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Molecular dynamics simulation on mechanical property of carbon nanotube torsional deformation*

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In this paper torsional deformation of the carbon nanotubes is simulated by molecular dynamics method. The Brenner potential is used to set up the simulation system. Simulation results show that the carbon nanotubes can bear larger torsional deformation, for the armchair type (10,10) single wall carbon nanotubes, with a yielding phenomenon taking place when the torsional angle is up to 63°(1.1rad). The influence of carbon nanotube helicity in torsional deformation is very small. The shear modulus of single wall carbon nanotubes should be several hundred GPa, not 1 GPa as others reports.

Keywords: carbon nanotube, molecular dynamics, Brenner potential function, torsional deformation

PACC: 6148, 6185, 4630, 0630M

1. Introduction

Since 1991 when Iijima discovered the carbon nanotube using the electricity arc method by chance,[1] carbon nanotubes have found comprehensive application in the foreground of many fields, such as mechanics, materials, electronics, micromanipulation and hydrogen storage, because of their excellent and inimitable characteristics. Especially in the aspect of the nano-mechanical system, the carbon nanotube has exhibited its superiority and tremendous developing perspective in the nano-industry,[2−5] so it has become the focus of research of many specialists.

In a real engineering application process, the torsional deformation of the materials is a hackneyed situation. So research on its torsional mechanical property has very important theoretical meaning and value in use. But since the carbon nanotube is a nanomaterial, its diameter is several nanometres to a few tens of nanometres only, so it is hard to analyse by the traditional experimental methods.[6−11] Up to now, the studies about the torsional property of single wall carbon nanotubes have not been performed in correlative experimental reports. So this paper plans to research into the mechanical property of the carbon nanotube by the molecular dynamics simulation method.

At present, because the Brenner potential which describes the covalent bond function is obtained by experimental method, its main function is to describe the valence-bond structure and characteristics of diamond, graphite and hydrocarbon; especially, it can be used to calculate valence-bond formation and the fracture process between carbon atoms,[8−16] and it is useful to research into the mechanical property of carbon nanotube torsional deformation. In order to further research into the mechanical property of carbon nanotube torsional deformation, based on interactions of C atoms, we use the Brenner semi-empirical potential,[7,17−20] the carbon nanotube acting forces between C–C atoms are deduced in detail for different axial directions. The results we obtained from simulation experimental research of the carbon nanotube torsional deformation are different from others. We think that this experimental result accords with the real carbon nanotube actual torsional deformation process.

2. Computational methods

The calculation of acting forces between atoms is the core of the whole simulation, it takes 90% calculating time, and it is crucial to the correctness and

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veracity of the simulation results. According to this simulation of the molecular dynamics we make use of the Brenner potential function, and the acting forces of the carbon nanotubes between C–C atoms are deduced as follows:

$$F_i = -\sum_{j\neq i} \frac{\partial V_{ij}}{\partial r_{ij}} \cdot \frac{x_i - x_j}{r_{ij}}, \tag{1}$$

where V_{ij} is given by the Brenner potential as

$$V_{ij} = V_{\mathrm{R}}(r_{ij}) - \bar{B}_{ij} V_{\mathrm{A}}(r_{ij}) \tag{2}$$

and r_{ij} is the distance between atoms C_i and C_j, $x_i - x_j$ is the projection of r_{ij}. The force component in the x direction is given by

$$\begin{aligned}\frac{\partial V(r_{ij})}{\partial x_i} = {} & \{f'_{ij} A_1 \exp[-A_2(r_{ij} - R_0)] - f_{ij} A_1 A_2 \exp[-A_2(r_{ij} - R_0)] - f'_{ij} \bar{B}_{ij} A_3 \exp[-A_4(r_{ij} - R_0)] \\ & + f_{ij} \bar{B}_{ij} A_3 A_4 \exp[-A_4(r_{ij} - R_0)]\} \frac{x_i - x_j}{r_{ij}} - f_{ij} A_3 \exp[-A_4(r_{ij} - R_0)] \frac{\partial \bar{B}_{ij}}{\partial x_i},\end{aligned} \tag{3}$$

where $A_1 = D_{\mathrm{CC}}/(S_{\mathrm{CC}} - 1)$, $A_2 = (2S_{\mathrm{CC}})^{1/2}\beta_{\mathrm{CC}}$, $A_3 = D_{\mathrm{CC}} S_{\mathrm{CC}}/(S_{\mathrm{CC}} - 1)$, $A_4 = (2/S_{\mathrm{CC}})^{1/2}\beta_{\mathrm{CC}}$, $f'_{ij}(r_{ij}) = \partial f_{ij}(r_{ij})/\partial r_{ij}$. D_{CC}, S_{CC} and R_0 are parameters, and the function f_{ij}, which restricts the pair potential to nearest neighbours, is given by Brenner's paper[21].

