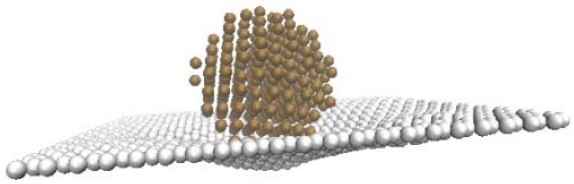

Fig. 4 The deformation shapes at maximum deflections on SLGSs in MD simulation

III. Results and Discussion for Nanotube

The maximum transverse dynamic deflection of MD simulation is graphically shown for a different nanotubes aspect ratio (length/diameter) in Fig. 5 with zigzag and armchair SWCNTs.

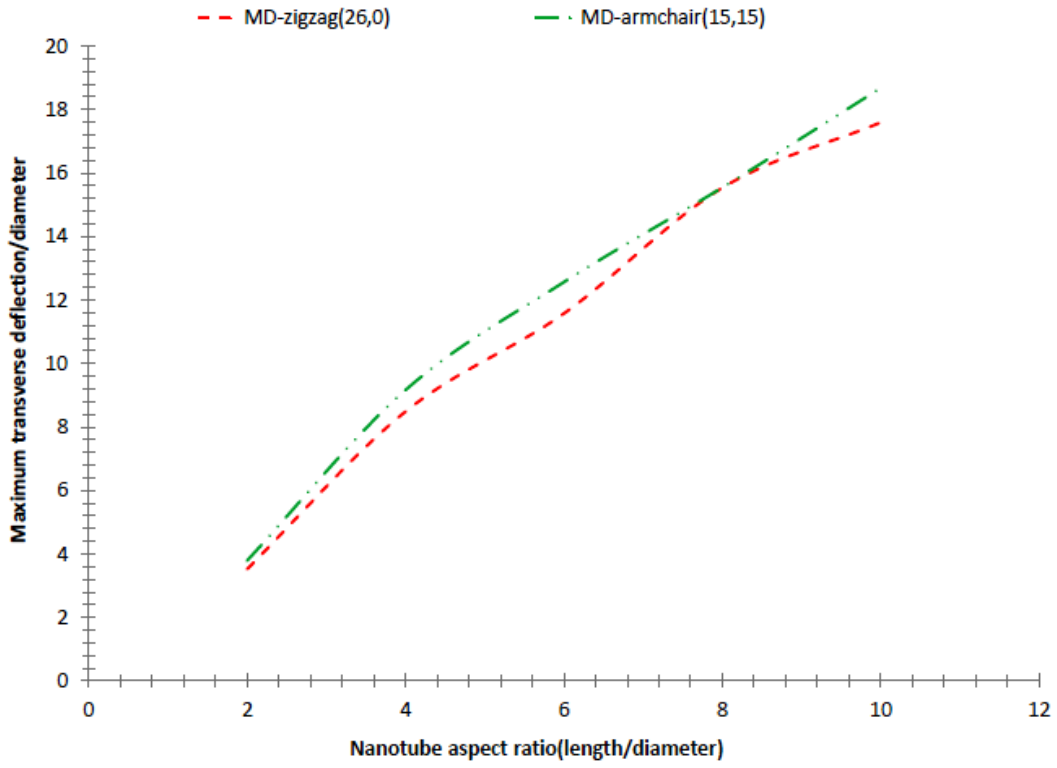

Fig. 5 The maximum dynamic deflections versus nanotube aspect ratio of MD simulations for the clamped zigzag (26, 0) and armchair (15, 15) nanotubes

Fig. 5 shows that the maximum dynamic deflection in the center of the nanotube is increased when the nanotube aspect ratio is increased for these boundary conditions. In order to study the dynamic behavior of SWCNTs, the nanotube with a clamped-free boundary condition is simulated, as shown in Fig. 6.

The results of MD simulations for the armchair (15, 15) and zigzag (26, 0) nanotube with a clamped-free boundary condition are graphically compared, as shown in Fig. 7. It can be found that in contrast to the pervious boundary conditions, the clamped-free boundary condition make a relatively a significant difference between the armchair and zigzag nanotube due to the difference in the chirality.

