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RESEARCH ARTICLE

SIMULATION STUDIES ON EFFECT OF TEMPERATURE ON UNIAXIAL DEFORMATION OF SINGLE ATOMIC LAYER GRAPHENE (SALG) SHEET

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ABSTRACT

Molecular dynamics (MD) simulation studies were carried out on a single atom layer graphene sheet to get an insight into the temperature dependent uniaxial deformation. Uniaxial deformation was performed on a 50 nm x 50 nm graphene sheet in zig-zag mode at a constant temperature and a constant engineering strain rate of 0.001 per second. It was observed that failure strain and ultimate stress at failure strain decreased with increasing temperature. Although the variation in mechanical properties with temperature was small, it became significantly large for 1200K and 1500K. The results have been validated using existing mathematical models.

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INTRODUCTION

Molecular Dynamics (MD) simulations have been performed in this study using LAMMPS with the adaptive intermolecular reactive empirical bond order (AIREBO) potential to understand the atomistic level mechanical behaviour and fracture properties of single atom layer graphene sheet (Plimpton, 1995; Stuart, 2002). Simulations were performed under various temperatures to study the mechanical behaviour of graphene sheet. AIREBO potential was selected for simulation because it has been widely reported in the literature that it shows actual mechanical behaviour of grapheme (Zhao, 2009). The breaking of carbon-carbon bonds and their reformation in graphene sheet are also accurately simulated using this potential. In the present work, uniaxial tensile test of graphene along the zig-zag direction was performed on a 50x50 nm^2 size graphene sheet having 1008 atoms with periodic boundary condition. The atomic coordinates of graphene sheet were obtained using a *scilab* program and the data was used to make an input *read data* file for LAMMPS. There was no specific reason to choose this size of graphene sheet. MD Simulation was performed using Isothermal-Isobaric (NPT) ensemble at the specified temperature (300K, 600K, 900K, 1200K and 1500K) for 250 ps with a time step of 0.5 fs.

The system was equilibrated for 30 ps (during this time energy and temperature of the system became almost constant except for small fluctuations maybe due to the kinetic energy of atoms) before performing uniaxial tensile test in a controlled deformation along the zig-zag direction of the structure by applying the strain rate of 0.001 ps^{-1}. Strain (ϵ) was calculated by using the change in the sheet dimension in the x-direction while stress was calculated using the change in potential energy (PE) with respect to the change in strain applying the following formulae,

$$\epsilon = \Delta L_x / L_x \text{ and } \sigma = \frac{1}{V}\left[\left(\frac{\partial PE}{\partial \theta}\right)\right]$$

L_x is the sheet length in x-direction. The strain is applied to the system at every time step of 0.5 fs and the resulting potential energy of the system (PE, in eV) is recorded at a constant temperature. The deformation was run for 250 ps since the fracture strain of graphene is achieved well within this time frame. The radial distribution function (RDF) of the system at 300K is shown in Fig 1a. RDF was recorded after every time step of 5 ps. Three curves have been plotted, representing three different stages of deformation. Immediately after equilibration and before the deformation run was started, atoms were placed in an equilibrium position and a sharp peak was obtained at 1.42 angstrom which is the C-C bond distance. As soon as the strain approached the fracture strain, the atoms got displaced as is evident from the decrease in the amplitude of RDF as well as the shifting of C-C distance to a different value. After fracture,

