

Effect of Defects on Mechanical Properties of Graphene under Shear Loading Using Molecular Dynamic Simulation

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Graphene sheet including single vacancy, double vacancy and Stone-Wales with armchair and zigzag structure was simulated using molecular dynamics simulation. The effect of defects on shear's modulus, shear strength and fracture strain was investigated. Results showed that these shear properties reduce when the degrees of all kinds of defects increase. The dangling bond in SV and DV defected graphene leads to decrease its mechanical properties especially shear strength and fracture strain where the role of weak interatomic bonds are important. The vacancies in DV defected graphene are also next to each other and slide over each other under shear deformation results to less shear strength than that of SV defected graphene. Results can be useful in tuning the mechanical properties of graphene-based materials that is a key-role parameter in designing and fabrication of nanomechanical systems. However, the maximum and minimum reduction occurs for single vacancy and Stone-Wales defects, respectively. It was also found that distinction between shear properties of zigzag and armchair structures is preserved in defected graphene.

Keywords: Graphene, Simulation, Shear's modulus, Defect

INTRODUCTION

Graphene is a two dimensional sheet with covalent bonds of carbon atoms. It is a noticeable material due to its mechanical, electrical, thermal and optical properties. Graphene is found in different carbonized forms and nanotubes made by wrapping graphene sheets. Based on the repeating units it can be divided to armchair and zigzag graphene. The remarkable structure and particular properties of graphene make a vast applications in different fields such as sensors, batteries, transistors, solar cell, as well as gas separation membranes [1-4]. The unique mechanical property of graphene has been reported such as elastic properties and high intrinsic strength [5], which is important for the practical applications. The main feature is due to the structural integrity of the hexagonal graphene lattice and strong in-plane sp^2 bond between carbon atoms. There are

some techniques to fabricate graphene layers such as mechanical exfoliation of graphite [6], chemical exfoliation of graphite [7,8] and chemical sedimentation of graphite vapor on metal surfaces [9-11]. Preparation of graphene sheets is still a challenging task, and defects are inescapably present in the graphene materials for different synthesis methods. Previous reports have shown that structural defects have a great effect on the chemical, electronic and magnetic properties [12-14], but the influence of various defects on the mechanical properties of graphene has not yet been well investigated and needs more study.

Three highest structural defects which appear during growth can be classified into: incomplete bonding defects, topological defects and heterogeneous defects. The simplest defects in graphene sheets are single vacancy (SV) and double vacancy (DV) [15,16], resulting from missing carbon atoms. No atom is removed or added to the sheet in stone-Wales (SW) [17] defect. Four hexagons are transformed into two pentagons and two heptagons by

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rotating one of the C-C bonds by 90°.

Shear's modulus, as the most important properties, is a measure of the hardness of an elastic material in engineering design. Shear's modulus of defect-free and functionalized graphene has been investigated by experimental and computational research [18,19]. However, the shear's modulus of defective graphene has not yet been well studied. The structural defects have enormous effects on the shear's modulus of graphene. There are different types of stress: tension or tensile stress, compression or compressive stress and shear stress. Shear's modulus describes the material response to shear stress and stiffness of material under tensile or compressive stress. In the case of graphene, with the reduced dimension, it is more logic to define the in-plane stiffness instead of the classical 3D Young's modulus.

In this work, to investigate the effects of structural defects on shear's modulus of graphene, we perform MD simulations of SV, DV and SW defects for armchair and zigzag graphene sheets. The effects of these defects on the characteristics of graphene under shear for different degree of defects are studied.

MODELS AND COMPUTATION METHODS

In this research, a pristine graphene sheet with dimensions of $x = 50 \text{ \AA}$ and $y = 50 \text{ \AA}$ is simulated by MD simulation. The adaptive intermolecular reactive bond order (AIREBO) potential [20] is applied using LAMMPS software [21]. For shear replacement, the x positions of all atoms at the top layer are changed by the rate of 10^{-4} \AA/ps (Fig. 1). Here, MD simulations are accomplished in the NVT (the volume and the temperature are constant) and NPT (the pressure and the temperature are constant) ensemble and time step size in all cases is 1 fs. Finally, strain energy per volume (u) is calculated based on Eq. (1) [22].

$$u = 1/2G\varepsilon^2 \quad (1)$$

Where ε is strain and G is shear's modulus.

The defect degree of vacancies is the number of atoms which have been removed from the pristine graphene sheet. When an atom is removed from its lattice position, the lattice bonding geometry around the vacancy changes and a

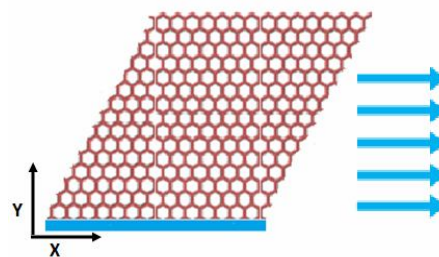


Fig. 1. Displacement of graphene nano sheets.

lower energy state is generated. Consequently, reconstruction of vacancy defects in the graphene sheets takes place. The diffusion and reconstruction of vacancy defects in graphene layers have been investigated theoretically [23,24]. The SV defect reconstruction modifies two of the three dangling bonds of the missing atom, but one dangling bond is open. There are no dangling bonds in the graphene with DV defects and it is such as pristine graphene sheet. SW displacement means rotating one of the C-C bonds by 90° and considering two defected atoms.

