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# Residual strain in graphene: Study of temperature and crack effect

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## KEYWORDS

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Molecular dynamics;  
Residual strain;  
Center cracked.

**Abstract.** Graphene is a thin sheet with special properties and complicated mechanical behavior. It is 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 at the center of graphene sheets were considered. Stress-strain curves of defected graphene sheets with different tension strain rates were plotted. The results showed that cracks would lead the graphene to fracture sooner. In addition, increasing temperature leads to a decrease in the Young's modulus of graphene and graphene fracture 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 is subject to more plasticity behavior in case of temperature increase.

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## 1. Introduction

After years of graphene exploration, researchers are still showing increasing interest in the study of graphene due to its unique properties, such as high thermal conductivity (5000 W/mk) [1], large surface area (2600 m<sup>2</sup>/g) [2], and high elastic modulus (1000 GPa) [3], and it is recognized as one of the key materials for creating electronic devices in the future [4]. Moreover, single-layer graphene layers are widely used for developed materials and nanocomposites [5]. Studying mechanical properties of graphene is interesting for researchers. Lee et al. [6] found Young's modulus of graphene with 0.335 nm thickness, about  $1 \pm 0$  TPa, and mechanical strength of  $130 \pm 10$  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 production and can affect mechanical properties of these carbon allotropes. Therefore, it is very important to study the defect effect on 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 the effect of crack on graphene sheets. Le and Batra [13] proved that the initial length of the crack and the loading speed were effective in the growth rate of the cracks. Fan et al. [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. This study focused 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 and Volokh [16] work. They pulled

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graphene in two directions to study the effect of cracks on graphene. Wang et al. [17] studied effect of Stone-Wales defects on strength of graphene. Their results indicated a relative decline in graphene strength. Lia-Jin et al. [18] studied center cracks in graphene using continuum mechanics. They could determine strain energy release in graphene by applying graphene tensions.

The effect of temperature on graphene has been studied by some researchers. Yong et al. [19] studied the effect of temperature on mechanical properties of graphene. The results showed that increasing temperature significantly changed the strength of graphene. Li and Chou [20] studied non-cracked graphene sheet experimentally and found Young's modulus and failure strength of graphene. Dewapriya et al. [21] studied the effect of temperature on free-edged graphene sheet using molecular dynamic simulation. Their results showed that higher temperature led to lower Young's modulus.

In this paper, residual strain of graphene sheet at different temperatures is studied. In addition, the effect of the temperature on center cracked graphene and without-cracked graphene is investigated. For this purpose, four different cracks are created on the graphene sheets; for each crack, the graphene sheet is stretched with three different strain rates. Effect of temperature on mechanical properties of graphene (at different strain rates) is 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 at a cut-off distance less than  $r_{ij}^{\max}$  (for C-C bond,  $r_{ij}^{\max}$  is equal to 2 Å). Each pair of atoms with covalent bonding operates under the following potential [22]:

$$E_{ij}^{\text{REBO}} = V_{ij}^R(r_{ij}) + b_{ij} V_{ij}^A(r_{ij}), \quad (1)$$

where  $V_{ij}^R$  and  $V_{ij}^A$  are repulsion and attraction potential which act between  $i, j$  atoms, and  $b_{ij}$  is bond-order term of potential function. The total potential energy is obtained through the following equation:

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} \left[ E_{ij}^{\text{REBO}} + E_{ij}^{\text{LJ}} + \sum_{k \neq i, j} \sum_{l \neq i, j, k} E_{ijkl}^{\text{tors}} \right], \quad (2)$$

where  $E_{ij}^{\text{LJ}}$  is Lennard-Jones potential for non-bonded atoms, and  $E_{ijkl}^{\text{tors}}$  is torsional interaction potential:

$$E_{ijkl}^{\text{tors}} = f_c(r_{ij}) f_c(r_{ik}) f_c(r_{jl}) \varepsilon \left[ \frac{256}{405} \cos^{10} \left( \frac{\phi}{2} \right) - 0.1 \right], \quad (3)$$

