RESEARCH ARTICLE

Stress-strain behavior of two-layer graphene with different chirality

Mohsen Motamedi [1,*], A.H. Aghili [2]

[1] Faculty of engineering, university of shahreza, Isfahan, Iran

[2] Department of Mechanical Engineering, Faculty of Engineering, University of Shahreza, Shahreza, Iran

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ABSTRACT

Graphene is a two-dimensional sheet containing carbon atoms arranged as a honeycomb lattice. Graphene has been recently the subject of much interest due to its unique mechanical, thermal, and electrical properties. The experimental method for calculating the mechanical properties of graphene is complex because of its nanoscale lateral dimension, so the use of the theoretical method for calculating the properties of monolayer graphene has also received much attention recently.

In this study, two-layer graphene with two different chirality angles was modeled by molecular dynamics in LAMMPS software. In summary, this research involves producing the primary structure, balancing the sample, applying the axial tensile test, and extracting the stress-strain graph from the sample. The simulated graphene has a value of 102.2*100.8 Å and an interlayer distance is 3.4 Å.

The results showed that as the number of sheets increased, the amount of Young's modulus was more than that of the single-layer graphene. In addition, the fracture strength of the two-layer armchair graphene is greater than the fracture strength of the two-layer zigzag graphene. Then, by increasing the chirality angle, the fracture strength decreases. Finally, it was shown that by increasing the chirality angle in two-layer graphene from 0 ° (armchair) to 30 ° (zigzag), the Young's modulus value increases, while by increasing the chirality angle in single-layer graphene from 0 ° to 30 °, the Young's modulus does not change significantly.

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INTRODUCTION

Nowadays, carbon structures have a wide range of diversity and applications. Graphite, diamond, amorphous carbon, carbon nanotubes and graphene are different forms of carbon structures. Graphene is the newest form of the multi-dimensional graphite carbon family.

A 2D graphene sheet contains atoms of carbon which is arranged as a honeycomb [1-3]. Graphene has attracted much attention in recent decades due to its unique mechanical, thermal, and electrical properties [4-7]. Graphene is widely used in manufacturing electrical, nanoelectric and nano-electromechanical systems (NEMSs) because of its crystalline structure and strong electrical properties [8-9].

Among its special mechanical properties are an important advantage for its use in the structure of various materials. These properties include high Young's modulus (about 1100 GPa), fracture resistance (about 125 GPa) and good thermal conductivity. These incredible properties lead to the use of graphene instead of carbon fibers to reinforce the composites [10-12].

Graphene properties have been calculated through both experimental and numerical or theoretical methods.

Lee et al. [13] have created a crack in the center of a single-layer graphene sheet by atomic

* Corresponding Author Email: *motamedi@shahreza.ac.ir*

force microscopy (AFM) and so they have experimentally shown that one of the toughest materials is graphene, so that the modulus value of a monolayer graphene with thickness of 0.335 nm was reported 1.0±0.1 TPa and graphene fracture strength was reported 130 GPa.

Because of the complexity of the experimental method for calculating the mechanical properties of graphene because the lateral dimension of graphene is nanoscale, the use of the theoretical approach for calculating the properties of single-layer graphene has also received much attention recently.

Hernandez et al. [14] have calculated the Young's modulus of graphene equals 1.206 TPa by the orthogonal bending method.

Using density function theory coupled with local density approximation, Leo et al. [15] found that at small strain scales, graphene has an isotropic elastic response with an elastic modulus of 1050 GPa and a Poisson ratio of 0.186 based on DFT-LDA results. In addition, Van Lir et al. [16] reported value of Young's modulus of a single-layer graphene equals to 1.11 TPa by using Ab intio calculations.

Molecular dynamics simulation is an important atomic-scale numerical method that can investigate the chemical and physical properties of materials. In this method, the molecular motion of each particle is calculated in solid, liquid, and gas models, and the properties are obtained based on statistical theories of mechanics [17].