$$\frac{\partial \bar{B}_{ij}}{\partial x_i} = \frac{1}{2}\left(\frac{\partial B_{ij}}{\partial x_i} + \frac{\partial B_{ji}}{\partial x_i}\right) + \frac{\partial f_{ij}}{\partial x_i} (= 0), \tag{4}$$

$$\begin{aligned}\frac{\partial B_{ij}}{\partial x_i} = {} & -\delta_i \left[1 + \sum_{k(\neq i,j)} G_i(\theta_{ijk}) f_{ik}\right]^{-\delta_i - 1} \sum_{k\neq(i,j)} \left\{ f_{ik} \frac{2a_0 c_0^2 (1 + \cos\theta_{ijk})}{[d_0^2 + (1 + \cos\theta_{ijk})^2]^2} \right. \\ & \left. \times \left[\frac{r_{ij}^2 - r_{ik}^2 + r_{jk}^2}{2r_{ij}^2 r_{ik}} \cdot \frac{x_i - x_j}{r_{ij}} + \frac{r_{ik}^2 - r_{ij}^2 + r_{jk}^2}{2r_{ik}^2 r_{ij}} \cdot \frac{x_i - x_k}{r_{ik}}\right] + f'_{ik} G_i(\theta_{ijk}) \frac{x_i - x_k}{r_{ik}} \right\},\end{aligned} \tag{5}$$

where $G_i(\theta_{ijk})$[21] is a function of the angle between bonds $i - j$ and $j - k$. Similarly

$$\frac{\partial B_{ji}}{\partial x_i} = -\delta_j \left[1 + \sum_{k(\neq i,j)} G_j(\theta_{jik}) f_{jk}\right]^{-\delta_j - 1} \sum_{k\neq(i,j)} \left\{ f_{jk} \frac{2a_0 c_0^2 (1 + \cos\theta_{jik})}{[d_0^2 + (1 + \cos\theta_{jik})^2]^2} \cdot \frac{\partial \cos\theta_{jik}}{\partial x_i} \right\}, \tag{6}$$

$$\frac{\partial \cos\theta_{jik}}{\partial x_i} = \frac{r_{ij}^2 - r_{jk}^2 + r_{ik}^2}{2r_{ij}^2 r_{jk}} \cdot \frac{x_i - x_j}{r_{ij}} - \frac{r_{ik}}{r_{ij} r_{jk}} \cdot \frac{x_i - x_k}{r_{ik}}, \tag{7}$$

r_{ij} and r_{jk} are associated through B_{ij}, so the contribution of $\dfrac{\partial V(r_{jk})}{\partial x_i}$ cannot be neglected

$$\frac{\partial V(r_{jk})}{\partial x_i} = -f_{jk} A_3 \exp[-A_4(r_{jk} - R_0)] \frac{\partial \bar{B}_{jk}}{\partial x_i}. \tag{8}$$

The total acting forces of atom i in the x direction is calculated as follows:

$$F_x^i = -\sum_{j\neq i} \frac{\partial V(r_{ij})}{\partial x_i} - \sum_{j\neq i} \sum_{k(\neq i,j)} \frac{\partial V(r_{jk})}{\partial x_i}. \tag{9}$$

The total acting forces of atom i in the y and z direction can be obtained by the same method.

The molecular dynamics stimulation for this torsional experiment can be divided into three steps: initialization, relaxation and imbalanced evolvement. The initialization is to regulate the original condition,

but the requirement for atomic original velocity and position is not too rigid, because the system would lose all the memory of the atomic initial state. The established system during the initialization may not have the desired energy, and it may not correspond to any balance state of the system. In order to drive the system to reach the balance state, a relaxation process would be needed. When it reaches balance state, the external load can be executed on the system to simulate the demanded status. Finally, we can count the macroscopical physical quantity such as force, position and velocity between atoms during the simulating process by analysing all characters of the system.