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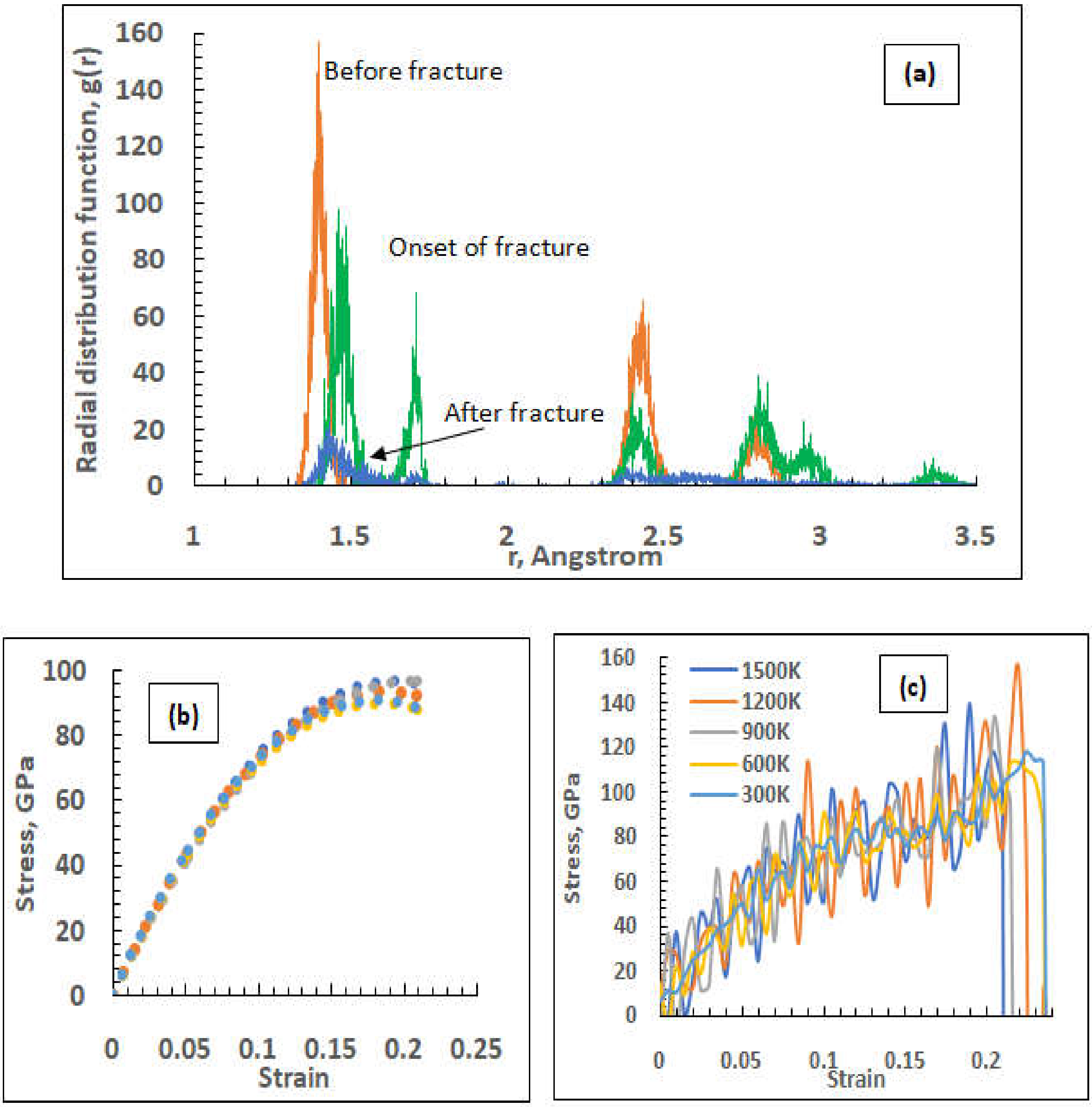
the C-C atoms drifted apart resulting not only in a diffused peak but also shifted to an arbitrary position. The stress-strain curves for various temperatures ranging between 300 K and 1500 K are shown in Fig. 1(b). These curves have been drawn using the best fit values of the data obtained through MD Simulation. Since the fluctuations in simulation data (Fig 1c) were large and not rendering a clear picture, best fit values of stress were plotted against strain increment. As is evident from the figure, a non-linear stress-strain curve is obtained for graphene.