Zaeri et al. [18] have calculated the mechanical properties of single walled carbon nanotubes by molecular dynamics simulation. They have investigated the effect of nanotube chairality. diameter and nonlinearity of interatomic interactions.

By molecular dynamics and studying the intrinsic thermal vibrations of graphene, Jiang et al. [19] have obtained Young's modulus of the single-layer graphene. Moreover, the different effects such as model size, temperature and isotopic irregularity on Young's modulus of Graphene have been investigated using this method. For example, in this study it is shown that the Young's modulus of graphene increases with increasing temperature in the range (500-1000 °C).

Zhao et al. [20] have investigated the changes in strength of graphene fracture caused by changes in temperature, strain rate and crack length using molecular dynamics method, fracture kinetic analysis with elastic nonlinear relation and quantum fracture mechanics theory. The results show that the temperature up to 1200 K does not change much the Young's modulus of graphene. However, the fracture strength and fracture strain of graphene reduce considerably with increasing temperature. In addition, with increasing temperature to more than 1200 K, the Young's modulus declines and the material becomes softer so that at a temperature of about 2400 K the Young's modulus is 0.9 TPa. This result indicates that graphene is a very tough material compared to other materials even at very high temperatures.

By creating nanoscale cavities in monolayer graphene, the Young's modulus of graphene has been approximately calculated 1 TPa by molecular dynamics simulation [21].

By using MD, researcher has investigated the effects of defect, temperature and strain rate on the mechanical properties. By consideration of three types of defects including SV, DV and SW, They indicated that the existence of defects leads to remarkable decrease in the Young's modulus, fracture strength and fracture strain of graphene. It's found that for 1.67% defect concentration, the elastic modulus decrease from 106 to 55.5 GPa for graphene containing SV [22].

The researchers also investigated the effect of size and chirality on the properties of single-layer graphene by molecular dynamics. The results show that in small deformations (strains smaller than 0.5), chirality has no effect on linear elastic behavior of graphene [23]. However, with increasing strain, the chirality effect can be observed, so that the fracture strain is calculated 0.13 for the armchair model and 0.2 for the zigzag model [24].

Graphene is not limited to just one layer. Graphene is also bilayer and multilayer and the study of their properties is very important. In this paper, we investigate the effect of chirality (armchair and zigzag structure) on the elastic properties of bilayer graphene using the MD method. In this regard, bilayer graphene is investigated in two directions: armature (chirality angle of 0 °) and zigzag (chirality angle of 30 °).

MOLECULAR DYNAMICS SIMULATION

Molecular dynamics simulations have been performed by LAMMPS software [25]. In this simulation, the carbon-carbon covalent bond has been defined using the AIREBO potential [26]. This potential has utilized the potentials of REBO, Lennard Jones and the torsional interaction:

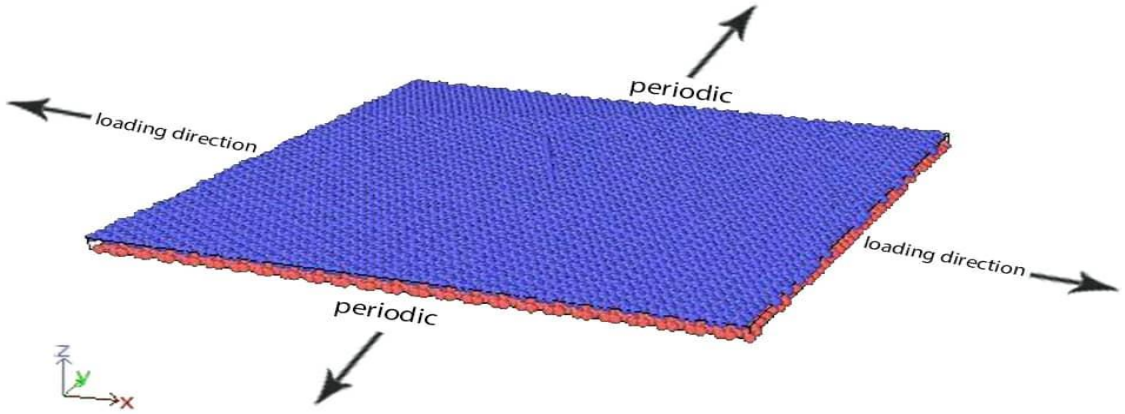

Fig. 1. Bilayer graphene and boundary conditions

$$E=\frac{1}{2}\sum_{i}\sum_{i\neq j}\left[E_{ij}^{REBO}+E_{ij}^{LJ}+\sum_{k\neq j\,L\neq i,\,j,k}\sum E_{kijl}^{TORSION}\right]$$

E_{ij}^{REBO} is the REBO potential, E_{ij}^{LJ} is the Lennard Jones potential and $E_{kijl}^{TORSION}$ is the torsional interaction potential.

The three right-hand statements show covalent bonding forces, interatomic interaction, and the effect of the dihedral angle. Lennard Jones potential has been also used to define non-bonded potentials between individual carbon atoms (between two layers), which is defined as follows:

$$E=4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right]$$

So that r is the distance between the atoms of carbon in the various layers, ε is the potential well's depth, σ is the equilibrium distance where the interatomic potential is zero. The values of Lennard Jones potential parameters, which are commonly used in modeling multilayer carbon structures, are considered as ε = 2.4 meV and σ = 3.4 Å based on the compressibility and distance between graphene sheets [27].for the REBO potential the total potential energy of system is given by:

$$E_{REBO}=\sum_{\mathrm{i}}\sum_{j=i+1}\left[E_R(r_{ij})-\bar{b}_{ij}E_A(r_{ij})\right]$$

Where r_{ij} is the distance between pairs of nearest nearby atoms i and j, $\bar{b}_{ij}$ is a many-bond empirical bond-order terms between atoms I and j that is derivable from Huckel electronics structure theory, E_R and E_A are the replusive and attractive pair terms, respectively,

$$E_R(r)=f_c(r)\left(1+\frac{\mathcal{Q}}{r}\right)A\exp(-\propto r)$$

$$E_A(r)=f_c(r)\sum_{n=1}^{3}B_n e^{-\beta_n r}$$

Wherein the parameters $\mathcal{Q}$, A, $\propto B$, β are utilize to fit the pairs, the quantity of these parameters are given in ref [28], and f_c is a cut off function.

To calculate the effect of the bond potential on the neighboring atoms, a function called the cut off function is used in most experimental potentials whose effect is very important when examining the fracture process. In this paper, the atomic cutoff radius is 2 Å for the REBO part of the potential [29].

COMPUTATIONAL DETAILS

The model used in the molecular dynamics simulation to apply axial traction on the bilayer graphene is as follows in Fig. 1. The simulated graphene has a value of 102.2*100.8 Å in directions of y and x and interlayer distance of 3.4 Å [30], respectively.

For investigation of the mechanical properties of the graphene bilayer, the axial tensile test is simulated using the method of applying deformation on the model. Prior to applying tensile on the created model which is shown in Fig. 1, both systems were equilibrated at 300 K at 30,000

time steps. The time step used in this simulation is equal to 1 femtosecond under NPT ensemble (using constant pressure-temprature by means of Nose-Hoover barostat and thermostat method) and pressure of zero bar with periodic boundary condition in three directions of x, y and z . During the tensile simulation of this specimen, the simulation box is stretched along the direction of x at a constant strain rate of 10^{-2}/PS and used under the NPT ensemble tensile at 300 K. This constant strain rate is applied to the structure every time steps. When applying the tensile test of boundary conditions in only two directions y, z is considered periodic. The stress is calculated along the x (axial stress) at every strain step. The engineering strain is also obtained at every time increment by multiplying the total loading time by the rate of applied strain. According to the Hook rule, the slope of the stress-strain curve in the linear part is equal to the elastic modulus of the bilayer graphene in direction of load application.