RESULTS AND DISCUSSION

Figure 2 shows the shear strength versus fracture strain for ideal armchair and zigzag graphene. It can be seen that the shear strength is 74.53 and 88.63 GPa and fracture strain is 0.26 and 0.32 for armchair and zigzag, respectively. Figure 3 displays the strain energy versus fracture strain for the ideal zigzag and armchair directions of graphene sheet. The result of shear's modulus is 205.9 and 198.78 GPa for zigzag and armchair structure, respectively, consistent with previous report [25]. To study the effects of single vacancy, double vacancy and Stone-Wales defects on shear's modulus, we created 1 to 5 defects of SV, DV and SW types in the graphene sheets. Shear's modulus versus defect degree for armchair and zigzag structure is investigated.

The results showed that shear strength and fracture strain is decreased by increasing the defects of all three kinds of defects, as shown in Figs. 4 and 5. Regarding the figures, a decreasing trend in shear strength and fracture strain, simultaneously with increasing the defected degree, is observed for zigzag and armchair structure. This decreasing trend indicates the reduction of sheets' strength which has more defects degree. In the SW defect

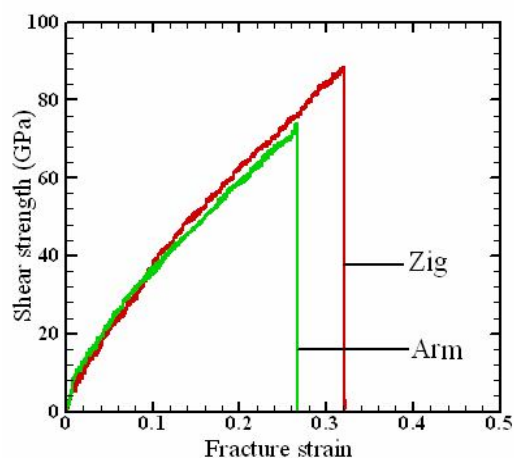


Fig. 2. Shear strength vs. fracture strain for ideal armchair and zigzag graphene.

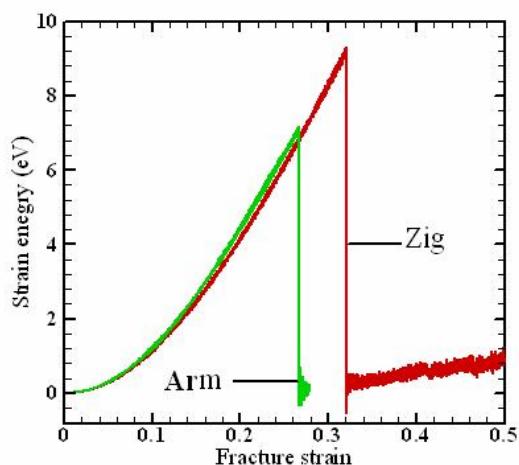


Fig. 3. Strain energy vs. fracture strain for ideal armchair and zigzag graphene.

interatomic sp^2 bonding is preserved by two heptagons and two pentagons. Therefore, SW defects have smaller effect on the stress and strain of graphene than vacancy defects. But for vacancy defects, there are dangling bonds near the carbon atoms, resulting a decrease in the shear's modulus. Moreover, since the graphene with SV defects has more dangling bonds than graphene with DV defects, its shear's modulus is much smaller than graphene with DV defects.

The strain energy for defected sheets in zigzag and armchair structures and the shear's modulus in terms of

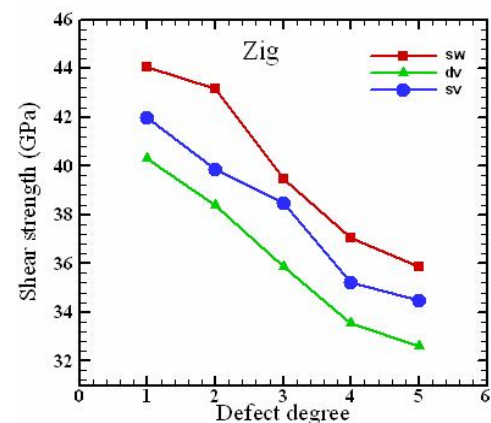
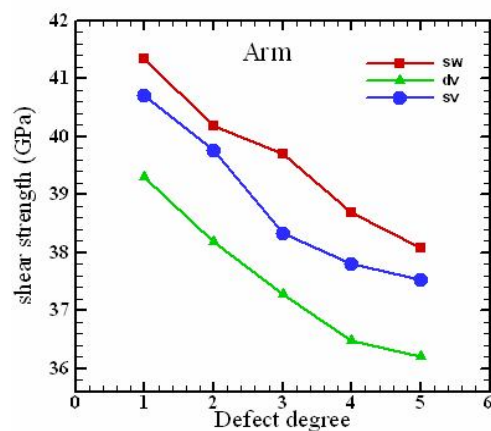


Fig. 4. Shear strength vs. defect degree for defected armchair (top) and zigzag (down) graphene nano sheet.

strain were calculated. Figures 6 and 7 show shear's modulus versus defect degree for zigzag and armchair structures, respectively.