3. Torsional simulation experiment of the carbon nanotubes

The torsional deformation of the materials is a hackneyed situation. In a nano-mechanical system, such as carbon nanotube AFM tips and nano-cutting-tool etc., the carbon nanotubes have comprehensive foreground application. So research on the characteristics of the carbon nanotubes such as length, compression and torsion has important significance. Due to limitation of the experimental condition, up to now, there is no experimental report about the torsional property of single wall carbon nanotubes (SWNT).

3.1. The model of torsional experiment

In order to analyse status of torsional deformation of the SWNT, two-end-ringent armchair type (10,10) and zigzag type(20,0) SWNT experimental models are established separately in this paper: their atomicity is 1000, the diameter of armchair type (10,10) is 13.58 Å, its length is 60.27 Å, the diameter of zigzag type (20,0) is 15.67 Å, its length is 53.29 Å, the system temperature is 300 K, its calculated model is shown in Fig.1. In Fig.1, the atomic coordinate of the

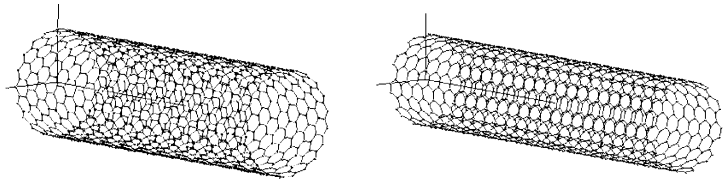


Fig.1. Zigzag and armchair carbon nanotubes images of topological structure.

carbon nanotube is created by geometrical method and arranged according to the perfect crystal lattice structure. The atomic initial velocity is decided by Maxwell distribution at the requested temperature. Velocity calibration is used to incarnate the temperature contribution. Verlet velocity arithmetic is used to calculate the kinetic equation.

During the calculating process, first one-end of the carbon nanotube adopts fixed boundary conditions, its two circles including 40 atoms are fixed, and two circles of another end of the carbon nanotube including 40 atoms are rotated to a small angle (φ) round the sectional centre at a time (see Fig.2). In simulating

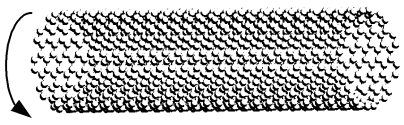


Fig.2. Torsion model of the carbon nanotube.

the experimental process, firstly we make the system up to thermodynamic equilibrium under the given temperature, and this stage has 5000 molecular dynamics time-steps(2.5 ps); after finishing thermodynamic equilibrium, then torsional displacement load is added, the revolution angle is $0.1^\circ(\varphi = 0.1^\circ)$ at a time. After adding a time load, relaxation which has 35 molecular dynamics time-steps proceeds. The torsional angle of the nanotube is 120° in the end of the torsional process.

3.2. Experiment results

Figure 3 is a torsional structure image of the carbon nanotube in the torsional process. From Fig.3 we can see that the torsional process of the carbon nanotube is similar to the torsion of a macroscopical hollow cylinder. When it reaches a definite torsion angle, the tube-body is not columniform any more, and corrugation appears; the more torsion proceeds, the bigger the distortion becomes, and it turns to a screw twisted column, though even in this case, the

C–C bond warps, but it does not rupture; this shows that the stability of C–C bond is very good, it is not easily destroyed. From the whole simulation process, we can know that the carbon nanotube can bear more large torsional deformation.

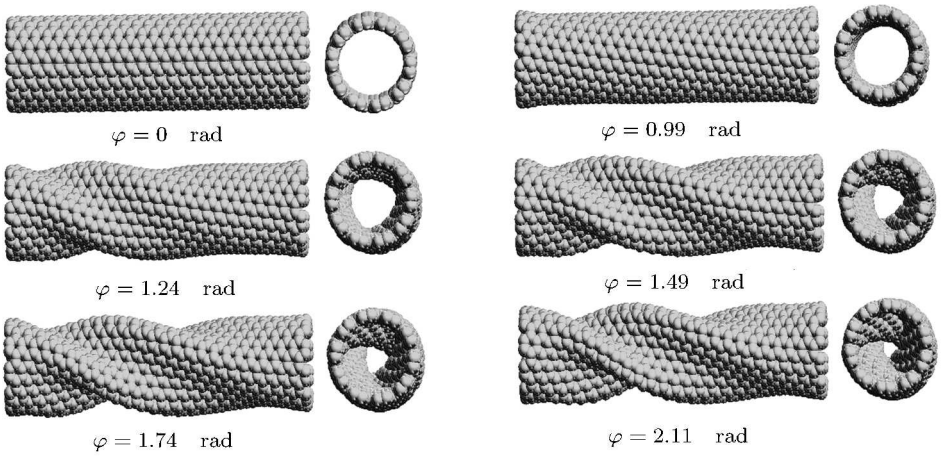


Fig.3. Structure image of torsion with torsion angle change.