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

In order to block the effects of size on graphene properties, graphene sheet was considered as  $9.997 \times 9.947 \text{ nm}^2$  dimensions [23]. Molecular dynamics simulation was conducted using LAMMPS package and AIREBO potential function. This potential enjoys 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 Å [24]. To measure the mechanical properties of graphene sheet, an axial tensile test was 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 completely fixed. The strain rate has great effect on the mechanical properties of graphene and crack growth. Therefore, three different strain rates were considered to apply to graphene sheet including 0.0005, 0.005, and 0.05  $\text{ps}^{-1}$ , and the time step was 0.001 ps for each one. All simulation steps were carried out at four different temperatures of 200, 500, 800, and 1200 K.

The Young's modulus was reported in experimental results between 0.5 to 2 TPa [25]. However, most research studies have reported on Young's modulus close to 1 TPa [26]. The value of Young's modulus has been reported in various papers, as shown in Table 1.

In this paper, the stress-strain curve for graphene was obtained using molecular dynamics method (Figure 1) according to the slope of the curve; the value of the Young's modulus was obtained as about 870 GPa (Figure 2). This value is in good agreement with that in other experimental and theoretical researches; it is particularly in agreement with the value obtained from experimental work of Zhang et al. (891 GPa) [38].

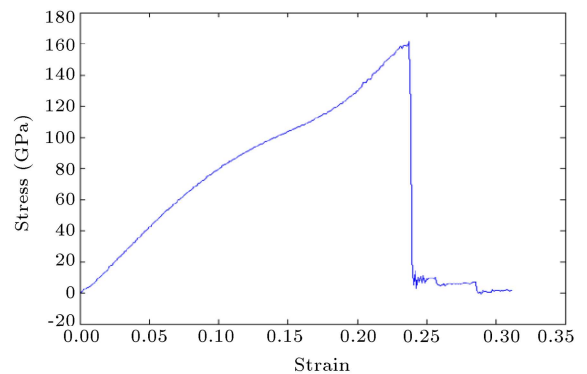
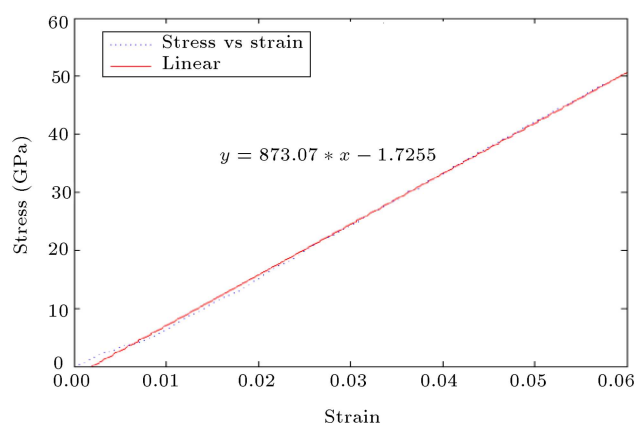


Figure 1. Stress-strain curve of graphene sheet.

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

References	Method	Young's modulus (GPa)
Reddy et al. [27]	Continuum models	669
Shokrieh and Rafiee [28]	Continuum models	1040
Arroyo and Belytschko [29]	Continuum models	694
Kudin and Scuseria [30]	Ab initio and Quantum	1021
Lier et al. [31]	Ab initio and quantum	1115
Liu et al. [32]	Ab initio and quantum	1050
Gao and Hao [33]	Ab initio and quantum	600
Yanovsky et al. [34]	Ab initio and quantum	737
Ni and Bu [35]	MD simulations	1100
Tsai and Tu [36]	MD simulations	912
Georgantzinos et al. [37]	Finite element method	1367
Li and Chou [20]	Structural molecular mechanics	1033
Lee et al. [6]	Experiment	1000
Yupeng and Pan [38]	Experiment	891

**Figure 2.** Slope of stress-strain curve.

### 2.1. Effect on temperature on graphene sheet strength

The effect of temperature on stress-strain curve of graphene was studied at four temperatures of 200, 500, 800, and 1200 K. For each temperature, three strain rates were considered: 0.0005, 0.005, and 0.05  $\text{ps}^{-1}$ . The results are shown in Figure 3.