Strength reduction is the result of modules decreasing due to increasing the defect degree. Again the SW defected sheets showed the least reduction and single vacancy defected sheets showed the most reduction. This effect could be explained in terms of the hardness of the C-C bonds in the graphene sheets, due to geometrical reconstruction. All of this indicates that the SW could be the strongest.

The variation of the mechanical properties of graphene sheets for zigzag and armchair structures was observed. But even in the presence of defects, zigzag has higher shear's

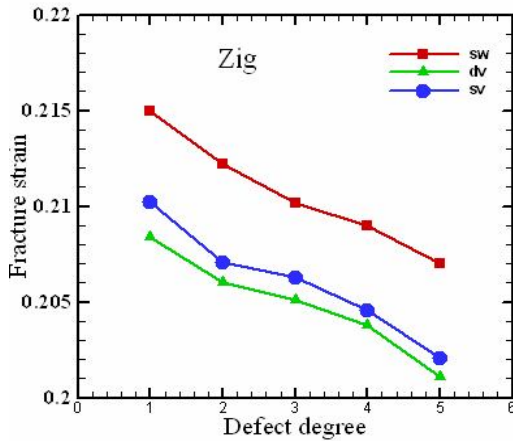
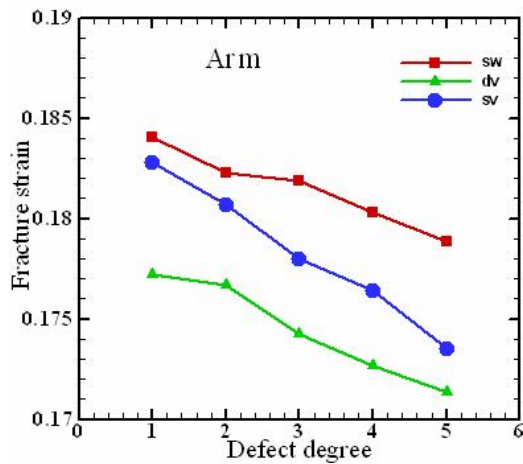


Fig. 5. Fracture strain vs. defect degree for defected armchair (top) and zigzag (down) graphene sheet.

modulus than armchair structure. This property could lead to important consequences regarding the defected structure because the existence of defects could make it soft or stiff.

CONCLUSIONS

In summary, using molecular dynamics simulation it is shown that shear's modulus, shear strength and fracture strain of defected graphene decrease when the grade of defects increases depending on the type of defect. It is found that the SW defect has the least effect on the shear properties of graphene compared to that of the SV and DV defects because of no dangling bond in SW defected graphene. The dangling bond in the SV and DV defected

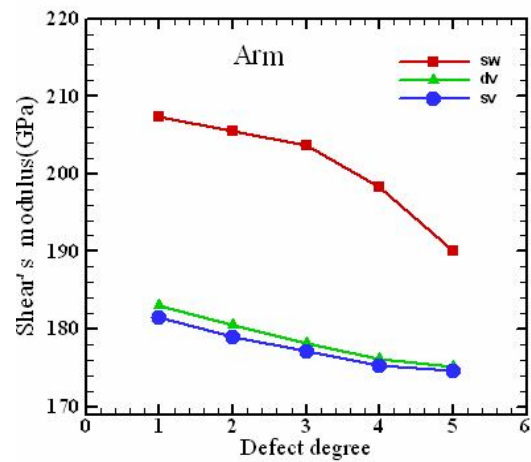


Fig. 6. Shear's modulus vs. defects degree for armchair graphene sheet.

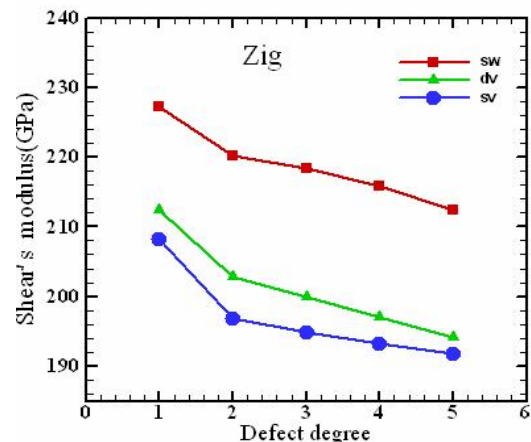


Fig. 7. Shear's modulus vs. defects degree for zigzag graphene sheet.

graphene leads to decrease the mechanical properties especially shear strength and fracture strain where the role of weak interatomic bonds are important. The vacancies in DV defected graphene are also next to each other and slide over each other under shear deformation results to less shear strength than that of SV defected graphene. Results can be useful in tuning the mechanical properties of graphene-based materials that is a key-role parameter in designing and fabrication of nanomechanical systems.

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