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Chirality- and size-dependent elastic properties of a single-layered graphene sheet

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This article mainly uses a structural mechanics approach to analyze the elastic properties of a single-layered graphene sheet (SLGS). Besides, the space frame structure is also adopted to model the interatomic forces of the carbon–carbon bonds. By means of the finite element method, the elastic properties of SLGS on the basis of different chirality and size are measured. According to the results, the elastic properties of SLGS are size- and chirality-dependent, which is in consensus with the literature.

Key words: Single-layered graphene sheet, Elastic properties, Chirality

INTRODUCTION

Based on its one atomic layer thickness, graphene is considered as a two-dimensional (2D) material which consists of carbon atoms set in a honeycomb lattice structure. After it was primarily isolated in 2004 [1], it has received significant attention due to its interesting physical properties like high levels of thermal conductivity [2], stiffness, strength [3], etc. Besides, multilayer graphene also possesses attractive physical characteristics [4-5].

By using experimental and theoretical methods, numerous studies have been carried out on the elastic properties of SLGS. Frank *et al*. proved the Young's modulus of graphene nearly 0.5 TPa with a nanoindentation experiment using atomic force microscope (AFM) [10]. In a similar approach, Lee *et al*. obtained the Young's modulus of graphene approximately equal to 1TPa [3]. By tip-induced deformation experiments Cristina found that the Young's modulus of free monolayer graphene reaches 0.25TPa [6]. From the perspective of theories, the molecular dynamics method was applied to study the Young's modulus of different chirality graphenes by Q.X.Pei *et al*., they also found that the armchair graphene is 0.89TPa and the zigzag graphene is 0.83TPa [7]. In addition, Hao Bu *et al*. also applied a molecular dynamics method (empirical Tersoff potential) to calculate the Young's modulus of graphene up to 1.24TPa [8]. *AB initio* DFT method was resorted by Fang Liu *et al*. to compute the Young's modulus and Poisson's ratio showing that the values are 1.05TPa and 0.186, respectively [9]. In addition,

Reddy adopted a continuum mechanics approach to figure the Young's modulus of non-equilibrium and equilibrium, showing that the values are 1.0 TPa and 0.7 TPa, respectively [11]. Li explored a structural mechanics approach that uses space frame structures to model the carbon nanotubes, therefore he expected that the Young's modulus of monolayer graphene was 1.0 TPa [12].

On the basis of molecular structural mechanics, Young's modulus and Poisson's ratio of SLGS was analysed by atomic simulation approach in this work. For this purpose, an equal structural beam was used to imitate the interatomic forces of the carbon–carbon bonds. The equal beam mode with different chirality and size will be used to study the Young's modulus and Poisson's ratio of SLGS.

MODEL

Theoretical foundation molecular mechanics and structural mechanics

Graphene can be considered as a large molecule made up of lots of carbon atoms arranged regularly, each of them being in a force field from the standpoint of molecular mechanics [12]. The force field, created by nucleus-nucleus and electron-nucleus interactions, controls the motions of atoms. As usual, the force field, expressed as a means of steric potential energy, only replies on the comparative position of the nucleus. In Fig. 1, diverse kinds of potential energy are shown. For the system, its whole potential energy under consideration can be calculated as [13]:

$$U_{Total}=\sum U_r+\sum U_\theta+\sum U_\phi+\sum U_\omega+\sum U_{vd\omega} \quad (1)$$

where $U_{vd\omega}$, U_ω , U_ϕ , U_θ and U_r are energies, relative to van der Waals nonbonding

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interaction, bond torsion, inversion, angle variation and bond stretching, respectively. Generally, the first term is of very little importance compared with the other four terms, which primarily contribute to the whole steric energy. Compared with other terms, the torsion and inversion energies have great importance for graphene which is subjected to in-plane tension loading. Consequently, the sum of angle variation and bond stretching, further represented by harmonic functions under small deformations of linear elasticity, can be used to fairly accurately calculate a monolayer graphene's whole potential energy [14-15]:

$$U_r = \frac{1}{2}k_r(r-r_0)^2 = \frac{1}{2}k_r(\Delta r)^2 \qquad (2)$$

$$U_\theta = \frac{1}{2}k_\theta(\theta-\theta_0)^2 = \frac{1}{2}k_\theta(\Delta\theta)^2 \qquad (3)$$

where k_θ and k_r stand for the force constants, separately relative to angle variation and bond stretching; θ and r stand for bond-angle and inter-atomic distance after deformation, respectively; θ_0 and r_0 refer to bond angle and distance before deformation, respectively.

