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MOLECULAR DYNAMICS STUDY ON MECHANICAL PROPERTIES OF GRAPHENE SHEETS WITH A HOLE

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The molecular dynamic simulation is used to study the fracture behavior of graphene sheets with a hole subjected to uniaxial tensile loading. In this simulation, the hole diameter of 0, 0.44, 0.88, and 1.84 nm are chosen to investigate the effect of the diameter of the hole on the mechanical properties of graphene sheets. The results show that when the diameter of the hole increases, the maximum stress and strain of graphene sheets decrease. The Poisson's ratio increases when the diameter of the hole increases. However, the Young's modulus decreases with increasing the hole diameter. Furthermore, when the ratio of hole diameter to width of the graphene sheets decreases, the stress concentration factor increases. This trend is consistent with the theoretical analysis. These results are useful for engineering applications of graphene materials.

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1. Introduction

Graphene, is composed of a two-dimensional (2D) planar sheet of covalently bonded carbon atoms arranged in honeycomb lattice, can form 1D carbon nanotubes or 3D graphite. Graphene is currently the material of intense research due to its exceptional mechanical and electrical properties [1-4]. Accordingly, graphene has great promise for novel photonic devices and mass sensors in nanobiological devices and nanomechanical systems [5-7].

The electronic behavior of graphene can be influenced by its mechanical properties [8]. In recent years, many researchers have experimentally studied the mechanical behaviors of graphene structures. In addition, some researchers have used molecular dynamics (MD) method to investigate its mechanical properties. For example, Gao and Hao [9] investigated the mechanical properties of zigzag graphene and armchair graphene nanoribbon under tensile and compressive loading with MD and found that the critical loading of the zigzag graphene is larger than that of the armchair graphene. Scarpa et al. [10] studied the transverse mechanical deformation of bilayer

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graphene. Zhong et al. [11] performed MD to investigate the thermal conductivity of graphene nanoribbons and found that single-layer graphene has better ballistic transport property than the multilayer graphene.

The graphene has been shown to have very high intrinsic strength. However, the mechanical properties of graphene structures with holes or cutouts, may occur in the engineering applications, are still poor understood. Only very few reports are available for the graphene structures with discontinuous geometries [12]. In this article, the fracture responses of graphene sheets with a circular hole subjected to tensile loading are study. In addition, the effects of different diameters of the hole on the Young's modulus and Poisson's ratio, and stress concentration factor of the graphene sheets are also discussed.

2. Simulation method

The structure of armchair graphene has a hole with different diameters, *d*, of 0, 0.44, 0.88, and 1.84 nm, respectively, in its middle center, and the corresponding simulated system consists of 2296, 2290, 2272, and 2194 carbon atoms with the dimensions around l = 9.9 nm and w =5.8 nm as shown in Fig. 1. In this simulation, the Tersoff potential [13,14] is used to model the interaction between the carbon atoms. 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 tensile loading and thus the system maintains at the temperature of 300 K.

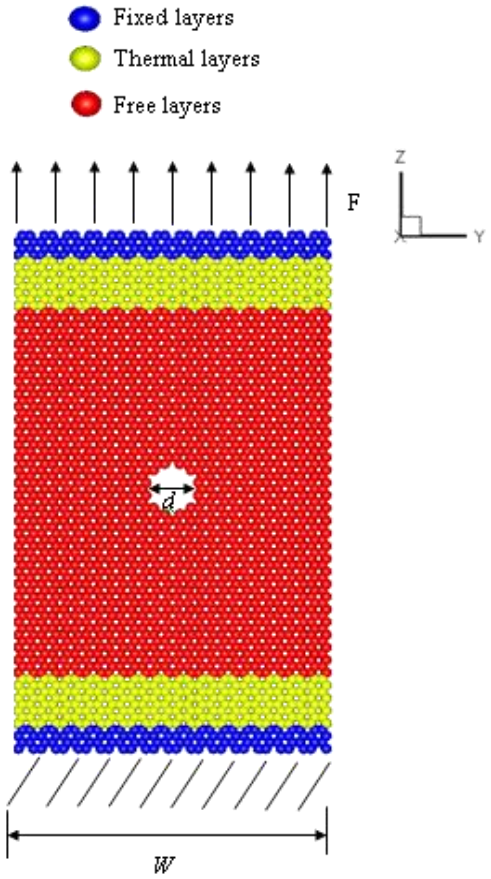

Fig. 1. Schematics of MD of graphene sheets with a hole diameter subjected to uniaxial tensile loading.

