Residual strain in graphene: study of temperature and crack effect

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Abstract. Graphene is a thin sheet with special properties and complicated mechanical behavior. It’s important to study graphene experimentally and theoretically. Stone–Wales defects, cracks and atom vacancy are popular defects in carbon allotropes especially in graphene. In this paper, residual strain in graphene was discussed. At first, stress-strain curve of non-defected graphene sheet was obtained using molecular dynamics simulation and effect of temperature on mechanical properties of graphene was obtained. Then, four different cracks were considered in center of graphene sheets. Stress-strain curves of defected graphene sheets with different tension strain rates were plotted. The results showed that cracks lead to the graphene to fracture sooner. Also, increasing temperature lead to the Young’s modulus of graphene decreases and graphene fractured at lower strain. On the other hand, residual strain of non-defected and cracked graphene increased by increasing temperature from 200 K to 1200 K. It means that graphene had more plasticity behavior by increasing temperature.

Keywords: Graphene; stress-strain curve; Molecular Dynamics; Residual strain; Center cracked;

1. Introduction
After years of graphene exploration, the interest of researchers in the study of graphene is still rising because of unique properties of graphene such as high thermal conductivity (5000 W/mK) [1], large surface area (2600 m$^2$/g) [2], high elastic modulus (1000 GPa) [3] and is recognized as one of the key materials for realizing electronic devices in future [4]. Also, single-layer graphene layers, are widely used for developed materials and nanocomposites [5]. Studying mechanical properties of graphene is interesting for researchers. Lee at al. [6] found Young’s modulus of graphene, with 0.335nm thickness, about $1 \pm 0.1$ TPa and mechanical strength $130 \pm 10$ GPa.

Results show that Stone-Wales defect and vacancy defect exist in graphene and carbon nanotubes. These defects can be created because of stress or during of production and can effect on mechanical properties of these carbon allotropes. Therefore, it’s very important to studying the defect effect in mechanical behavior of graphene sheets [7-11]. For this purpose, Jiang et al. [12] used molecular dynamics (MD) simulation and finite element method to investigate effect of crack on graphene sheets. Minh-Quy Le et al. [13] proved that the initial length of the crack and the loading speed are effective in the growth rate of the cracks. Na Fan [14] used numerical methods to investigate the fracture behavior of graphene sheets. Theodosiou and Saravanous [15] studied the crack effect on graphene using nonlinear finite element simulation. In this work, the focus was on the crack path in the graphene, and different states were examined. Theoretical method and then the continuum molecular mechanics method were used in Tuleubekov et al. [16] work. They pulled graphene in two directions to study effect of cracks on graphene. Effect of Stone-Wales defects on strength of graphene was studied by Wang et al. [17]. Their results indicate a relative decline in graphene strength. Lia-Jin and coworkers [18] studied center cracks in graphene using continuum mechanics. They could determine releasing strain energy in graphene by applying graphene tensions.

There are some studies about the effect of temperature on graphene. Yong Ge and his colleagues [19] studied temperature effect on mechanical properties of graphene. The results showed that
increasing temperature change the strength of graphene, significantly. Zhang [20] used molecular dynamics method to study multi-layer graphene and showed that increasing temperature had inverse effect on graphene strength. Dewapriya et al. [21] studied effect of temperature on free-edged graphene sheet using molecular dynamic simulation. Their results showed that higher temperature lead to lower Young’s modulus.

In this paper, residual strain of graphene sheet in different temperature was studied. Also, the effect of the temperature on center cracked graphene and without-cracked graphene has been investigated. For this purpose, four different cracks were created on the graphene sheets, and for each crack, the graphene sheet was stretched with three different strain rates. Effect of temperature on mechanical properties of graphene (in different strain rates) will be investigated using molecular dynamics method.

2. Molecular Dynamics Simulation

Initially, using the molecular dynamics method, we study the effect of the center crack on the mechanical properties of the graphene. For this purpose, The AIREBO (adaptive intermolecular reactive empirical bond-order) potential function is considered. AIREBO works in cut-off distance less than $r_{ij}^\text{max}$ (for C-C bond $r_{ij}^\text{max}$ is equal to 2 Å). Each pair of atoms with covalent bonding operates under the following potential [22]:

$$ E_{ij}^{\text{REBO}} = V_{ij}^R(r_{ij}) + b_{ij} V_{ij}^\Lambda(r_{ij}) $$

(1)

Where $V_{ij}^R$ and $V_{ij}^\Lambda$ repulsion and attraction potential which act between $i$, $j$ atoms. $b_{ij}$ is bond-order term of potential function. The total potential energy is obtained from the following equation:
\[ E = \frac{1}{2} \sum_i \sum_{j \neq i} \left[ E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_k \sum_{i,j,k,l} E_{ijkl}^{tors} \right] \]

Which \( E_{ij}^{LJ} \) is Lennard-Jones potential for non-bonded atoms. \( E_{ijkl}^{tors} \) is torsional interaction potential:

\[ E_{ijkl}^{tors} = f_c(r_{ij}) f_c(r_{ik}) f_c(r_{jl}) \varepsilon \left[ \frac{256}{405} \cos^{10}(\phi/2) - 0.1 \right] \]

Where \( f_c \) is bond-weight terms, \( \varepsilon \) is the depth of the potential well in Lennard-Jones function and \( \phi \) in Dihedral angle.