The curves overlapped each other at low strains (elastic region) showing no difference in the tensile modulus. However, at larger strains (non-linear region) the difference between curves became slightly visible. Though the temperature did not influence the tensile properties of graphene, the fracture strength and fracture strain decreased significantly with the increase in temperature (Fig. 1d,e). The fracture strain, as well as stress, at 1500K (higher temperature) was lower compared to the values at 300K (room temperature). The figure also shows a comparison of the data obtained in the present study with that obtained theoretically for a pristine graphene sheet

Table 1. Effective moduli (GPa) of graphene sheet at different temperatures obtained in the present study

Temp(K)	300K	600K	900K	1200K	1500K
Poisson's ratio (m)	0.15	0.24	0.22	0.13	0.10
D_g (GPa)	-2793.9	-2686.4	-2275.4	-2660.6	-2563.9
E_g (GPa)	1007.7	983.3	940.0	999.8	998.7
L_{11} (GPa)	1030.8	1043.4	987.9	1017.0	1008.8
L_{12} (GPa)	154.63	250.4	217.3	132.2	100.8
L_{22} (GPa)	438.1	396.5	385.2	442.4	453.9
N_{11} (GPa)	-11695.9	-12099.2	-10050.9	-11011.4	-10463.8
N_{12} (GPa)	-263.1	-696.9	-486.4	-186.0	-104.6
N_{22} (GPa)	0	0	0	0	0



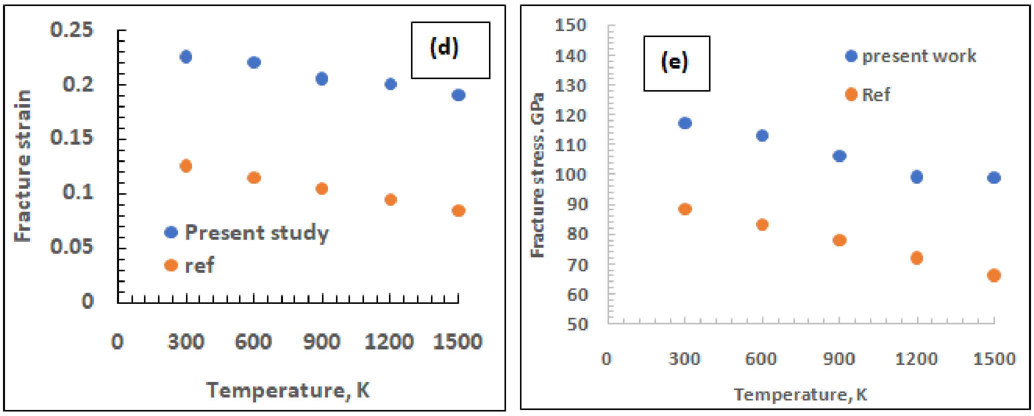


Fig 1. (a) Radial distribution function of graphene sheet during deformation (b) Stress-strain curves (fitted values) at different temperatures (c) Stress-strain curves drawn using simulation data (d) Fracture strain at different temperature (e) Fracture stress at different temperature