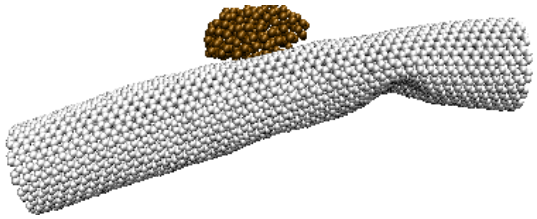

Fig. 6 Deformation of MD simulation for the nanotube with a clamped-free boundary condition and L/d=6

IV. Results and Discussion for Graphene

It can be observed from the MD simulation results that generally; chirality does not have a considerable influence on the value of the maximum center deflection of SLGSs. However, in the case of rectangular SLGSs, it is seen that the deflection of armchair SLGSs are a little higher than those of zigzag SLGSs. The impact response of graphene is governed by the striker/plate mass ratio, where the small striker mass is independent of the graphene boundary conditions and may be treated as an impact on an infinite graphene sheet. Large striker mass caused quasi-static behavior, where the load and deflection essentially have the same relation as under a concentrated static load. Therefore, quasi-static impact response occurs when the striker mass is larger than the mass of the graphene. Small and large striker mass displacements are graphically compared with MD simulation, as shown in Fig. 8.

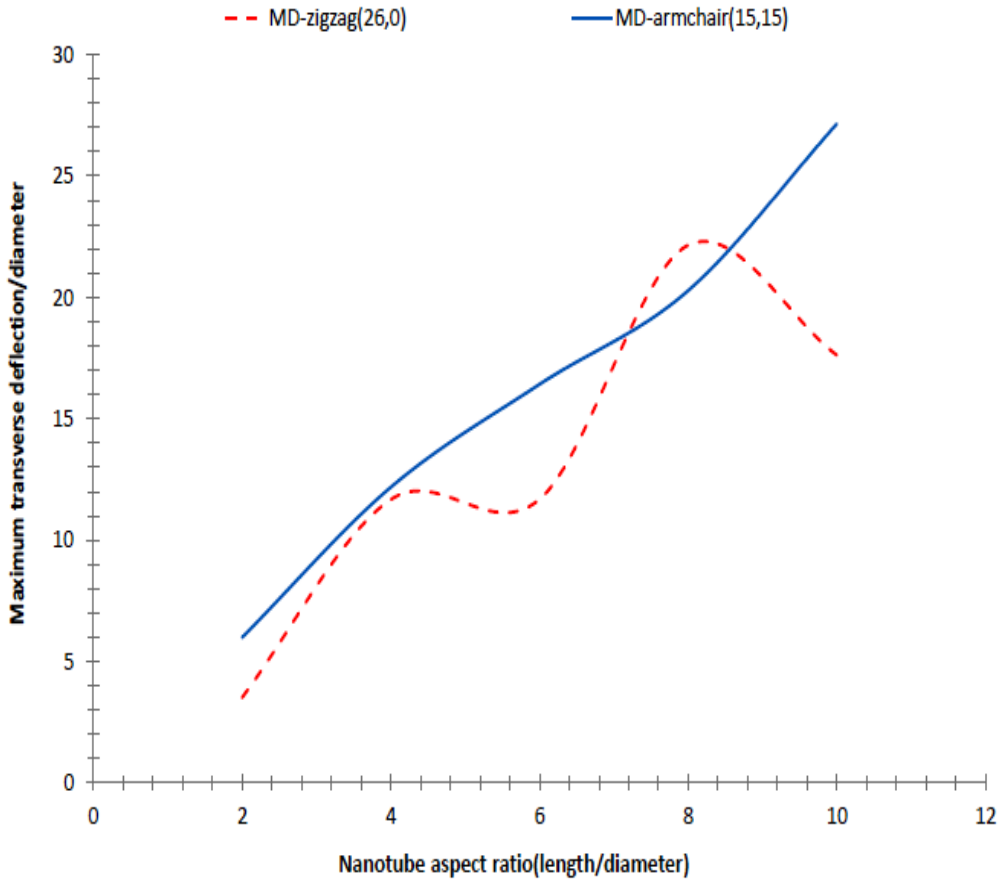

Fig. 7 The results of MD simulations for the armchair (15, 15) and zigzag (26, 0) with a clamped-free boundary condition