As shown in Figure 3, increasing temperature leads graphene to failure at lower strain. By calculating the Young's modulus of graphene in each temperature, it can be found that increasing temperature leads to a decrease in strength of graphene (Table 2). A comparison of these results with other studies' results shows good agreement. Yong et al. [19] studied temperature effect on mechanical properties of graphene. The results showed that increasing temperature changed the strength of graphene, significantly. In addition, Zhang and Pan [38] and Dewapriya et al. [21] studied effect of temperature on free-edged graphene sheet using

**Table 2.** Effect of temperature on Young's modulus of graphene.

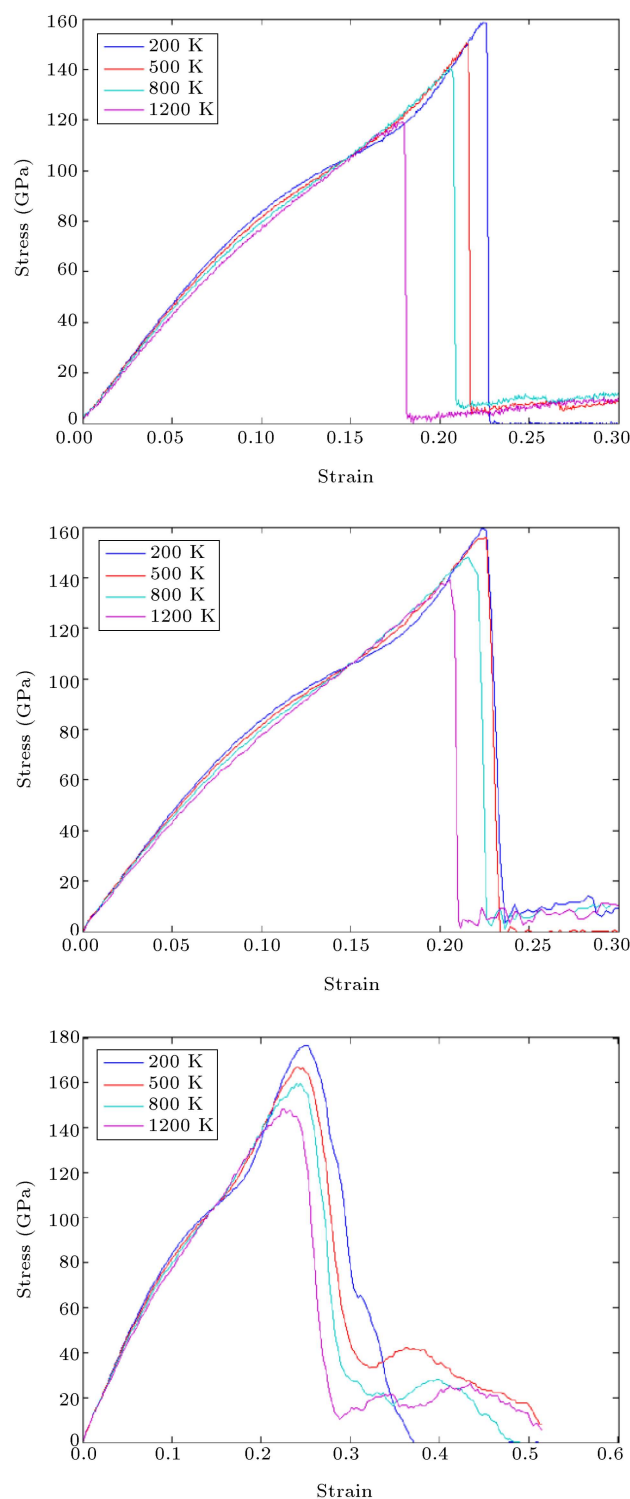
Temp. ( $^{\circ}\text{K}$ )	Young's modulus		
	0.0005 $\text{ps}^{-1}$	0.005 $\text{ps}^{-1}$	0.05 $\text{ps}^{-1}$
200	0.92023	0.93002	0.93989
500	0.89607	0.90576	0.92307
800	0.87107	0.88469	0.90186
1200	0.84139	0.85679	0.87101

molecular dynamic simulation. Their results showed that higher temperature led to lower Young's modulus.