In the simulation process the energy change is shown in Fig.4. From Fig.4, we can see that the external

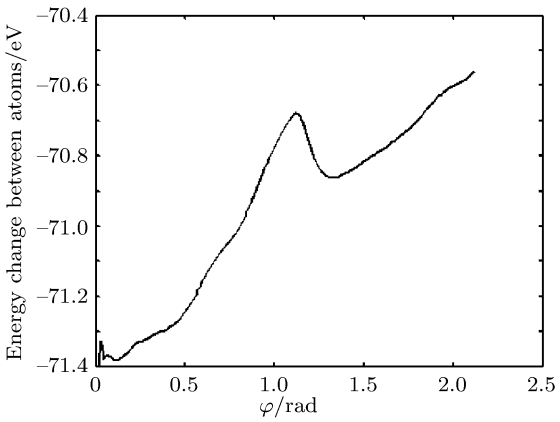


Fig.4. Energy change in torsion in simulation process.

load keeps continual and leads to an increase of energy. When it reaches a definite torsion angle, which is about 63° (1.1rad), it exceeds the range of elastic deformation of the carbon nanotube torsion, and the yielding phenomenon appears; at this time energy begins to release and the carbon nanotube becomes destabilized. Energy increases again with further torsion, that is because carbon nanotube has released accumulative strain energy by the change of the structure, the distortion caused by the torsion is not acute any more, so energy increases again.

The change of radial distribution function (RDF) during the simulation is shown in Fig.5; it shows that the bond-length basically keeps the original size, and also shows that C–C bond does not fracture easily in the torsion process: the curve rises since 2.2 Å, which shows that the bonds are broken at this length. Its mean square displacement curve is shown in Fig.6, the curve all along shows increasing tendency, this shows that the atom makes diffusion movement at all times in the torsional process and it is reasonable.

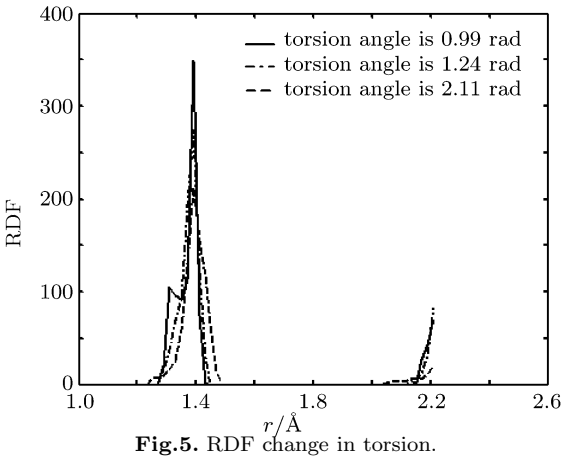


Fig.5. RDF change in torsion.

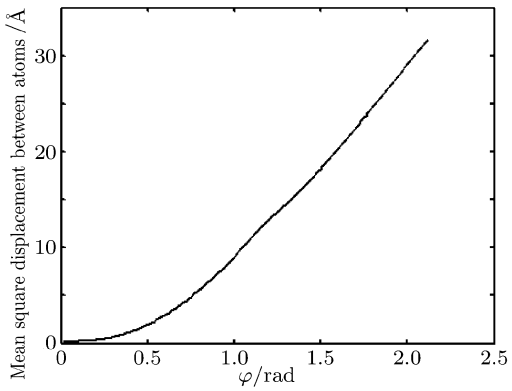


Fig.6. Mean square displacement curve in torsion.

The simulation experimental results show that

the carbon nanotubes can bear prodigious torsional deformation and C–C bond fracture does not occur, we can thus know that the carbon nanotubes have huge ability of anti-torsion.

3.3. Torsion of the different helicity carbon nanotubes

In order to research the influence of the helicity on carbon nanotube torsional deformation, we change the carbon nanotube type into the zigzag type (20,0) model, then proceed with the same relaxation and load process; the structure change in the torsional process is shown in Fig.7. Figure 8 shows the energy change in torsion.