DISCUSSION AND RESULTS

Fig. 2 shows the stress-strain curve of zigzag and armchair bilayer graphene under simple tensile test. According to Fig. 3, the Young's modulus value for armchair graphene has been approximately obtained 1.2 TPa and the Young's modulus value for zigzag graphene has been approximately obtained 1.42 TPa. These values have been obtained by calculating the slope of the stress-strain graph of bilayer graphene under tensile test. The Young's modulus of both zigzag and armchair bilayer graphene are shown in Table 1.

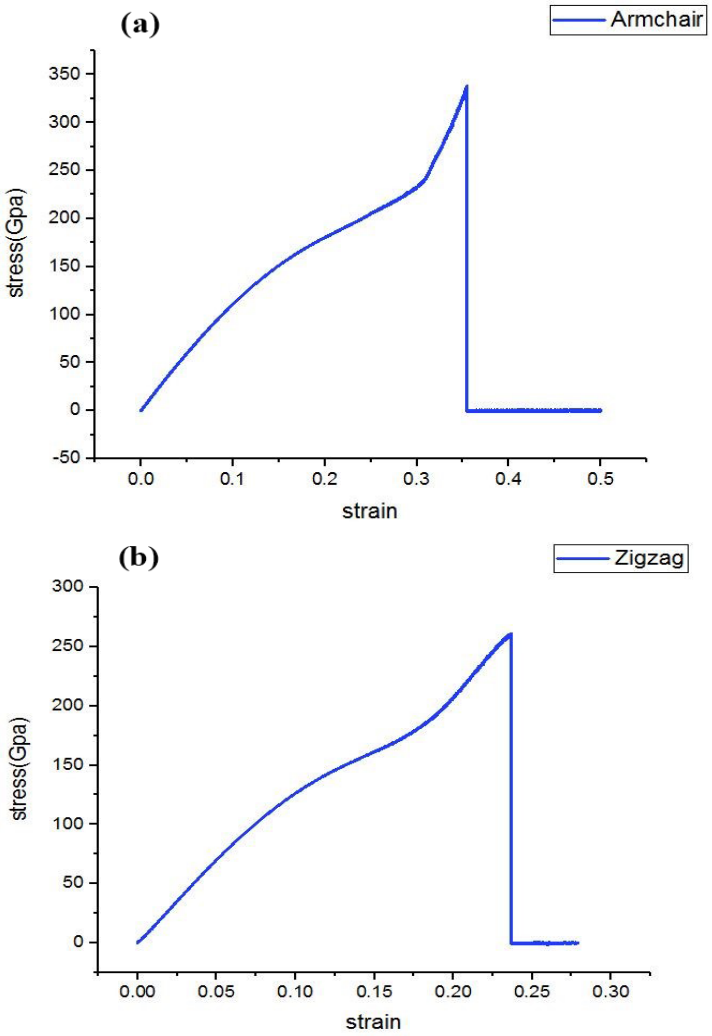

Fig. 2. The stress-strain curve of (a) armchair and (b) zigzag bilayer graphene under simple tensile test at temperature of 300 K

