Molecular Dynamics Study of Mechanical Properties of Monolayer Graphene Sheet

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1. Introduction

The main problem for the advancement of nuclear fusion is the plasma surface interaction (PSI). In the experimental fields of plasma confinement, a portion of hydrogen plasma flows into the divertor walls, which are protected by the layers of polycrystalline graphite or carbon fibre composite. The hydrogen plasma with weak incident energy erodes these carbon walls. The hydrocarbon molecules produced from the erosion of hydrogen and carbon surface tend to become impurities and can affect the plasma confinement. [1] To better understand the properties of the carbon plasma wall facing material, the mechanical properties of graphene which is an atom thick monolayer of carbon atoms is first studied in detail. Graphene has attracted extensive research investigations since its discovery in 2004, due to its remarkable electrical, thermal, chemical and mechanical properties: high elastic modulus (1.02 TPa) and intrinsic strength (130 GPa) [2]; high thermal conductivity (5000 W/mK) [3]; high charge carrier mobility at room temperature (15,000 cm^2/Vs) [4]; and high specific surface area (2630 m^2/g) [5], which makes it good for potential applications in nano devices such as sensors and resonators and as graphene-based composites and so on [2-5]. In order to maximize its potential, mechanical properties of graphene such first be studied in detail. In this paper, the effect of different parameters such as simulation time step, temperature, chirality and strain rate on the mechanical properties such as Young's modulus and fracture stress on monolayer graphene sheets is studied.

2. Methodology

All the molecular dynamics (MD) simulations presented in this paper have been performed using large-scale atomic/molecular massively parallel simulator (LAMMPS) [6] and the AIREBO (Adaptive Intermolecular Reactive Empirical Bond Order) [7] potential is used for the uniaxial tensile tests on the graphene sheet. In the MD simulations, a uniformly distributed

tensile force is applied along the x-axis of monolayer graphene sheets. The geometrical model is a rectangle with length 4.96 Å and width 1.12 Å, and the total number of atoms is 252. Periodic boundary conditions are imposed along x, y and z directions. Prior to applying the loading condition, the monolayer graphene structure was left to isotropically relax to zero pressure in x, y and z directions at a temperature of 300K for 100,000 time increments using constant pressure-temperature by means of Nose-Hoover barostat and thermostat method. [8,9] The loading condition was applied by extending the periodic simulation box size in the x direction under constant strain rates, while the y and z direction was altered to reach zero stress using NPT Nose-Hoover method. Virial stresses in the x direction (uniaxial stress) were calculated at each strain level. The engineering strain at each time step was calculated by multiplying the total time of loading simulation by the applied strain rate. Using the Hooke's law, the slope of the initial part (strain < 3%) of uniaxial stress-strain curve is equivalent to the elastic modulus of monolayer graphene along the loading direction.

