Digest Journal of Nanomaterials and Biostructures Vol. 7, No. 4, October-December 2012, p. 1811-1816

TEMPERATURE EFFECT ON MECHANICAL PROPERTIES OF GRAPHENE SHEETS UNDER TENSILE LOADING

TE-HUA FANG , WIN-JIN CHANG[a*], JHIH-CHIN YANG[b]
Department of Mechanical Engineering, National Kaohsiung University of Applied Sciences, Kaohsiung 807, Taiwan
[a]*Department of Mechanical Engineering, Kun San University, Tainan 710, Taiwan*
[b]*Institutue of Mechanical and Electromechanical Engineering, National Formosa University, Yunlin 632, Taiwan*

The aim of this article is to study the Young's modulus and Poisson's ratio of graphene sheets using the molecular dynamics simulation. In the simulation, the graphene sheets subjected to a uniaxial tensile loading at different temperatures is performed until failure occurres. The results show that the failure strain of the graphene sheets decreases with increasing temperature. A nonlinear relation between the stress and strain is obtained. In addition, Poisson's ratio of graphene sheets increases as the temperature increases. However, Young's modulus decreased with increasing temperature.

(Received October 9, 2012; Accepted November 13, 2012)

Keywords: Molecular dynamics; Temperature effect; Mechanical property; Graphene sheets

1. Introduction

In recent years, graphene has attracted great scientific interest because of its excellent mechanical, chemical, and thermal properties [1-4]. In addition, due to its outstanding electronic properties, graphene may be viewed as a possibility for replacing silicon in future electronic nanodevices [5]. The electronic behaviour of graphene can be influenced by its mechanical properties [6]. Therefore, the study of the mechanical behaviours of graphene is important and valuable for exploring its application in electronic and other fields.

With the rapid development of computer technology over the past years, molecular dynamics (MD) simulation has been very effective in simulating the mechanical properties of nanostructured materials and in recognizing the microscopic mechanisms and offering insights into microscopic behaviours [7-13]. In recent years, MD simulation has also been used to study the mechanical properties of graphene [14-18]. For example, Jiang et al. [14] investigated the Young's modulus of graphene with the intrinsic thermal vibration in graphene by molecular dynamics and obtained that the results agree very well with the experiment data. Li [16] studied the stretchability of grapheme nanoribbons through molecular dynamics simulations and found that they can be considerably strengthened by a small twist angle. Erdogan et al. [17] performed the tight-binding molecular dynamics to study the structural changes of grapheme nanoribbons under uniaxial stretching.

* Corresponding author: changwj@mail.ksu.edu.tw

In this article, molecular dynamics simulation is used to study the mechanical properties of graphene sheets under uniaxial tensile loading. The Young's modulus and Poisson's ratio at temperatures of 200, 300, 400, and 500K are investigated.

2. Simulation method

The armchair graphene sheets consists of 2296 carbon atoms with the dimensions around l = 9.9 nm and w =5.8 nm as shown in Fig. 1. Two layers of atoms on the top and bottom are fixed and four layers of thermostat atoms closed to the fixed layers are set to dissipate any excess heat generated during the tensile loading and thus the system maintains a set temperature. The Tersoff potential [19] is used to model the interaction between the carbon atoms.

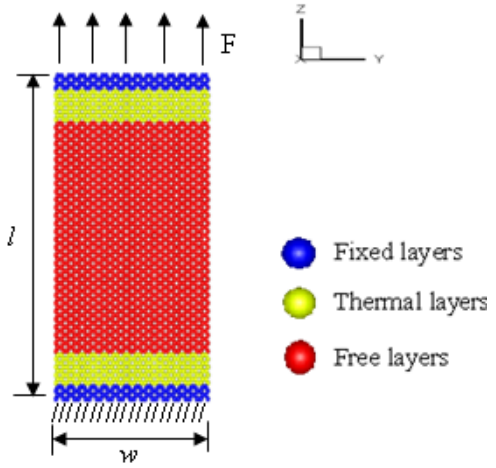

Fig. 1. Schematics of MD of graphene sheets subjected to a uniaxial tensile loading.