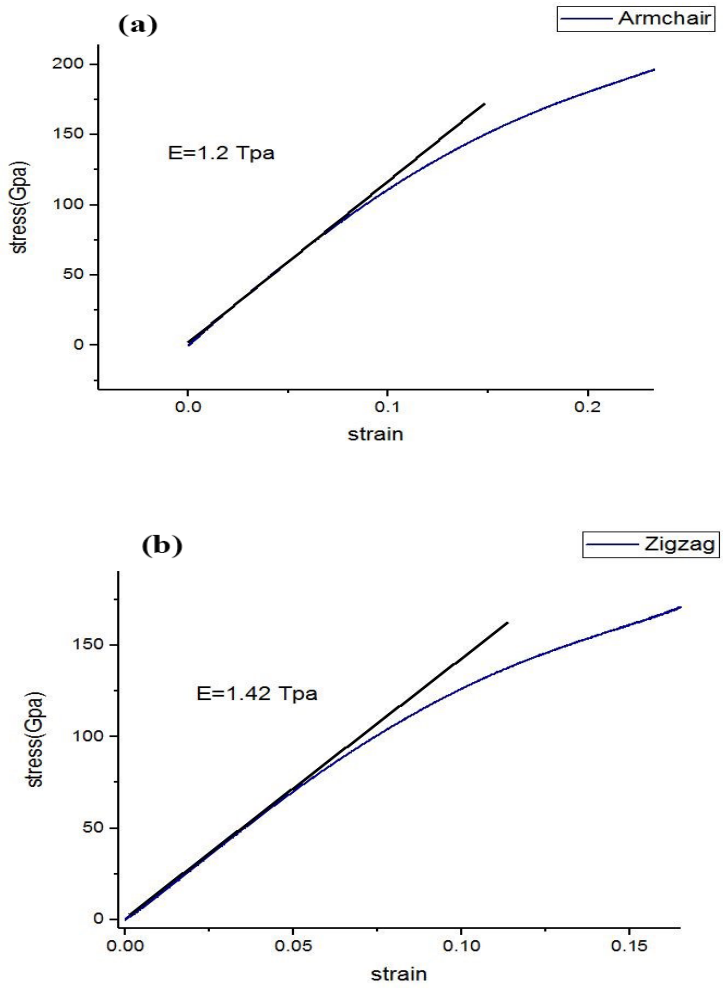

Fig. 3. The slope of stress-strain curve of bilayers of (a) armchair and (b) zigzag in the elastic zone

Table 1.Young's modules of bilayer graphene

Graphene Structure	Size[Å]	Young's Modulus[TPa]
zigzag	102.2*100.8	1.42
armchair	102.2*100.8	1.2

According to Fig. 2, the ultimate stress tolerated by armchair bilayer graphene was 338 GPa, which occurs at a strain of 0.35 (Å/Å) and the ultimate stress tolerated by zigzag bilayer graphene was 261 GPa, which occurs at a strain of 0.23 (Å/Å),Table(2).

According to the stress-strain diagrams of the specimens in Fig. 2, the ultimate stress tolerated by zigzag two-layer graphene is lower than that tolerated by armchair bilayer graphene. Under equal strains, zigzag graphene can tolerate more stress.

Fig. 4 shows the model changes under the tensile test at fracture moment. According to Fig. 4, the fracture accrues near to one side of it.

The result of this study indicates that by increasing the number of graphene sheets from one layer to two layers, the Young's modulus value of 1 TPa in bilayer graphene increases to 1.2 TPa in armchair bilayer graphene and 1.4 TPa in zigzag bilayer graphene that is in good agreement with previous study [31].

Table 2. The Ultimate stress and strain of bilayer graphene

Graphene Structure	Ultimate Strain	Ultimate Stress[GPa]
zigzag	0.23	261
armchair	0.35	338