3. Results and Discussion

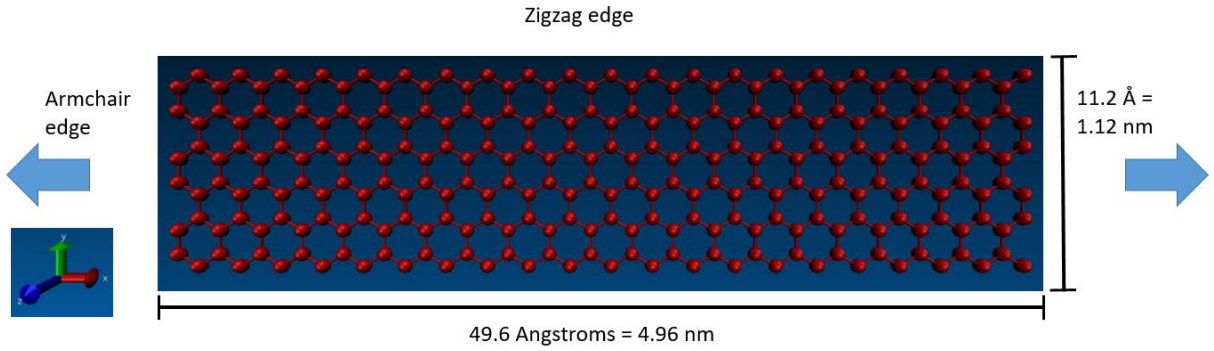

Figure 3.1 Monolayer graphene sheet showing the zigzag and armchair edges

The time step is the length of time between two consecutive iterations in a MD simulation. A time step should be less than 10% of the vibration period of an atom and, time step of 0.5 fs to 0.8 fs provides good results in carbon nanotube and graphene simulations [10]. In order to investigate the effect of time step on the simulation of the uniaxial tensile test of graphene, a set of MD simulations were performed on a 5 nm by 1 nm graphene sheet with time steps of 0.1 fs, 0.3fs, 0.5fs, 0.8fs and 1 fs. All other MD parameters were kept constant, such as 300K for temperature and strain rate at $1 \times 10^9\ s^{-1}$. The results are shown in Figure 3.2. It can be seen that the Young's modulus of the zigzag direction is consistently higher than that of the armchair direction. However, the fracture stress and strain are both higher for armchair direction. Also, as the time step increases, the fracture stress increases for armchair and zigzag directions.

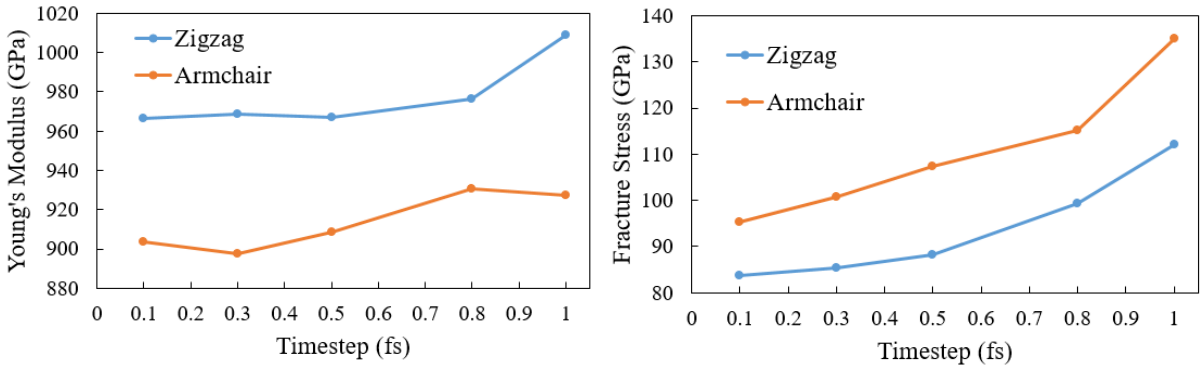

Figure 3.2 Effect of time step to Young's modulus and fracture stress of armchair and zigzag directions.

In MD simulations, a tensile test is performed by applying strain to the nanostructure at a constant strain rate [10,11]. Strain rate of the order of 10^9 is generally used in MD simulations. In order to investigate the effect of strain rate on the failure point of graphene, a set of MD simulations were performed under the strain rates of 0.0005 ps^{-1}- 0.005 ps^{-1}. From Figure 3.3, it can be seen that as the strain rate increases, the Young's modulus and the fracture stress also increases.