As the strain rate increases, the Young's modulus shows an increasing trend with the strain rate. In addition, the strain rate effect is more obvious at higher temperature. For example, at 200 K, the Young's modulus increases by about 2% for strain rate variation from 0.0005  $\text{ps}^{-1}$  to 0.05  $\text{ps}^{-1}$ . However, at 800 K, the Young's modulus increases by about 3.5% for strain rate variation from 0.0005  $\text{ps}^{-1}$  to 0.05  $\text{ps}^{-1}$ . This is the reason why, at a higher strain rate, graphene has shorter relaxation time to experience the thermal fluctuation and, thus, the graphene is harder.

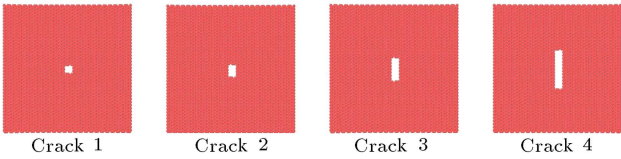
### 2.2. Center cracked graphene sheets

To investigate the effect of temperature on mechanical properties of center-cracked graphene, four types of cracks were considered in different sizes. The cracks are located at the center of the graphene sheet and are visible in Figure 4. The size of graphene sheet is  $9.997 \times 9.947$  nm, and the cracks are located at the center of sheet, with the respective length and width of 0.7 and 0.6 for Crack 1, 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.



**Figure 3.** Effect of temperature on stress-strain curve of graphene sheet with strain rates of 0.0005, 0.005, and 0.05 ps<sup>-1</sup>, respectively.

The effect of temperature on stress-strain curve of center-cracked graphene was studied at four temperatures of 200, 500, 800, and 1200 K. For each temperature, three strain rates were considered: 0.0005, 0.005, and 0.05 ps<sup>-1</sup>. The stress-strain curves for Crack 1



**Figure 4.** Graphene sheets with center cracks.

**Table 3.** Effect of temperature on Young's modulus of cracked graphene.

Temp. (°K)	Young's modulus		
	0.0005 ps <sup>-1</sup>	0.005 ps <sup>-1</sup>	0.05 ps <sup>-1</sup>
200	0.90591	0.91090	0.92047
500	0.88028	0.89167	0.90584
800	0.85923	0.86373	0.87997
1200	0.82048	0.83190	0.84432

are shown in Figure 5. It can be found that increasing temperature leads to a decrease in strength of center-cracked graphene (Table 3).

As observed, temperature changed the strength of center-cracked graphene. By changing temperature from 200 K to 1200 K, the Young's modulus increases by about 10%.

In addition, by comparing Tables 2 and 3, it can be concluded that Crack 1 (in Figure 4) reduces the Young's modulus by about 2.5%. In addition, the failure occurs at lower strain at high temperatures. Figure 6 shows the stress-strain curves of four cracked graphenes compared with non-cracked one.