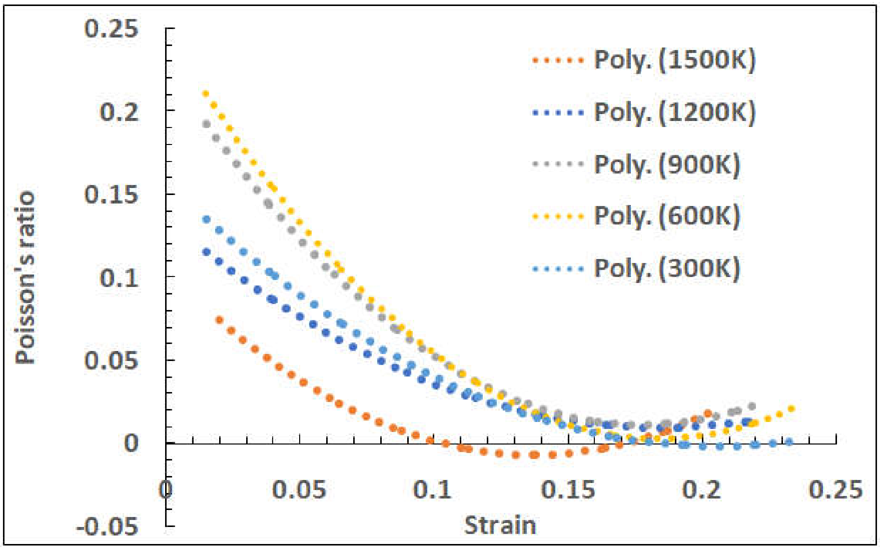


Fig.2. Variation of poisson's ratio with strain at different temperatures

using kinetic theory of fracture (Zhao, 2010). Although the trend appears to be similar, there is a large difference in the values of fracture strain and stress obtained theoretically using the following formulae (Halsey, 1945; Arrhenius, 1989; Wei, 2003).

$$\tau = (\tau_0/n_s) \exp ((U_o - \gamma\sigma)/k_B T) \qquad (1)$$

(where lifetime is the time taken for a stressed solid to breakdown, σ is tensile stress, T is absolute temperature, τ_0 (=0.001ps) is the vibration period of atoms in solid, n_s(1.5xNumber of atoms) is the number of sites available for the state transition, U_o(=4.94 eV)is the interatomic bond dissociation energy, and $\gamma = qV$ (=8.49 Å^3), where V is the activation volume and q (=1) is the coefficient of local overstress, and k_B is the Boltzmann constant). For a time varying tensile stress in a uniaxial tensile test, the fracture is initiated when

$$\int_0^{tr} \frac{dt}{\tau(T,\sigma(t))} = 1 \qquad (2)$$

where t_r is the time to failure (Zhao, 2010). Eqs 1 and 2 have been used to obtain analytical expression for fracture strain (ϵ_r) and σ_r for graphene as follows,

$$\sigma_r (\dot{\epsilon},T)=ak_BT/(\gamma a+kT) \{(Uo/\gamma) + (b(\tau_0/n_s)\dot{\epsilon}) ((\gamma a/kT) + 1)\} \quad (3)$$

where$\dot{\epsilon}$ is the strain rate.

$$\epsilon_r = (1/b)(\exp(\sigma_r/a) - 1) \qquad (4)$$

In eqs. 3 and 4, a (=1.11x 10^{11} Pa) and b (=9.69) are the regression coefficients obtained from the time varying stress versus-strain curve. Using these constants, the values obtained for $_r$and ϵ_r of graphene as a function of temperature has been plotted in Fig1(d,e). In the present work, however, instead of this approach, mathematical relations reported elsewhere (Elmarakbia, 2016) have been used. It has been reported that since, the stress-strain curve for the graphene sheet follows a non-linear behaviour, stress can be written in matrix form as

$$\{\sigma \}= \{L_g\}\epsilon + \{N_g\}\epsilon^2 \qquad (5)$$

where L_g is the linear stiffness tensor and N_g is the non-linear stiffness tensor.

$$L_g = Eg/(1 - m^2) \begin{pmatrix} 1 & m & 0 \\ m & 1 & 0 \\ 0 & 0 & \frac{1-m}{2} \end{pmatrix} \qquad (6)$$

$$N_g = 4D_g/(1-m^2)^2 \begin{pmatrix} 1 & m^2 & 0 \\ m^2 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (7)$$