To determine Young's modulus and Poisson's ratio of graphene sheets, the boundary atoms on the bottom edge of the system are fixed and a positive displacement Δl with a stretch rate of 5 m/s in the z direction when the force F is applied to the atoms on the top edge. A nonlinear relation between the tensile stress σ_z in the z direction and the strain ε_z can be expressed as follows:

$$\sigma_z = E\,\varepsilon_z + D\,\varepsilon_z^2 \tag{1}$$

where E and D are, respectively, the Young's modulus and the nonlinear elastic modulus of the graphene sheets. The presence of the second-order term leads to a decrease of stiffness and the value of D is typically negative [20]. σ_z can be calculated through F/A, where $A = w\,h$ represents the cross-sectional area and h denotes the thickness of the graphene sheets, which is usually taken as 0.34 nm. The tensile strain ε_z is obtained from $\varepsilon_z = \Delta l / l$. In addition, Poisson's ratio ν can be obtained from the following equation:

$$\nu = -\frac{\varepsilon_y}{\varepsilon_z} = -\frac{\Delta w / w}{\Delta l / l} \tag{2}$$

where ε_y is the lateral strain in the y direction and is determined from $\Delta w / w$.

3. Results and discussion

In this article, we investigate the fracture behaviour of graphene sheets subjected to a tensile loading at temperatures of 200, 300, 400, and 500 K. Fig. 2 depicts the snapshots of graphene sheets induced a tensile stress until failure at various temperatures. After defect deformations such as vacancies and topological defects in the graphene sheets, the crack took place when the further loading was increased. The kinetic energy is transferred into strain energy through the deformation during the tensile loading. Therefore, increasing the temperature decreases the strain energy because of the increasing kinetic energy. This results in a decrease in the strain to failure for a higher temperature condition. In addition, it can be seen that the fracture occurs at the interface of the fixed layers and thermal layers.