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. In order to describe the simulated data, a nonlinear elastic response of the graphene sheets is considered. The nonlinear behavior 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 is the Young's modulus and D is the third-order elastic modulus and reflects the nonlinear elastic behavior of graphene sheets. The presence of the second-order term leads to a decrease of stiffness and the value of D is typically negative. In addition, σ_z is determined 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 longitudinal strain ε_z is calculated from $\varepsilon_z = \Delta l / l$. Accordingly, 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 $\Delta w / w$

In addition, the maximum stress of the graphene sheets is induced at the hole edge due to stress concentration. A stress concentration factor is used to estimate the stress distribution near the hole. In the simulation, the stress concentration factor $\overline{K}_t$ is defined as the ratio of maximum stress at the hole edge to nominal applied stress. It can be expressed in the following form:

$$\overline{K}_t = \frac{\sigma_m}{\sigma_0} \tag{3}$$

Where σ_m is the maximum stress before the spontaneous crack fracture. σ_0 is the nominal applied stress. For a structure with a larger hole, σ_m is smaller, but σ_0 is larger due to the geometry effect.

3. Results and discussion

3.1. Fracture behavior under tensile loading

In this article, we investigate the fracture behavior of graphene sheets with a hole diameter of 0, 0.44, 0.88, and 1.84 nm at the temperature of 300 K. Fig. 2 depicts the snapshots of graphene sheets subjected to tensile loading inducing a tensile stress until failure for various diameters of the hole. After defect formation such as vacancies and topological defects in the graphene sheets, the crack takes place when the further loading was increased. The kinetic energy is transferred into strain energy through the deformation during the tensile loading. The graphene sheets with a larger diameter have lower strain energy. This results in a decrease in the strain to failure for a larger diameter of the hole. In addition, it can be seen that the fracture occurs at the interface of the fixed layers and thermal layers along the transverse direction for the graphene with a small hole or even no hole. When the hole becomes larger, the main fracture occurs at the hole along the transverse direction. This indicates that the nominal applied stress is higher for the graphene sheets with a larger hole.

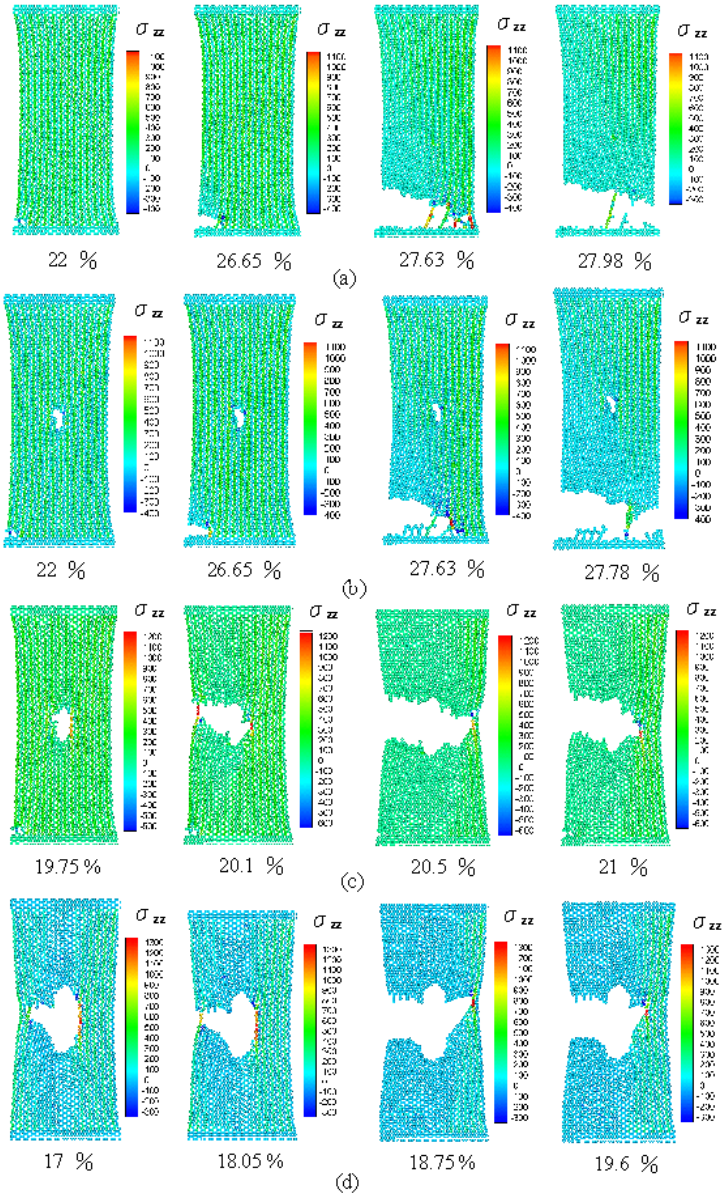

Fig. 2. The snapshots of graphene sheets with a hole diameter of (a) 0 nm, (b) 0.44 nm, (c) 0.88 nm, and (d)1.84 nm subjected to a tensile stress until failure.