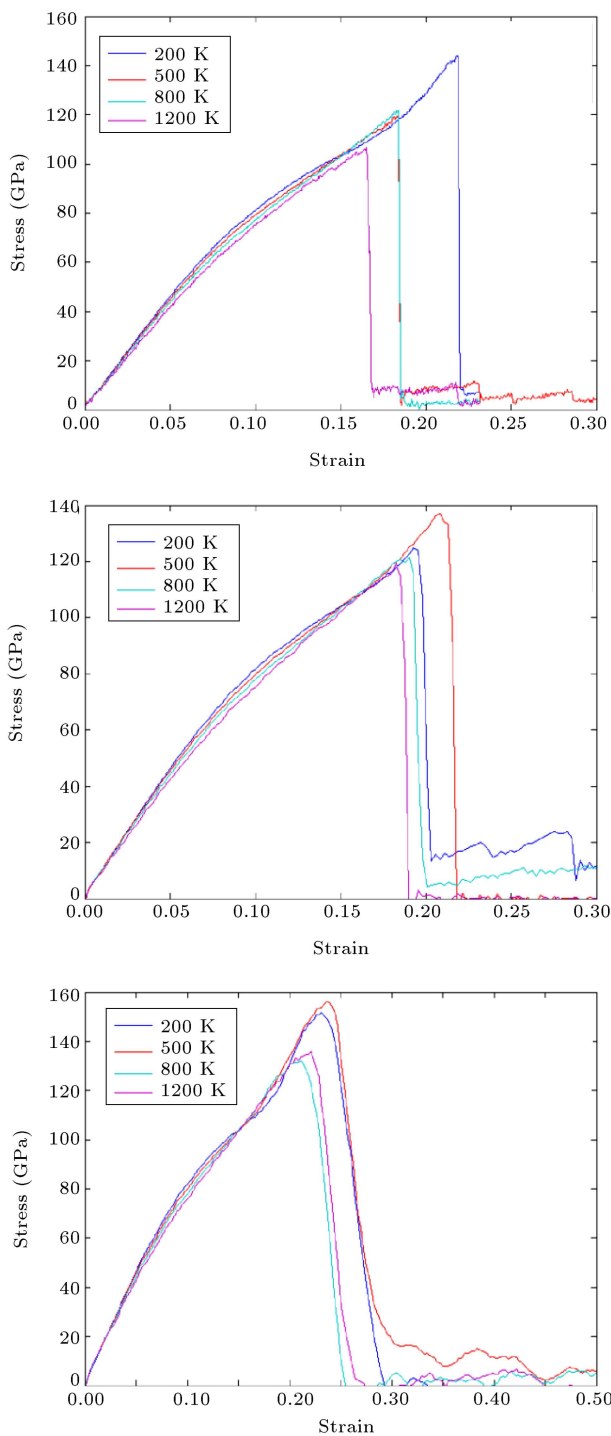
Some curves continue to fluctuate after failure, because energy is accumulated in the graphene in the pulling process that is being released.

Li and Chou [20] studied non-cracked graphene sheet experimentally and found Young's modulus and failure strength of graphene about 1 TPa and 130 GPa, respectively. In addition, Zhang and Pan [39] obtained fracture strength of graphene sheet about 140 GPa. In this work, fracture strength of graphene sheet was obtained about 155 GPa, which has good agreement with the mentioned experimental works.

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

### 2.3. Effect of temperature on residual strain of graphene

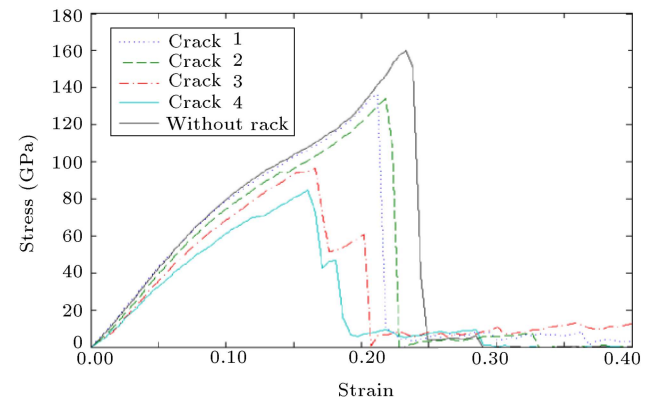
Residual strain is the strain at which the graphene does not return to its original size after the deforming force has been removed. Some parameters, such as temperature, strain rate, and crack, have an important



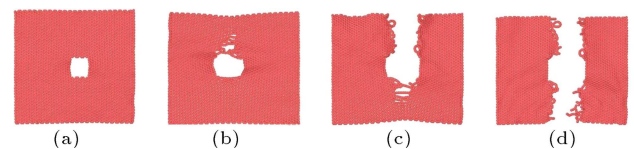
**Figure 5.** Effect of temperature on stress-strain curve of cracked graphene sheet with Strain rates of 0.0005, 0.005, and 0.05  $\text{ps}^{-1}$ , respectively.

role in residual strain. In this work, the effect of temperate and center crack was studied on residual strain graphene.

