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Mechanical properties of single layer graphene nanoribbons through bending experimental simulations

Weidong Wang, a Cuili Shen, Shuai Li, Jiaojiao Min, and Chenglong Yi
School of Electrical and Mechanical Engineering, Xidian University, China
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Molecular Dynamics (MD) simulations of bending experiments have been carried out for graphene nanoribbons in order to measure their mechanical properties. Based on the continuum theory, one physical model is established for a double-clamped single layer rectangular graphene film and the relation between the centerline deflection and the concentrated force has been derived. During MD simulations, the Airebo potential is utilized to describe the C-C atomic interactions of graphene, and the concentrated radial forces were exerted on the centerline of a graphene nanoribbon. After the simulations, a set of Young’s moduli is calculated based on the presented relation between the centerline deflection and the concentrated force, with an average value of 1.034 TPa, and the maximum stress of graphene is also obtained as 137.09 GPa. © 2014 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution 3.0 Unported License. [http://dx.doi.org/10.1063/1.4868625]

I. INTRODUCTION

Graphene is a kind of carbon material with one monolayer of carbon atoms arranged in a two-dimensional honeycomb lattice. It was discovered and successfully isolated from bulk graphite just a few years ago. It is the basic unit for building other dimensional carbonaceous materials, such as zero-dimensional fullerenes, one-dimensional carbon nanotubes, and three-dimensional graphite Ref. 1. The successful synthesis of single layer graphene and the experimental observation of Dirac charge carrier properties in graphene-based devices awakened an enormous interest in this two-dimensional carbonaceous material Ref. 2. Due to its unique electronic, structural and mechanical properties, graphene has become an important candidate for numerous potential applications, ranging from chemical sensors, composites, spintronic devices, transparent electrodes for light-emitting diodes and photovoltaics, to mechanical resonators Refs. 3–5.

The superior mechanical properties of graphene make it ideally suited for NEMS applications, such as in pressure sensing and fabrication of nanoresonators Ref. 3. So the mechanical properties of graphene have become one of the current research hotspots Ref. 6, and have been investigated using experimental and theoretical approaches. Poot et al. measured the nanomechanical properties of graphene sheets suspended over circular holes by using an AFM Ref. 7. Blakslee et al. reported the Young’s modulus of bulk graphite to be about 1.06 TPa Ref. 8. Using nanoindentation by an atomic force microscope, Frank et al. and Lee et al. measured the Young’s modulus and ultimate strength of multiple layer and monolayer graphene, and reported that graphene has the highest Young’s modulus of about 1 TPa Refs. 9 and 10. In addition to experimental methods, numerical simulation has become a powerful tool in the research on the mechanical behavior of nanomaterials. Using first principles methods, Liu et al. computed the Young’s modulus and Poisson’s ratio of graphene under tension as 1.050 TPa and 0.186, respectively Ref. 11. Sakhaee-Pour studied the elastic properties and bending mechanical behavior of graphene films using molecular structural mechanics Refs. 12 and 13. Han et al. investigated the stretching properties of graphene through molecular dynamics (MD) simulation, and got an elastic modulus of 1.031 ~ 1.058 TPa and tensile strength of

aCorresponding Author: wangwd@mail.xidian.edu.cn
Their findings suggest that graphene sheets can sustain very large bending and stretching prior to the occurrence of fracture, while the variation of the values of the elastic modulus has not yet reached a consensus. Compared with other simulation methods, the MD method has irreplaceable advantages, and it can quantitatively simulate the dynamic process that happens in a real solid. Moreover, MD is a more effective way than experimental methods of investigating the mechanical properties of nanoscale material graphene.

Bending experiments are another good approach to determining the mechanical properties of materials. Some investigations of bending experiments have been carried out for graphene Refs. 16–21, but the values of the mechanical properties obtained differ greatly from the simulation results based on other principles. For example, Hod et al. studied the mechanical properties of the bending deformation of narrow graphene nanobelts using the method of concentrated force loading, and got the Young’s modulus of graphene as about 7.0 TPa Ref. 16, which differs greatly from the conclusions obtained through the stretching method. In view of this situation, this article will perform some MD simulations of the bending experiment on graphene nanoribbons by means of concentrated force loading to measure the mechanical properties of graphene.

