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# Effect of temperature on deformation of carbon nanotube under compression*

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The mechanical behaviour of carbon nanotubes is one of the basic research fields on the nanotube composites and nano machinery. Molecular dynamics is an effective way for investigating the behaviour of nano structure. The compression deformation of carbon nanotubes (CNTs) under different temperature is simulated, by using the Tersoff–Brenner potential to describe the interactions in CNTs. The results show that thermal fluctuations may induce the strained CNT to overcome the local energy barrier and develop the plastic deformation.

**Keywords:** carbon nanotube, molecular dynamics, plastic deformation
**PACC:** 6148, 6185, 5225L, 6220F

## 1. Introduction

Much research has been performed on the nanotube structures concerning their mechanical and electrical properties.[1−4] Due to the special hexagonal structure and $sp^2$ hybridization of C—C bonds, the carbon nanotubes (CNTs) have some outstanding mechanical properties, such as high modulus, extreme flexibility and strength. Therefore, the CNTs have wide application in nano-scale devices and composite materials.

Molecular dynamics (MD) simulations on the axial compression deformation of CNTs have been made by Yakobson.[5] The results show that the CNTs exhibit the super-elastic characteristic up to axial strain as large as 20% without any defects or plastic deformation. However, previous atomistic simulations on this subject were generally conducted at zero temperature, not considering the temperature effect.

Our interest in this paper is the effect of temperature on the mechanical behaviour of CNTs under axial compression and to gain some information about the micro mechanisms of deformation.

## 2. Computational model

MD method is employed to study atomic motion in the objective system, and Newton dynamics function is used to determine the variation of instantaneous location and velocity of each atom. It is the most feasible method to find out the microscopic mechanism of deformation and the intrinsic characteristics of a structure, so in nano-scale, the MD method is widely used in numerical simulation of many physical processes.[6,7] The MD program named WMD is developed on Linux system by us. Carbon atoms are modelled with a classical multi-body Tersoff–Brenner potential which can reliably describe the main features of the mechanism of response of the CNTs.[8] The third-order prediction-correction algorithm is adopted for the kinetic function.[9]

The configuration of SWCNT is denoted by two numbers $(n, m)$ which describe how a graphite sheet rolls up to form CNTs. The (10,10) CNTs are simulated in this paper. The whole computational model includes 820 atoms and the length of the CNT is 4.92nm. The simulation process includes the following steps: the initial configuration is relaxed to reach the equilibrium state. To accomplish the compression, the motion of the last three rings at one end of the tube is restricted and the other end of the tube is shifted along the axis by 0.001nm in each step. The whole simulation process includes 1000 steps. Figure 1 shows the computational model.

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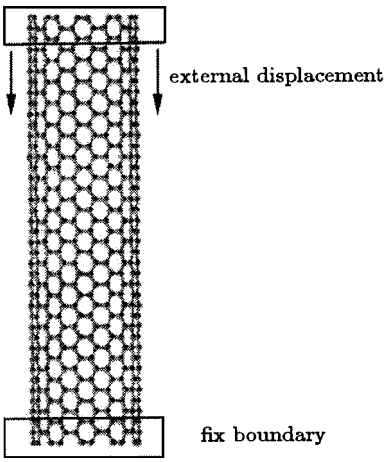



**Fig.1.** Computational model of CNT.

To simulate the mechanical behaviour of the CNT under different temperature, the Nose–Hoover thermostats are adopted to control the temperature during the simulation.[10,11] The idea of the method is to use a generalized variable to express the thermal interaction between the true system and the external heat bath and to set up a new extended system including the true system and the external heat bath. The Hamiltonian of the extended system can be expressed as[10]

$$H = \sum_{i=1}^{N} \frac{\boldsymbol{p}_{\nu i}\boldsymbol{p}_{\nu i}}{2ms^2} + E_{\rm tot} + \frac{\boldsymbol{p}_s^2}{2Q} + gk_{\rm B}T_0 \ln s, \qquad (1)$$

where $Q$, $p_s$ are, respectively, the mass and conjugate momentum of the variable $s$, $g$, $T_0$ and $p_{\nu i}$ are the freedoms of the extended system, the target temperature and the momentum of the particle in the extended system, respectively.