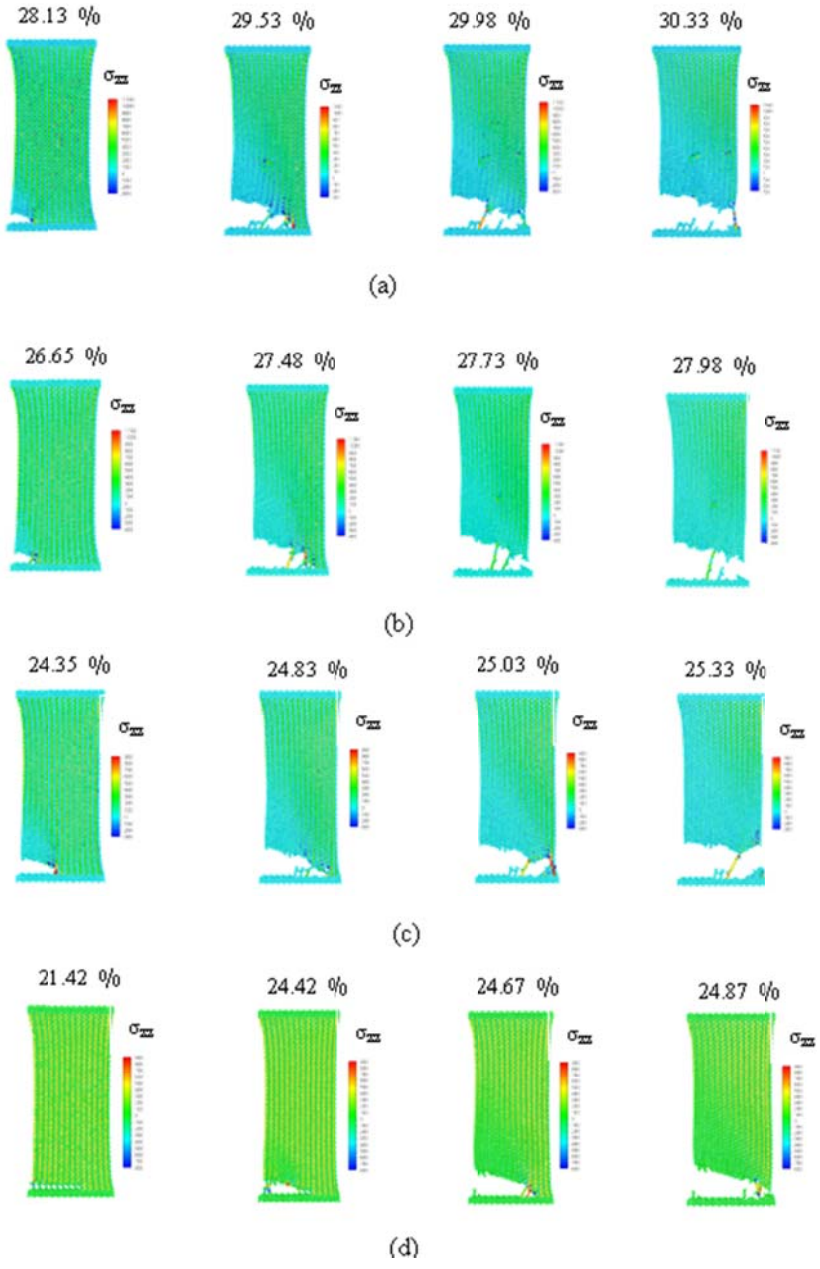

Fig. 2. The snapshots of graphene sheets induced a tensile stress until failure at temperatures of (a) 200K, (b) 300K, (c) 400K, and (d) 500K.

The temperature dependence of the stress-strain behaviour in the temperature range from 200 to 500 K is shown in Fig.3. The area under the stress–strain curve represents the strain energy per unit volume that the graphene sheets can absorb before failure. The nonlinear relation between the stress and strain is given by Eq. (1). The values of Young's modulus and elastic modulus for the graphene sheets are listed in Table 1. Because the binding energy between carbon atoms decreases as the temperature increases, it can be seen that Young's modulus of graphene sheets decreases with increasing temperature. In addition, the values of the third-order elastic modulus are all minus. The result is similar to that obtained by Ni et al. [21]. They found the averaged Young's modulus was 1.13 for the longitudinal mode of graphene sheets at temperature of 300K.

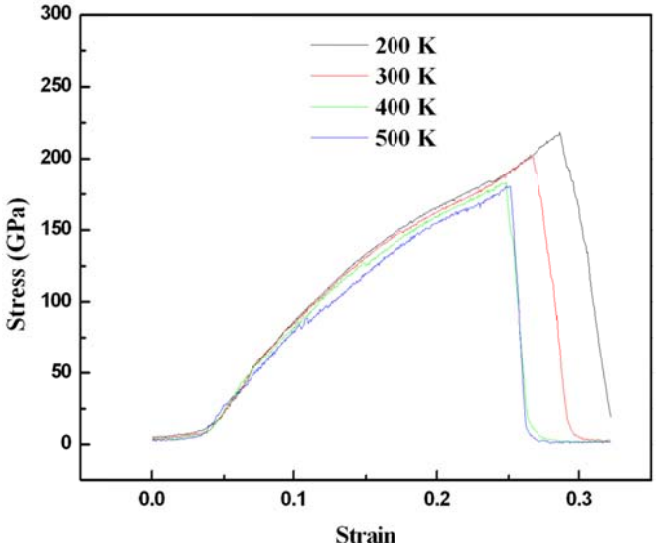

Fig. 3. The stress-strain curve of graphene sheets subjected to the tensile loading at different temperatures.

Table 1. The elastic constants of graphene sheets at different temperatures.

Temperature (K)	Young's Modulus (TPa)	Third-order Elastic Modulus (TPa)
200	1.184	-1.302
300	1.171	-1.295
400	1.148	-1.279
500	1.070	-1.066

The temperature effect on the Poisson's ratio of graphene sheets is illustrated in Fig. 4. The value of Poisson's ratio is smaller than that of a single-layer graphene obtained by Zhou and Huang [22]. This is due to the thickness effect. A thicker graphene is prone to deformation due to the applied force. In addition, the Poisson's ratio increases with increasing temperature. This is because a smaller strain in the z-direction is obtained at a higher temperature.