In order to avoid the effects of size on graphene properties, graphene sheet considered as 9.997 × 9.947 nm² dimensions [23]. Molecular dynamics simulation was done using LAMMPS package and AIREBO potential function. This potential has high accuracy in atomic interactions and reformation of atoms.

For covering the area round the crack in AIREBO potential function, the cut-off distance was considered as \( 2 \AA \) [24]. To measuring the mechanical properties of graphene sheet, an axial tensile test is used which can be performed on the basis of deformation control or force control. In the deformation control method, the strain applies to one graphene side while the opposite side is considered to be completely fixed. The strain rate has a great effect on the mechanical properties of graphene and crack growth. So, three different strain rates were considered to apply to graphene sheet which include 0.0005, 0.005, 0.05 ps⁻¹ and for each one the time step was 0.001 ps. All simulation steps were carried out at four different temperature 200, 500, 800 and 1200 K.

The Young’s modulus has been reported in experimental results between 0.5 to 2 TPa [25]. But most researches have reported Young’s modulus close to 1 TPa [26]. The value of Young’s modulus has been reported in various papers show in Table 1.
In this paper, we obtained the stress-strain curve for graphene using molecular dynamics method (Fig. 1) and according to the slope of the curve; the value of the Young's modulus was obtained about 870 GPa (Fig. 2). This value has good agreement with other experimental and theoretical researches. Specially, with the value obtained from experimental work of Zhang et al. (891 GPa) [38].

2.1. Effect on temperature on graphene sheet strength

The effect of temperature on stress-strain curve of graphene was studied at four temperature 200, 500, 800 and 1200K. For each temperature, three strain-rate were considered; 0.0005, 0.005, 0.05 ps$^{-1}$. The results can be seen in Fig 3.:

As shown in the Fig 3., increasing temperature lead graphene failure in less strain. By calculating the Young's modulus of graphene in each temperature, it can be find that increasing temperature lead to decrease strength of graphene (Table 2). Comparing these result by other studies shows good agreement. Yong Ge and his colleagues [19] studied temperature effect on mechanical properties of graphene. The results showed that increasing temperature change the strength of graphene, significantly. Also, Zhang [38] and Dewapriya et al. [21] studied effect of temperature on free-edged graphene sheet using molecular dynamic simulation. Their results showed that higher temperature lead to lower Young’s modulus.

As the strain rate increases, the Young’s modulus show an increasing trend with the strain rate. Also, the strain rate effect is more obvious at higher temperature. For example, at 200 K, the Young’s modulus are increased about 2% for strain rate variation from 0.0005 ps$^{-1}$ to 0.05 ps$^{-1}$. But, at 800 K, the Young’s modulus are increased about 3.5% for strain rate variation from 0.0005 ps$^{-1}$
to $0.05\text{ ps}^{-1}$. This because at a higher strain rate, graphene has shorter relaxation time to experience the thermal fluctuation and so the graphene is harder.

### 2.2. Center cracked Graphene sheets

To investigate the effect of temperature on mechanical properties of center cracked graphene, 4 types of cracks were considered in different sizes. The cracks are located in the center of the graphene sheet and are visible in Fig. 4. The size of graphene sheet is $9.97\times9.94\text{ nm}$ and the cracks are located at center of sheet, with length and width of 0.7 and 0.6 for crack1, 0.7 and 0.8 for crack 2, 0.7 and 1.95 for crack 3 and 0.7 and 3.16 for crack 4.

The effect of temperature on stress-strain curve of center cracked graphene was studied at four temperature 200, 500, 800 and 1200K. For each temperature, three strain-rate were considered; 0.0005, 0.005, 0.05 ps$^{-1}$. The stress-strain curves for crack-1 show in Fig. 5. It can be find that increasing temperature lead to decrease strength of center cracked graphene (Table 3)

As can be seen, temperature changed the strength of center cracked graphene. By changing temperature from 200K to 1200K, the Young’s modulus increase about 10%.

Also comparing Table 2 and Table 3, It can be concluded that crack-1 (in Fig. 4) reduces the Young’s modulus about 2.5%. Also, the failure happened in less strain in high-temperature. Figure 6 shows the stress-strain curves of four cracked graphene with comparing non-cracked one.