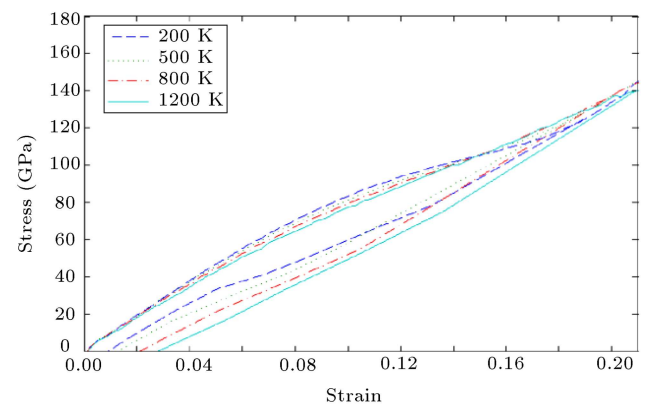
To this end, the effect of temperature on graphene strain was studied at four temperatures of 200, 500, 800, and 1200 K. The graphene was pulled to 0.2 strain by 0.0005  $\text{ps}^{-1}$  strain rate; then, the pulled



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



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

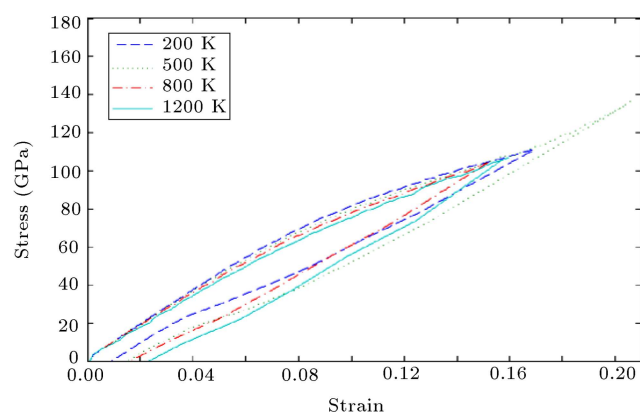


**Figure 8.** Effect of temperature on residual strain of graphene.

force was removed. Figure 8 shows the residual strain of graphene at different temperatures. By increasing temperature, the slope of stress-strain curve decreased; however, the residual strain increased. In other words, the residual strain increased from 0.01 to 0.028 when the temperature changed from 200 to 1200 K.

Therefore, it can be concluded that graphene at high temperatures experiences more plasticity behavior.

In addition, the effect of temperature on residual strain of center-cracked graphene was studied. For this aim, the graphene with Crack 1 (in Figure 4) was pulled at four different temperatures of 200, 500, 800, and 1200 K (Figure 9). As previously concluded, increasing temperature increased residual strain, too. However, as discussed before, cracked graphene has low residual strain because it is fractured at lower strain.



**Figure 9.** Effect of temperature on residual strain of center-cracked graphene.

### 3. Conclusion

This study investigated the effect of temperature on the residual strain of graphene. For this aim, the effect of temperature on graphene strain was studied at four temperatures of 200, 500, 800, and 1200 K. The result showed that residual strain increased from 0.01 to 0.028 when the temperature changed from 200 to 1200 K. Therefore, it can be concluded that graphene at high temperatures experienced more plasticity behavior. In addition, 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 were obtained as 870 GPa and 155 GPa, respectively, which had good agreement with those of 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 lower tensile strain.

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