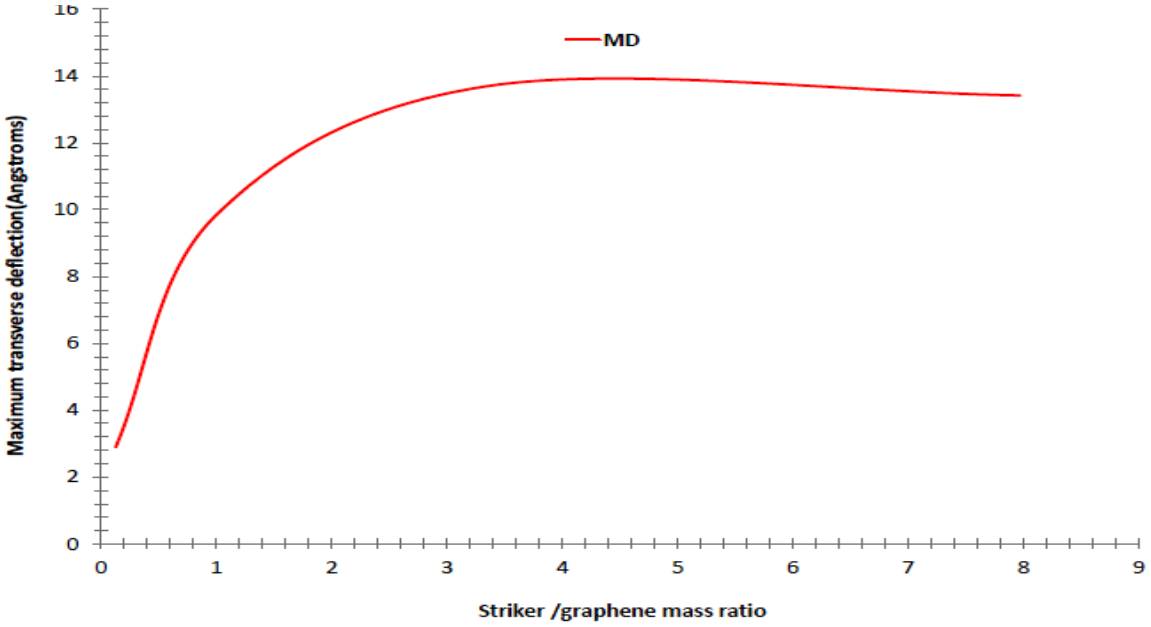

Fig. 8 The influence of striker mass on the dynamic deflections in MD simulation and analytical model

By increasing striker velocity to 15 Angstroms/picosecond, high local deformation occurred. Global deformation is not increased due to the damage caused in the graphene, as shown in Fig. 9.

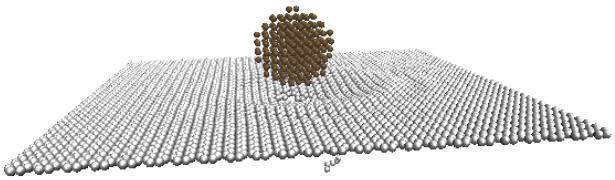

Fig. 9 The deformation shapes at maximum deflections on SLGSs in MD simulation

V. Conclusion

In this study, MD simulations were carried out for a series of armchair and zigzag SWCNTs to compare the results corresponding to each type of boundary conditions. Also, MD simulations were performed for a series of square and rectangular SLGSs with various values of side-length and chirality. Small striker mass is independent of the graphene boundary conditions and can be simulated as an impact on an infinite plate. For large striker mass, load and deflection essentially have the same relation.

The inclusion the deformation of the striker decreases deflection. The growth of the mass ratio increases the magnitudes of dynamic deflections.

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