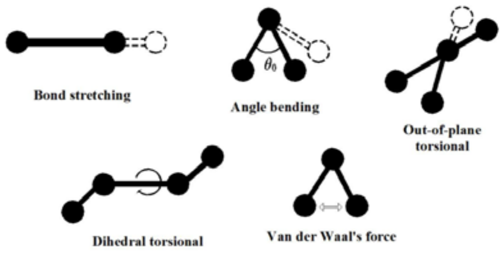

Fig. 1. Potential energy of carbon–carbon bonds

Structural mechanics

Twisting and stretching make up a whole beam's potential energy on the basis of structural mechanics. In Fig. 2, diverse loadings are shown which are used in a uniform beam generating potential energy. Under axial load, a uniform beam's strain energy, N , can be computed as:

$$U_A = \frac{1}{2}\int_0^L \frac{N^2}{EA}dl = \frac{1}{2}\frac{N^2L}{EA} = \frac{1}{2}\frac{EA}{L}(\Delta L)^2 \qquad (4)$$

where E is the Young's modulus of the uniform beam, U_A the tensile energy, A the beam's cross section, ΔL the length variation, and L the length of beam. In the beam, M produces strain energy in the application of pure bending load. U_M , the bending potential energy is given by

$$U_M = \frac{1}{2}\int_0^L \frac{M^2}{EI}dl = \frac{2EI}{L}\alpha^2 = \frac{1}{2}\frac{EI}{L}(2\alpha)^2 \qquad (5)$$

where α stands for the rotation angle of the end of the beam and I stands for its moment of inertia.

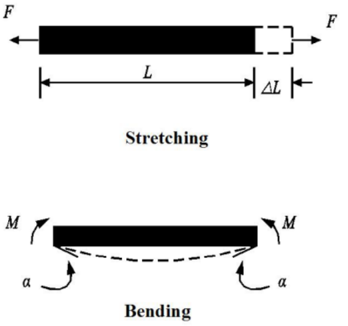

Fig. 2. Stretching and bending a of a uniform beam

Equivalent continuum space frame structures model

That is to say, the equivalencies of the relevant terms between molecular and structural mechanic systems are imposed because of the independency of the potential energy terms in those systems The equivalency of energy between diverse term states an equivalent structural beam. To model interatomic forces of the covalently bonded carbon atoms, an equivalent structural beam is used. Attributions of the beam according to force field constants, covalent stiffnesses, are as:

$$\frac{EA}{L} = k_r \qquad \frac{EI}{L} = k_\theta \qquad (6)$$

$\frac{EA}{L}$ and $\frac{EI}{L}$ stand for bending and stretching of the equivalent beams.

There is a possibility that the stiffnesses, which are defined in constants of force field terms, use the structural beam by the stiffness matrix method. Another method using the structural beam suggested the atomistic finite element [16]. It is pointed out that specified diameter and elastic modulus of the beam fulfill the probabilities of using the beam with the atomistic limited approach compared with the stiffness matrix method. *Via* replacing $A = \frac{\pi d^2}{4}, I = \frac{\pi d^4}{64}$ in Eq. (6) according to the force filed constants, the beam features are deduced as:

$$d = 4\sqrt{\frac{k_\theta}{k_r}}, E = \frac{{k_r}^2 L}{4\pi k_\theta} \qquad (7)$$

where E is the modulus of elasticity and d is cross section diameter. L is the length of beam which is regarded to be equal to the carbon atoms' distance in a covalent bond.

k_θ and k_r are equal to 8.76×10^{-10} Nnm/rad^2 and 6.52×10^{-7} N/nm,respectively, by employing the AMBER force field of molecular dynamics simulation [15-16]. 0.1412 nm is the distance between two contiguous carbon atoms [21]. We can get E= 5.488×10^{-6}N/nm^2 and d=0.146618 nm through solving the Eq. (7). Additionally, the ratio of Poisson is reasonably supposed to be 0.3.

To simulate the monolayer graphene nanofilms, the space frame structures, which are made up of beam elements, are shown in terms of the theoretical analysis in the part above. It is forecasted that the mechanical features of the SLGSs are size- and chirality-dependent [17-20]; so, the elastic properties are computed for the armchair sheets and zigzag in diverse sizes. Two geometric parameters, b and a, are described to specify every SLGS. b and a stand for side width and length of the SLGS, respectively. In Fig. 3, the diagram of the SLGSs studied in this research is shown.

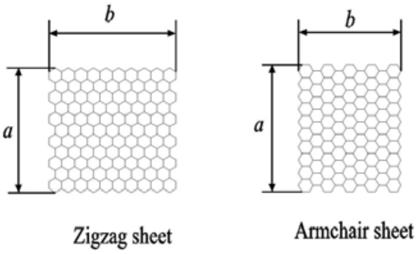

Fig. 3. Zigzag SLGS and armchair SLGS.