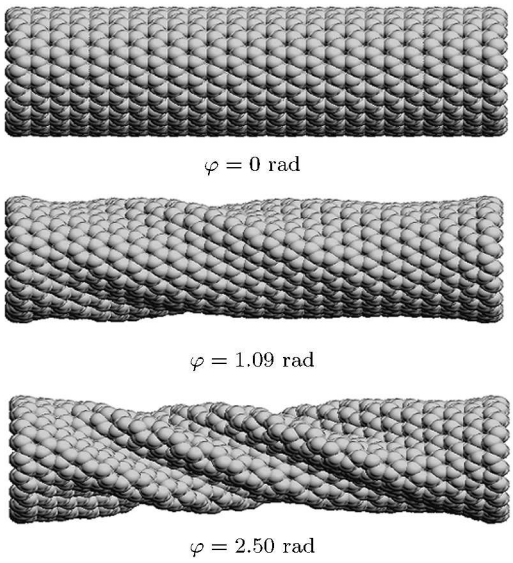


Fig.7. Zigzag structure change in torsion.

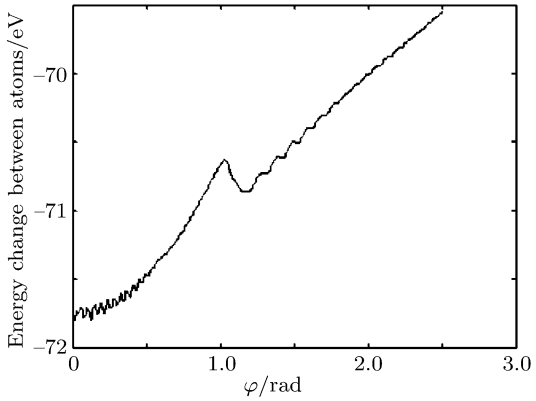


Fig.8. Energy change in torsion.

From Fig.7 we can find that its structure change is similar to that of the armchair type (10,10) model, and from Fig.8 we can see that energy presents a little oscillation during torsional initial stages and oscillation time is a little long, but helicity influence is small, and the yielding phenomenon takes place when the torsional angle is 1.1rad as in the situation of the armchair type (10,10) model. So the helicity influence on carbon nanotubes torsional nature can be neglected.

Computational formula of the carbon nanotube shear modulus G_θ is given as

$$G_\theta = \frac{1}{V_0}\frac{\partial^2 E}{\partial \gamma^2}, \tag{10}$$

where V_0 is equilibrium state volume, the function V_0 is given by

$$V_0 = 2\pi L R \delta R. \tag{11}$$

γ is given by

$$\gamma = \frac{R\varphi}{L}, \tag{12}$$

L is the length and R is the radius of carbon nanotube in equilibrium state, δR is thickness, but there is not unified standards about δR, $\delta R = 0.34\,\text{nm}$ is used in this paper which is the thickness of a graphite layer, E is strain energy, which is the increased system energy calculated by the Brenner potential, γ is shear strain.

According to torsional energy change of the armchair type carbon nanotube, after calculation, we obtain shear modulus of the simulation experiment model $G_\theta = 158.082 \times 1.6 \times 10^{-20}\text{J}/0.0088\,\text{nm}^3 = 287.4\,\text{GPa}$.

Salvetat *et al* used the AFM probe to touch SWNT fasciculus directly,[22] according to the force between the tip of the probe and tube-hank, the length of the carbon tube-hank and bending degree; he obtained Young's modulus of SWNT hank through the calculating method, then according to the relation between tube-hank and a SWNT hank, he obtained the shear modulus 1 GPa. However, the shear modulus is the intensity of comparative slippage of SWNT hank, and it is not shear strength itself; obviously this result is on the low side and unreasonable. With the development of experimental conditions, it will be testified that the shear modulus is about several hundred GPa.

4. Conclusions

Through the above analysis, some conclusions can be drawn as follows.

1) The carbon nanotube can bear great torsional deformation. For the armchair type (10, 10) SWNT, only when its torsional angle reaches 63° (1.1 rad)

does the carbon nanotube generate the yielding phenomenon, its shear modulus is 278.4 GPa at this time.

2) The influence of different helicity of the carbon nanotubes on the torsional deformation is small, and when the torsional angle is about 1.1 rad or larger, destabilization of carbon nanotubes appears.

3) The simulation experiments show that the shear modulus of SWNT should be several hundred GPa, but not 1 GPa as described by some reports.

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