Some curves continue to fluctuate after failure. The reason for this is energy accumulation in the graphene in pulling process that is being released.
Li and coworkers [20] studied non-cracked graphene sheet experimentally and found Young’s modulus and failure strength of graphene about 1TPa and 130 GPa, Respectively. Also, Zhang and coworkers [39] obtained fracture strength of graphene sheet about 140 GPa. In this work, fracture strength of graphene sheet was obtained about 155GPa which has good agreement with mentioned experimental works.

Fig. 7, depicts different frames from graphene initial loading to failure. A brittle fracture occurs without noticeable deformation and is characterized by rapid crack propagation (Fig.7d). The direction of crack is perpendicular to the direction of tensile strain and results in a relatively flat fracture surface.

2.3. Effect of temperature on residual strain of graphene

Residual strain is the Strain in which the graphene does not return to its original size after the deforming force has been removed. Some parameters like temperature, strain rate and cracked have important role in residual strain. In this work, effect of temperate and center crack were studied on residual strain graphene.

For this aim, the effect of temperature on graphene strain were studied at four temperature 200, 500, 800 and 1200 K. the graphene was pulled to 0.2 strain by 0.0005 ps$^{-1}$ strain-rate and then the pulled force was removed. Figure 8 shows the residual strain of graphene in different temperatures. By increasing temperature, the slope of stress-strain curve was decreased, but the residual strain was increased. In the other words, the residual strain was increased from 0.01 to 0.028 when the temperature was changed from 200 to 1200 K.

So, it can be concluded that graphene in high temperature has more plasticity behavior.
Also, the effect of temperature on residual strain of center-cracked graphene was studied. For this aim, the graphene with crack-1 (in Fig. 4) was pulled in four different temperature 200, 500, 800 and 1200 K (Figure 9). As previously concluded, increasing temperature will be increased residual strain, too. However, as discussed before, cracked graphene has less residual strain because it will be fracture in less strain.

3. Conclusion

In this study, effect of temperature on residual strain of graphene was studied. For this aim, the effect of temperature on graphene strain were studied at four temperature 200, 500, 800 and 1200 K. the result showed that residual strain was increased from 0.01 to 0.028 when the temperature was changed from 200 to 1200 K. So, it can be concluded that graphene in high temperature has more plasticity behavior. Also, the properties of graphene and the effect of center cracks were investigated using molecular dynamics. For this purpose, at first, the properties of graphene were obtained using the molecular dynamics method and the results were compared with experimental and theoretical researches. Young’s modulus and strength fracture of graphene sheet was obtained 870 GPa and 155 GPa, respectively, which had good agreement with other works. Then, the mechanical properties of graphene with center crack were investigated. The results showed that Young’s modulus of graphene decreased by increasing the crack length, and the fracture also occurred in less tensile strain.

References


Mohsen Motamedi is an assistant professor of mechanical engineering at University of Shahreza, Isfahan, Iran. He received his PhD degree from University of Tehran (2015). His research interests include nano-mechanics, finite element method, molecular dynamics simulation, composite and nano-composite materials and fracture mechanics.

Amin Esfandiarpour received the BS degree in solid state physics from Zanjan University, Zanjan, Iran, in 2007, and M. Sc. degrees in molecular-atomic physics from the University of Isfahan, Iran in 2010 and PhD from Payame Noor University (The center of graduate Study), Tehran, Iran, in 2015 and Post-doc in physics, from the University of Isfahan, Iran in 2018. His research interests is identifying mechanical and thermal properties of novel material based on molecular dynamics simulation and density function theory (DFT)
Figures’ captions:

Figure 1. Stress-strain curve of graphene sheet

Figure 2. Slope of stress-strain curve

Figure 3. Effect of temperature on stress-strain curve of graphene sheet with Strain rate 0.0005, 0.05 and 0.05 ps\(^{-1}\), Respectively

Figure 4. Graphene sheets with center cracks

Figure 5. Effect of temperature on stress-strain curve of cracked graphene sheet with Strain rate 0.0005, 0.005, 0.05 ps\(^{-1}\), respectively

Figure 6. Effect of center crack on stress-strain curve of graphene in 500 °K

Figure 7. Different frames of graphene loading from the beginning to the final failure

Figure 8. Effect of temperature on residual strain of graphene

Figure 9. Effect of temperature on residual strain of center-cracked graphene
Tables’ Captions:

Table 1. The value of Young's modulus has been reported in various papers

Table 2. Effect of temperature on Young’s modulus of graphene

Table 3. Effect of temperature on Young’s modulus of cracked graphene
Figure 1:
Figure 2:

\[ y = 873.77x - 1.7253 \]
Figure 3:
Figure 4:

Crack 1    Crack 2    Crack 3    Crack 4
Figure 5:
Figure 6:
Figure 7:
Figure 8:
Figure 9:
### Table 1:

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