3.2 Young's modulus and Poisson's ratio

The stress-strain curve of graphene sheets with a hole subjected to the tensile load for different diameters of the hole 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. A smaller strain at fracture is obtained for a graphene sheets with a larger hole as given in Fig. 2. In addition, its maximum stress at fracture is also lower for the graphene sheets with a larger hole. Therefore, the figure shows that the strain energy decreases with increasing diameter of the hole.

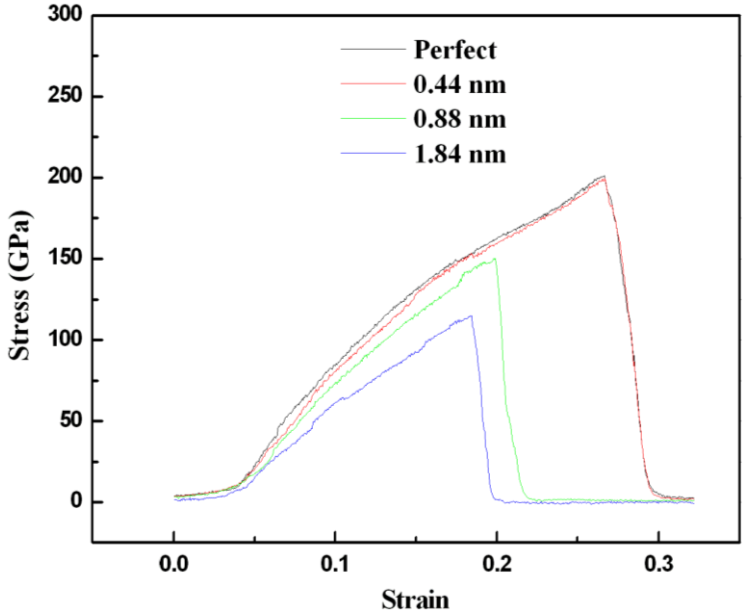

Fig. 3. The stress-strain curve of graphene sheets with a hole subjected to the tensile load for different diameters of the hole.

The values of Young's modulus and nonlinear elastic modulus for the graphene sheets are based on the relation between the stress and strain given by Eq. (1) and are listed in Table 1. It can be seen that Young's modulus of graphene sheets decreases with increasing diameter of the hole. This is because a larger hole in a structure leads to a weaker strength. In addition, the values of the third-order elastic modulus are all minus. This nonlinear elastic behavior of graphene is consistent with the previous experimental study [2].

Table 1. The elastic constants of graphene sheets with different diameters of the hole.

Hole diameter (nm)	Young's Modulus (TPa)	Third-order Elastic Modulus (TPa)
0	1.171	-1.295
0.44	1.157	-1.239
0.88	0.777	-0.571
1.84	0.603	-0.385

The effect of hole size on the Poisson's ratio of graphene sheets is illustrated in Fig. 4. The Poisson's ratio increases with increasing diameter of the hole. This is because a smaller strain in the z-direction of graphene sheets with a larger diameter of the hole is obtained as given in Fig. 2. This also indicates that the effect of the diameter of the hole on the lateral strain is smaller than the longitudinal strain.

3.3. Stress concentration factor

In practical applications of graphene sheets with cracks, the true stress caused by an external load can be calculated by using the theoretical stress concentration factor K_t as follows:

$$K_t = 2\sqrt{a/\rho} \tag{4}$$

where K_t is a function of the geometry of a crack. ρ represents the radius of the curvature at the crack tip and *a* denotes one-half the length of an internal crack. It is noted that K_t approaches infinity as the radius of curvature is close to zero.