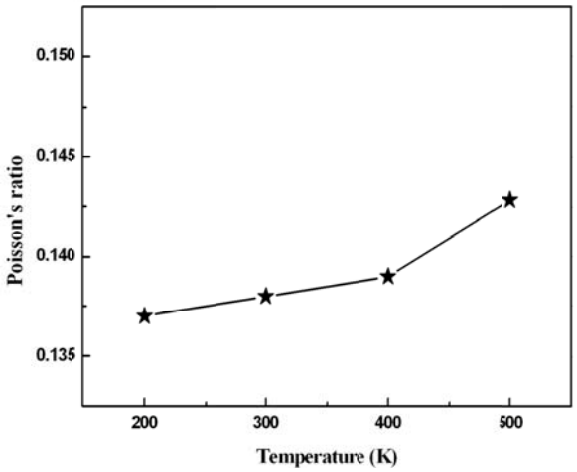

Fig. 4. The Poisson's ratio of graphene sheets subjected to the tensile loading at different temperatures.

3. Conclusions

The molecular dynamics simulation was used to study the Young's modulus and Poisson's ratio of graphene sheets at temperatures of 200, 300, 400, and 500 K. In the simulation, the graphene sheets subjected to a uniaxial tensile stress was performed until failure occurred. Based on the simulation, it was observed that the fracture occurs at the interface of the fixed layers and thermal layers. A decrease in the strain to failure was obtained for a higher temperature condition. In addition, Young's modulus of graphene sheets decreased with increasing temperature. However, the Poisson's ratio increased with increasing temperature.

Acknowledgment

The authors wish to thank the National Science Council of the Republic of China in Taiwan for providing financial supports for this study under Projects NSC 96-2628-E-150 -005 -MY3 and NSC 100-2221-E-168 -018.

References

[1] A. K. Geim, K. S. Novoselov, Nat. Mater. **6**, 183 (2007).
[2] C. N. R. Rao, A. K. Sood, K. S. Subrahmanyam, A. Govindaraj, Angew. Chem.(Int. Ed.), **48**, 7752 (2009).
[3] A. R. Ranjbartoreh, B. Wang, X. Shen, and G. Wang, J. Appl. Phys. **109**, 014306 (2011).
[4] K. Min and N. R. Aluru, Appl. Phys. Lett. **98**, 013113 (2011).
[5] R. V. Noorden, Nature **442**, 228 (2006).
[6] R. Miranda and A. L. Vázquez de Parga, Nature Nanotechnology **4**, 549 (2009).
[7] T. H. Fang, W. J. Chang, C. I Weng, Mater. Sci. Eng. A **430**, 332 (2006).
[8] W. J. Lee, S. P. Ju, and C. H. Cheng, Langmuir **24**, 13440 (2008).
[9] Y. H. Lin, T. C. Chen, Appl. Phys. A **92**, 571 (2008).
[10] T. H. Fang, W. J. Chang, C. M. Lin, W. C. Lien, Appl. Surf. Sci. **254**, 3436 (2008).
[11] T. H. Fang, W. J. Chang, S. H. Kang, J. H. Liou, Curr. Appl. Phys. **9,** 1241 (2009).
[12] T. H. Fang, W. J. Chang, and Y. C. Fan, Nano **5**, 231 (2010).

[13] T. H. Fang, W. J. Chang, and Y. C. Fan, Micro & Nano Lett.**6**, 214 (2011).
[14] J. W.Jiang, J. S. Wang, and B. Li1, Phys. Rev. B **80**, 113405 (2009).
[15] R. Faccio, P. A. Denis, H. Pardo,C. Goyenola, A. l. WMombru, J. Phys.: Condens. Matter **21**, 285304 (2009).
[16] Y. Li, J. Phys. D: Appl. Phys. **4**, 4954053 (2010).
[17] E. Erdogan, I. Popov, C. G. Rocha, G. Cuniberti, S. Roche, and G. Seifert, Phys. Rev. B **83**, 041401 (2011).
[18] Y. Zheng , L. Xu , Z. Fan , N. Wei, Z. Huang, J. Mater. Chem. **22**, 9798 (2012).
[19] J. Tersoff, Phys. Rev. Lett. **56**, 632 (1986).
[20] C. Lee, X. Wei, and J. W. Kysar, J. Hone, Science **321**, 385 (2008).
[21] Z. Ni, H. Bu , M. Zou, H. Yi, K. Bi, and Y. Chen, Physica B **405**, 1301 (2010).
[22] J. Zhou and R. Huang, J. Mech. Phys. Solids **56**, 1609 (2008).