II. METHOD AND SIMULATION PROCESS

A. Method

Being a kind of ideal two-dimensional material, graphene is different from bulk materials, and the elastic response of graphene must take nonlinear factors into account because the stress–strain response must curve over to a maximum point that defines the intrinsic breaking stress Ref. 10 and 17. An elastic response implies the existence of an energy potential that is a function of strain, which can be expressed as a Taylor series in powers of the strain. The lowest-order (quadratic) term leads to a linear elastic response. The third-order term gives rise to nonlinear elastic behavior. This kind of nonlinear elastic behavior under a uniaxial load can be expressed by

$$\sigma = E \varepsilon + D \varepsilon^2$$

where $\sigma$ is the symmetric second Piola–Kirchhoff stress, $\varepsilon$ is the uniaxial Lagrangian strain, $E$ is the Young’s modulus, and $D$ is the third-order elastic modulus. While in Ref. 10, the resulting force–displacement curve made by using the nonlinear elastic model was virtually indistinguishable from that of the linear model (where $D = 0$), nonlinear effects can be ignored while simulating the force–displacement response. Eq. (1) can be simplified as

$$E = \sigma / \varepsilon$$

Fig. 1 shows the diagram of double-clamped graphene nanoribbons. Region I is clamped; Region III is affected by a concentrated radial force; Region II is the zone of free movement.
Table I gives the model parameters of the single layer rectangular graphene film. Here, $L$ represents the length and $W$, the width of the graphene film.

For graphene loaded along its centerline by different concentrated radial forces, its bending stiffness (it is a 2D material) can be considered to be zero Ref. 18, and so the deformation of a double-clamped membrane is similar to that in uniaxial strain stretching. But unlike the stretching method, this beam bending method is to study the Young’s modulus of materials by measuring the bending deformation characteristics of the beam (i.e., the double end clamped graphene nanoribbons) Ref. 19 and 20. Here, the equivalent one-dimensional continuum model is presented to investigate the elastic behavior of a single layer graphene film, and the deformation mechanism diagram is shown in Fig. 2.

In the process of analysis, only the graphene film on the right side of the centerline was considered, due to symmetry. Denoting the concentrated radial force acting on the centerline of graphene by $F$ and the centerline deflection by $h$, denote the angle of $F$ by $\theta$ and its component by $F_1$. Then the axial strain $\varepsilon$ is

$$
\varepsilon = \sqrt{\frac{4(h/L)^2}{(L/h)^2}} + 1 - 1
$$

The normal stress $\sigma$ is

$$
\sigma = \frac{F_1}{W \times t}
$$

where $t$ denotes the effective thickness of the graphene, which is always taken as the layer spacing of the graphite crystal, i.e., 3.35 Å; $F_1$ is the magnitude of the effective axial tensile force, which is the component of $F$ exerted on the graphene film considered, and can be expressed as

$$
F_1 = F \times \cos \theta/2
$$

From Eqs. (2)–(4), the Young’s modulus, $E^{3D}$, can be derived,

$$
E^{3D} = \frac{F \times L \times \sqrt{4(h/L)^2 + 1}}{4 \times h \times W \times t \times \left(\sqrt{4(h/L)^2 + 1} - 1\right)}
$$

In the range of elastic deformation of the graphene film, the maximum stress $\sigma_{m}^{3D}$ can be calculated from Eq. (4) when both the concentrated radial force $F$ and the centerline deflection $h$ reach their maximum values.

$$
\sigma_{m}^{3D} = F_{\text{max}} \times \frac{\sqrt{4 + (L/h)^2}}{(4 \times W \times t)}
$$
B. The molecular dynamics simulation process

When performing MD simulations, we use the NVT ensemble and control the temperatures at the ideal temperature condition (0.01 K) during the simulations. In order to avoid the complex effects of atomic thermal fluctuations, the temperature is regulated by the Nosé–Hoover method and the time step is set to 1 fs.

The MD simulation process of a bending experiment on double-clamped graphene nanoribbons can be roughly divided into five steps, as shown in Fig. 3. Firstly, due to the modeling limitations of the LAMMPS used for these simulations, the graphene model should be imported from a physical model datum. Secondly, the simulation conditions are set up, including boundary conditions, potential functions, ensemble, temperature, time step, heating bath method, size and direction of the concentrated radial force, as well as the variable and format information for the output data.

Thirdly, one key step, referred to as the energy minimization and relaxation, should be carried out to ensure the accuracy of the simulation. System equilibrium is one of the basic requirements of MD simulations, thus before any MD simulations the ideal or theoretical system needs to evolve on its own to an equilibrium state without any force being applied to it. The process of reaching a stable equilibrium state in an MD simulation is called relaxation. Throughout the simulation, the initial atoms’ configuration is fully relaxed without any constraints, so that the system remains in the equilibrium state with lowest energy. This relaxation process needs 30 ps to achieve its natural balance state.