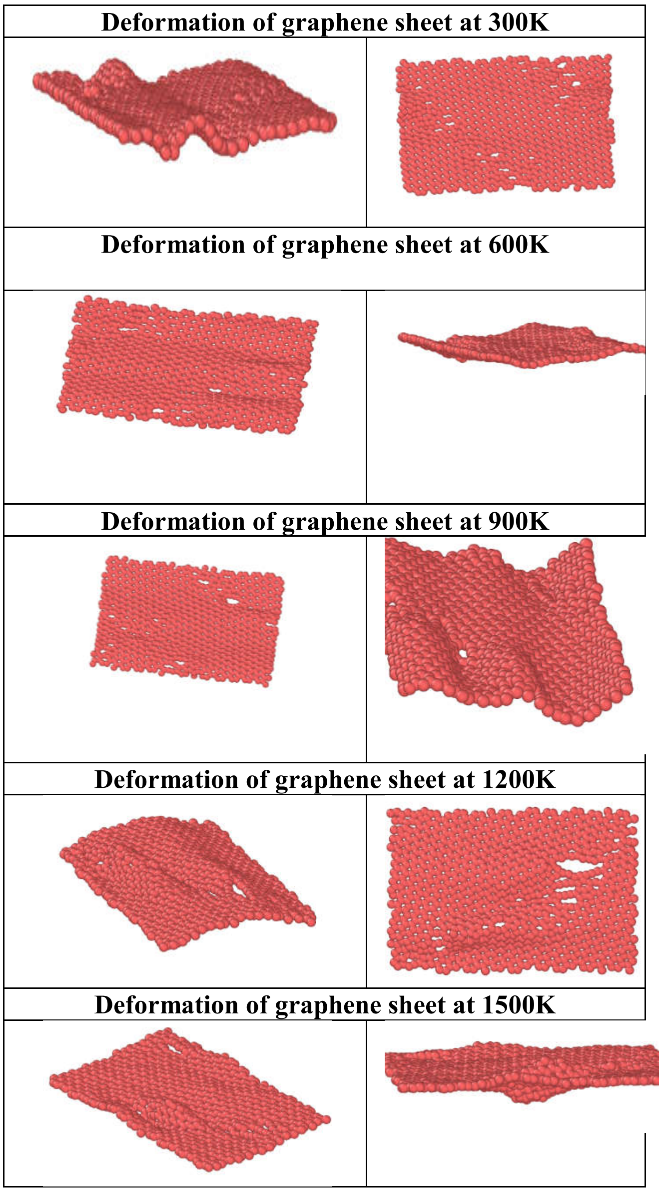


Figure 3. Ovito images of deformed graphene sheet at different temperatures

Using the Morse potential function and constants such as D = 0.6031 nN.nm, =26.25, $_2$ (=120 deg) as the angle of carbon bonds, r as the bond length 0.142 nm, t (0.34 nm) as the thickness of the graphene sheet, the constants E_g=1557.32 GPa, D_g=-4594.93 GPa and m = 0.2were obtained. Authors claimed that using these values, they were able to obtain a critical stress ($_{cr}$ = 132 GPa) and critical strain (ϵ_{cr}= 0.17) for graphene which were close to the reported values for graphene (Elmarakbia, 2016). In order to check the accuracy of the values obtained in the present work, we have substituted the values of E and D (obtained as regression coefficients of stress- strain curves of Fig 1b) in Eq.6 and 7 and calculated the effective moduli and its components L_{11} and N_{11} for different temperatures. The values for poisson's ratio (m) were obtained using Fig.2 in which the best fit values were plotted against strain at different temperatures. The values are shown in Table 1. It was observed that the effective moduli as well as poisson's ratio values match closely with the reported values for graphene (i.e. ~1TPa and 0.2 respectively). Figure 3 shows the images of deformed graphene sheet at different temperatures. Uniaxial tensile tests performed on a graphene sheet using controlled MD simulations showed that temperature significantly affects the mechanical properties of graphene sheet such as poisson's ratio, failure strain and moduli. These properties are higher at room temperature (300K) compared to that obtained at higher temperature (1500K).

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