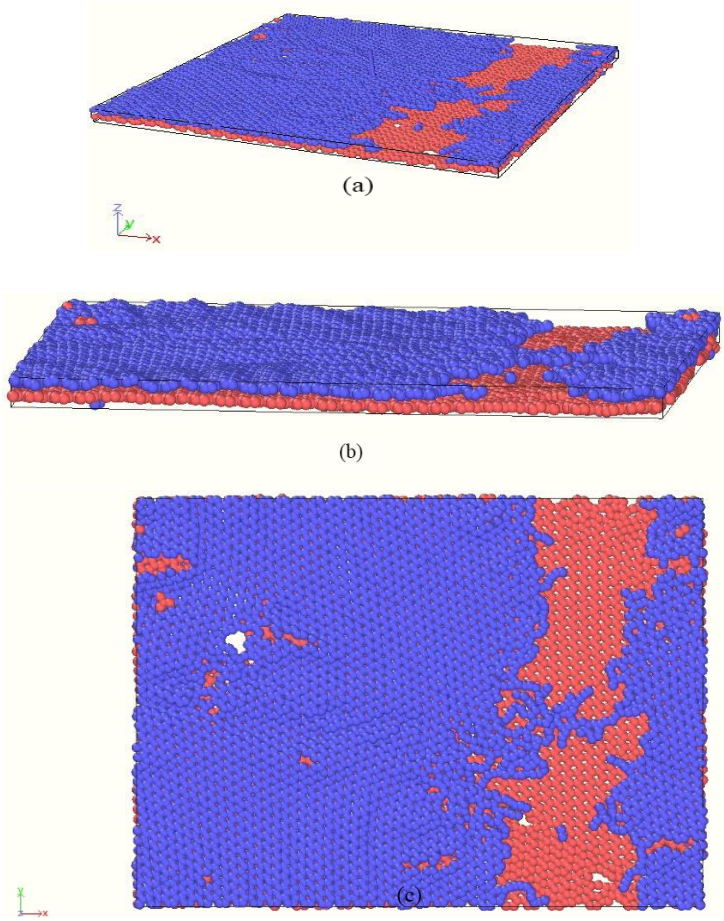

Fig. 4. The model changes under the tensile test at fracture moment

However, according to research of Mortazavi et al. [31], the Young's modulus decreases as the number of sheets decreases, but the amount of the Young's modulus of multilayer graphene is still higher than the Young's modulus of single-layer graphene. Consequently, by comparing these two studies, we conclude that with increasing number of sheets, the Young's modulus of bilayer graphene is higher than the Young's modulus of single-layer graphene,Table3. In addition, the fracture strength of the armchair bilayer graphene is 338 GPa and its fracture strain is 0.35, while the fracture strength of the zigzag bilayer graphene is 261 GPa. Comparison of these results and the values obtained from single-layer graphene [24] shows that the fracture strength of bilayer graphene is approximately 60% higher than the fracture strength of single-layer graphene.

In this study, the effect of chirality on Young's modulus and fracture strength of bilayer graphene has been also investigated. The results show that by increasing the chirality angle in bilayer graphene from 0 ° (armchair) to 30 ° (zigzag), the Young's modulus value increases, so that the Young's modulus value of the armchair bilayer graphene is equal to 1.2 TPa and the Young's modulus value of the zigzag bilayer graphene is equal to 1.4 TPa.

Table 3.Young's Modulus comparison of monolayer[24] and bilayer graphene.

Graphene Structure	Young's Modulus[TPa]
Zigzag monolayer	1.01
Zigzag bilayer	1.42
Armchair monolayer	1.01
Armchair bilayer	1.2

However, with increasing chirality angle in single-layer graphene from 0 ° to 30 °, the Young's modulus value does not change significantly [24].

According to the obtained results, the fracture strength decreases with increasing chirality angle. The fracture strength of armchair bilayer graphene (0 °) is 338 GPa and the fracture strength of zigzag bilayer graphene (30 °) is 261 GPa.

CONCLUSION

In the present study, bilayer graphene with two different chirality angles was modeled by molecular dynamics in LAMPS software. In summary, this research involves establishing the basic structure, balancing the sample, applying the axial tensile test, and extracting the stress-strain curve from the sample.

Initially, it was shown that when the number of sheets increase, the Young's modulus value of the bilayer graphene was higher than that of the single-layer graphene. In addition, the fracture strength of armchair bilayer graphene is 338 GPa and its fracture strain is 0.35, whereas the fracture strength of zigzag bilayer graphene is 261 GPa, which showed that the fracture strength of the bilayer graphene is approximately 60% higher than the fracture strength of single-layer graphene. The fracture strength also decreases with increasing chirality angle.

In following, it was shown that with an increase in the chirality angle in bilayer graphene from 0 ° (armchair) to 30 ° (zigzag), the Young's modulus value increased while by increasing the chirality angle in single-layer graphene from 0 ° to 30 °, the Young's modulus did not vary significantly.

CONFLICT OF INTEREST STATEMENT

All authors declare that no conflicts of interest exist for the publication of this manuscript.

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