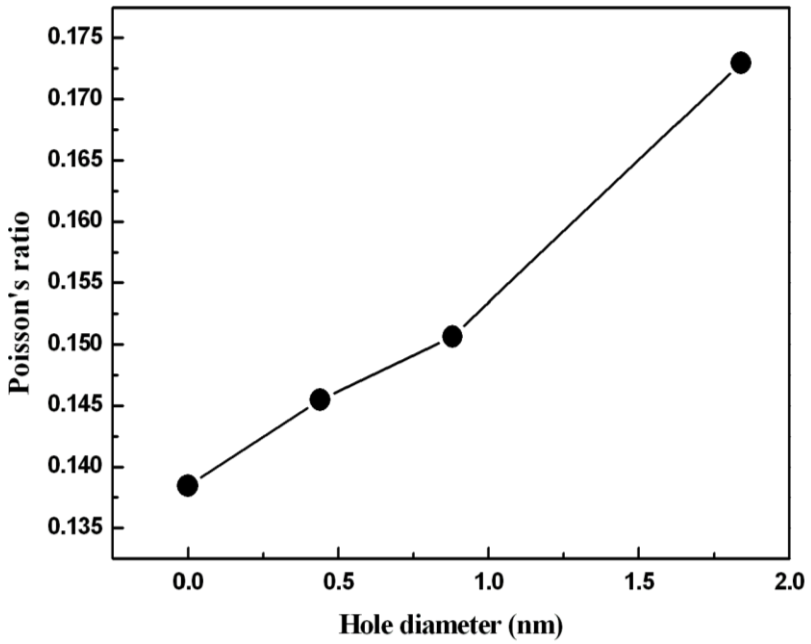

Fig. 4. The Poisson's ratio of graphene sheets with a hole subjected to tensile loading for different diameters of the hole.

Fig. 5 depicts the comparison of stress concentration factor obtained by using the MD simulation and theoretical analysis. The stress concentration factor is relative to the geometry parameter, which is expressed as the ratio of hole diameter to width of the graphene sheets, *d/w*. It can be seen that the stress concentration factor decreases with increasing the geometry parameter. This implies that even a small crack, it is critical and can induce a significant stress response. This should be noted in the nanostructure design. It can be seen that the stress concentration factor of MD simulation is generally higher than that of the theoretical analysis. The MD simulation is on the nano-meter scale and is different from the theoretical calculation, which is based on the continuum mechanics for the micro-meter scale. The precipitation of voids at grain boundaries is the main effect on the microstructures. However, the dislocation and atomic slipping become dominant for the nanostructures [15].

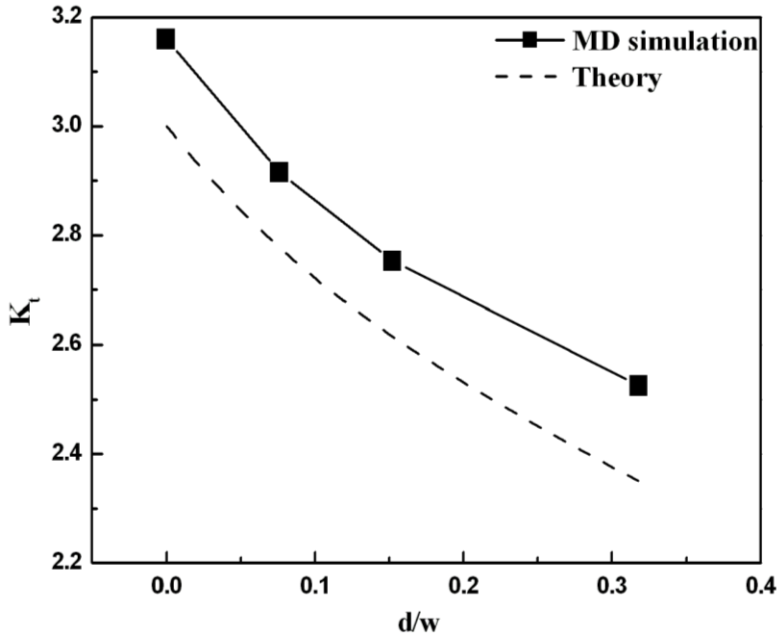

Fig.5. Comparison of stress concentration factor using the MD simulation and theoretical analysis.

4. Conclusions

The Young's modulus, Poisson's ratio, and stress concentration factor of graphene sheets with a hole were investigated using the molecular dynamic simulation. The graphene sheets subjected to uniaxial tensile stress was performed until failure occurred. The results showed that the maximum stress and strain decreased as the diameter of the hole increased. For the simulated cases, the maximum stress dropped from about 200 GPa to 100 GPa. The maximum strain was from 0.3 to 0.2. With increasing diameter of the hole, the Young's modulus of graphene sheets decreased, but its Poisson's ratio increased. In addition, the stress concentration factor decreased with increasing the geometry parameter *d/w*.

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