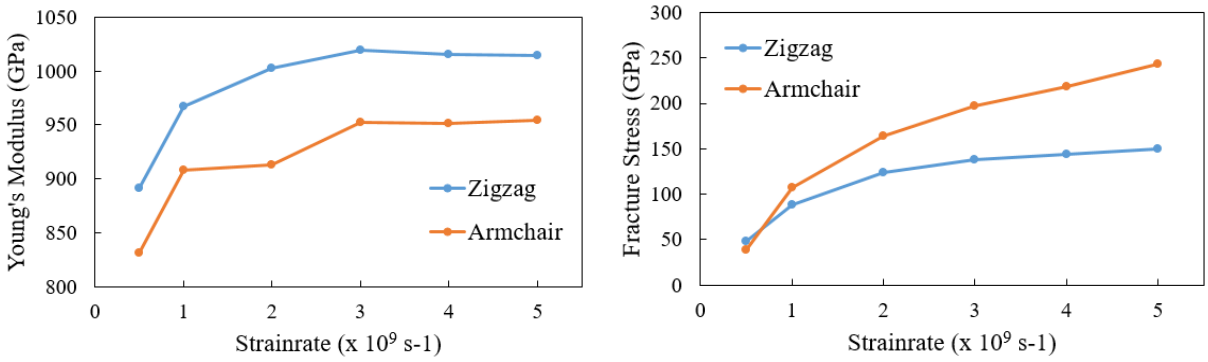

Figure 3.3 Effect of strain rate to Young's modulus and fracture stress of armchair and zigzag directions.

The effect of temperature on the mechanical properties of an armchair and zigzag graphene sheet is analysed for 100 K-1800K. The results are shown in Figure 3.4, for both edge directions, as the temperature increases, the Young's modulus decreases.

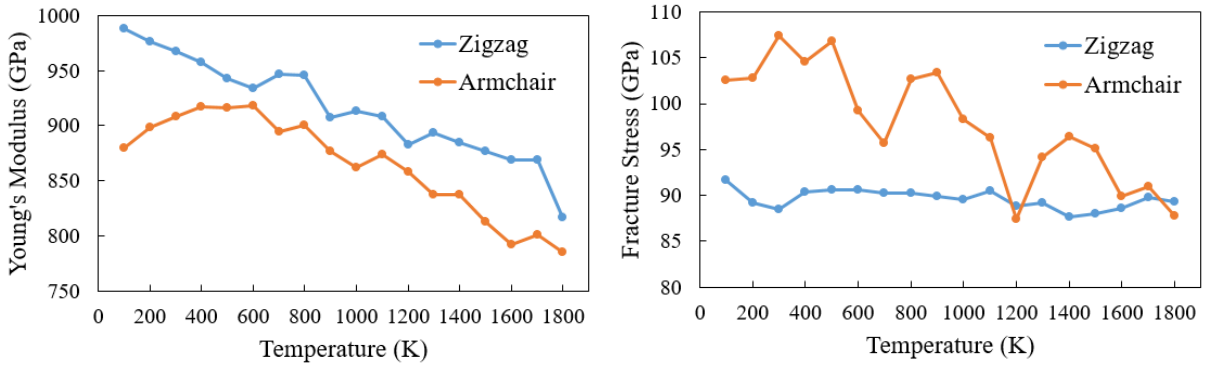

Figure 3.4 Effect of temperature to Young's modulus and fracture stress of armchair and zigzag directions.

4. Conclusion

The effect of different parameters such as edges or chirality, time step, strain rate and temperature on the mechanical properties of monolayer graphene sheets was studied. The results are as follows: The values of Young's modulus at room temperature obtained are 966.9 GPa and 908.3 GPa for armchair and zigzag graphene sheets, respectively. The simulation results reveal that as the temperature increased from 100 K to 1800 K, the elastic modulus declined from 879.5 GPa to 785.4 GPa for armchair and from 988.0 GPa to 816.9 GPa for zigzag. Also, the fracture stress dropped from 102.6 GPa to 87.7 GPa for armchair and from 91.7 GPa to 89.3 GPa for zigzag. Comparing the two chirality directions, armchair graphene sheet stores higher amount of strain energy compared to zigzag. The failure point of graphene sheets depends on the strain rates applied during the uniaxial tension. Results showed that as the strain rate is increased from $0.5 \times 10^9\ s^{-1}$ to $5 \times 10^9\ s^{-1}$, the Young's modulus increased by 14.8% in armchair and 12.1% in zigzag graphene sheets.

Acknowledgments

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