Fourthly, after the simulations, the system was found to be basically stable when the loading process of concentrated force was set to 150,000 time steps. It should be noted that the concentrated radial force is exerted on each atom and is denoted by $\mathbf{f}$ during the simulation processes, and then the total load $\mathbf{F}$ applied on Region III of the graphene nanoribbon equals $N_L \times \mathbf{f}$, where $N_L$ is the number of atoms in the loading Region III.

Finally, for the convenience of observing the bending experiment process and datum post-processing, the simulation results were set to be output every 100 time steps. The simulation values consist of the system temperature, the system total energy, the system kinetic energy, the system potential energy, the locations of each atom, and the centerline of the graphene nanoribbon, which are the objects of interest for researchers.
III. SIMULATION RESULTS AND ANALYSIS

A. System model during simulation

In order to guarantee the accuracy of the simulation, the double-clamped graphene nanoribbons should be relaxed completely before being affected by the concentrated radial force. Fig. 4(a) shows the system model after full relaxation. It can be found that a certain degree of fluctuations emerge in the unclamped region, which indicates that a single layer graphene nanoribbon is not a perfectly flat structure. The system model during the loading process of bending experiment is shown in Fig. 4(b). It can be observed that the centerline displacement of the graphene film becomes ever larger, and the degree of fluctuation becomes smaller and smaller gradually. Fig. 4(c) gives the system model of the steady state for the bending experiment. At that point in time, the bending deformation of the graphene film is at its largest, and the graphene film is not ruptured. It is obvious that the graphene nanoribbon was stretched as one flat plane, whose deflections at different sites are different from those of bulk materials, especially at the junctions between Region I and Region II. Due to the fact that the thickness is only that of a one-atom layer, the graphene could not bear torque loading, so that the torsion deformation occurred directly, despite its high elastic modulus.

B. Simulation curve

Fig. 5 gives the curves of the MD simulation results with the concentrated load of 0.6 eV/Å. It can be seen that the temperature finally reaches 0.01K in Fig. 5(a); the kinetic energy is close to
FIG. 5. Curves of MD simulation results: concentrated load 0.6 eV/Å.
zero and is directly proportional to the system temperature, as is shown in Fig. 5(b); Fig. 5(c) shows that the total energy and potential energy is so close that the contact ratio between them is very high. Obviously, after a total of about 180,000 time steps of simulation, the temperature, the total energy, potential energy, and kinetic energy of the system all tend to stable values, which indicates that the simulation results have stabilized.

### C. Results and analysis

As one standard 2-D material, the strain energy density of graphene can be represented by the energy per unit area rather than per unit volume Ref. 21. So the corresponding stress and elastic modulus can be expressed as $\sigma^{2D}$ and $E^{2D}$, with the units N/m. The traditional stress and elastic modulus of a 3-D bulk material can be obtained through these 2-D values by dividing each one by the effective thickness, which is always taken to be the layer spacing of the graphite crystal, i.e., 3.35 Å. Similarly, if the values of the 3-D elastic properties were being calculated, the corresponding 2-D stress and elastic modulus can also be obtained Ref. 22.

After MD simulations, different centerline deflection values of graphene nanoribbon were obtained, corresponding to the different concentrated radial loads. Meanwhile, according to Eq. (6), a set of Young’s modulus values were calculated, as shown in Table II, with an average value of 1.034 TPa. It should be pointed out that only if the concentrated force $F$ is no greater than 918.43 nN could the graphene nanoribbon make a complete recovery, that is to say, the graphene nanoribbon undergoes an elastic deformation stage during the bending experiments.

It was found that when the concentrated force $F$ equals 1122.52 nN, the graphene nanoribbons steps into a rupture state with a maximum centerline deflection of 67.5 Å. Thus, the maximum stress of graphene is also obtained as 137.09 GPa from Eq. (7). The values above, including Young’s modulus and the maximum stress, are in good agreement with the experimental results and numerical simulation results of the available literature Refs. 7–11, 14, and 15.

### IV. CONCLUSIONS

After carrying out Molecular Dynamics simulations of a bending experiment on a double-clamped single layer graphene nanoribbon, the mechanical properties of graphene were determined. One physical model was set up for a double-clamped single layer graphene film, and the relation between the centerline deflection and the concentrated force has been derived based on the continuum theory. The Young’s modulus values of graphene with different concentrated force loadings and its maximum stress were determined; the values obtained are consistent with the experimental results. In the future, different aspect ratios of graphene film will be considered in order to study the mechanical properties of graphene.

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