To study the elastic properties of SLGS, a space frame structure model is described. Normal stress to the atomistic model's free edge is used for the exploration of the elastic properties of the SLGS under tension. As a result, the continuum sheet's normal stress is presented as:

$$\sigma = \frac{nf}{bt} \qquad (8)$$

where n is the number of nodes exposed to the external forces, f is the magnitude of the tensile forces, t and b are the thickness and width of the SLGS, respectively. According to the strain and tensile stress, the Poisson's ratio and Young's modulus are calculated as:

$$E = \frac{\sigma}{\varepsilon_a} = \frac{\frac{nf}{bt}}{\frac{\Delta a}{a}} \qquad \nu = \frac{\varepsilon_b}{\varepsilon_a} = \frac{\frac{\Delta b}{b}}{\frac{\Delta a}{a}} \qquad (9)$$

where ε_a and ε_b stand for the tensile strain of SLGS, which are equal to the elongation ratios Δa and Δb to the original side length, a and b.

RESULTS AND DISCUSSION

Through the finite element method, we can detrmine the SLGS elastic properties. In Figs. 4-7, there are explanations of the Young's modulus and Poisson's ratio of SLGS with diverse size and chirality. The armchair graphene has 0.672 TPa and 0.435, and the zigzag graphene has 0.615 TPa and 0.388, respectively, on the condition that the SLGS width and length are 1.989 nm and 2.215 nm, respectively. This corresponds to the results in the references [11,21]. From the figures it can be perceived that with the gradually increasing size, the Poisson's ratio and Young's modulus increase or decrease. So we can prove that the SLGS elastic property is dependent on size. From Figs. 4 and 6 it is perceived that the Young's modulus of armchair graphene is constant (about 0.665TPa) and that of zigzag graphene increases from 0.615TPa to 0.700TPa, on the condition that the length varies and the width is constant. In the other case, the Young's modulus of armchair graphene increases from 0.672PTa to 0.708TPa, and that of zigzag graphene is constant (about 0.613TPa), on the condition that the width varies and the length is constant. From Figs. 5 and 7, we can see that there is a similar trend of the Poisson's radio for both armchair and zigzag graphene. In this way we can prove that the SLGS elastic property is dependent on chirality.

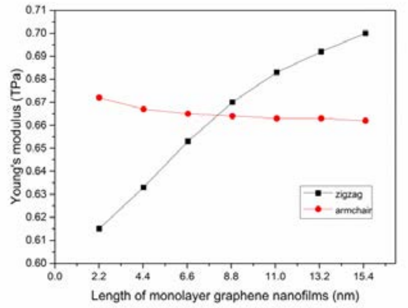

Fig. 4. Young's modulus of SLGS with the variation of length at constant width (1.989 nm).

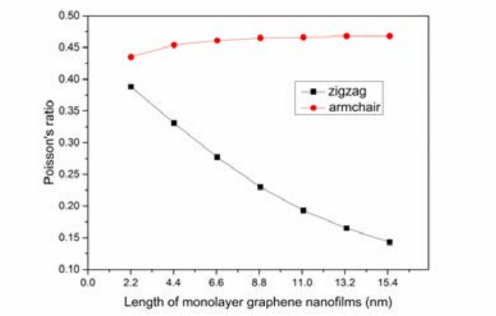

Fig. 5. Poisson's ratio of SLGS with the variation of length at constant width (1.989 nm).

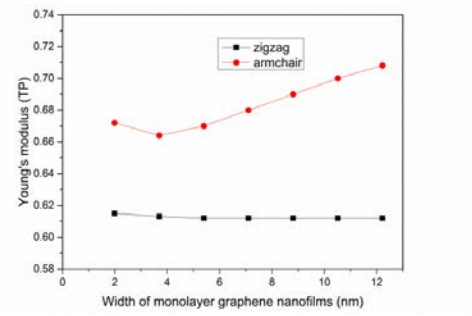

Fig. 6. Young's modulus of SLGS with the variation of width at constant length (2.215 nm).

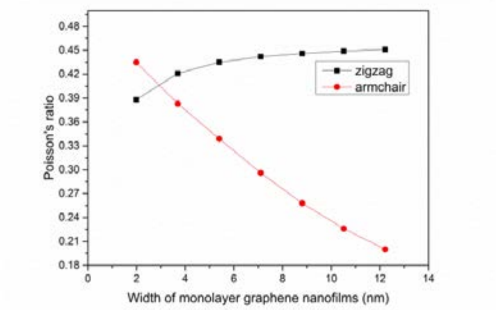

Fig. 7. Poisson's ratio of SLGS with the variation of width at constant length (2.215 nm).

CONCLUSIONS

The finite element model of equal continuum for the SLGS under exterior loads is presented. To this end, based on a SLGS action's atomistic analysis, the Poisson's radio and Young's modulus of the continuum model are computed. The armchair graphene is 0.672TPa and 0.435, and the zigzag graphene is 0.615TPa and 0.388, on the condition that the SLGS width and length are 1.989 nm and 2.215 nm, respectively. This corresponds to the results in the literature. So the method used in this paper is reasonable. On this basis, the elastic properties of SLGS with different chirality and size are calculated and it is found that with the size gradually increasing, the Poisson's ratio and Young's modulus increase or decrease, so we found that the SLGS elastic property is size-dependent. We also found that the SLGS elastic property is chirality-dependent.

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