The transformation from the variables of the true system $\{q_i, p_i, {\rm d}t\}$ to those of the extended system $\{q_{\nu i}, p_{\nu i}, {\rm d}t_\nu\}$ is performed according to the following relations

$$\boldsymbol{p}_i = \frac{1}{s}\boldsymbol{p}_{\nu i}, \quad \boldsymbol{q}_i = \boldsymbol{q}_{\nu i}, \quad {\rm d}t = \frac{1}{s}{\rm d}t_\nu.$$

The motion equations of the extended system can be obtained from the Hamiltonian of the extended system

$$\dot{\boldsymbol{q}}_i = \frac{\boldsymbol{p}_i}{m},$$

$$\dot{\boldsymbol{p}}_i = -\frac{\partial E_{\rm tot}}{\partial \boldsymbol{q}_i} - \eta \boldsymbol{p}_i,$$

$$\dot{\eta} = \tau^2 \frac{T(t) - T_0}{T_0}, \qquad (2)$$

$\eta$ being the damping coefficient of the heat bath. The instantaneous temperature of the system is $T(t) = \frac{1}{gk_{\rm B}} \sum_{i=1}^{N} m\dot{\boldsymbol{q}}_i^T \dot{\boldsymbol{q}}_i$. The relaxation coefficient of the heat bath is $\tau = \sqrt{\frac{gk_{\rm B}T_0}{Q}}$.

From the third equation in (2), we can see that if the instantaneous temperature $T(t)$ is higher than the target temperature $T_0$, the $\eta$ will be positive and the velocities of the atoms and the system temperature will descend. Conversely, if the instant temperature $T(t)$ is lower than the target temperature $T_0$, the $\eta$ will be negative and the velocities of the atoms and the system temperature will rise. This feedback mechanism keeps the temperature of the system constant. It is proved that the Nose–Hoover method can produce the true canonical ensemble.[11]

We use the WMD to perform a temperature adjustment test on the computational model of Fig.1. The condition of the temperature is 0, 300, 600, 900, 1200 and 1500K. 5000 steps (equal to 5ps in total) are relaxed at each temperature. The results are shown in Fig.2. As can be seen, the system temperature converges rapidly to the respective target values at each temperature and slightly oscillates around the corresponding temperature.

Using the Nose–Hoover thermostats to control the temperature during the simulation, we perform the MD simulations on the compression deformation of CNTs at 0, 300, 600, 900, 1200 and 1500K, respectively.

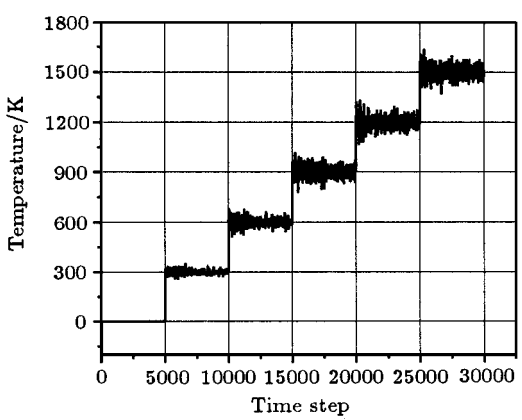



**Fig.2.** The evolution process of the system temperature.

## 3. Computational results

Previous experimental and theoretical research indicates that the CNT have high modulus and extremely high strength.[1,2,5] The atomistic simulations

on this subject are generally conducted at zero temperature. The results show that the CNTs buckle when the axial strain reaches a critical point. More studies indicate that the CNTs would recover their initial configurations after the external mechanical loads are removed and that no plastic deformations or defects are produced in the structure of CNTs even if the axial strain is as large as 15%.[5] The results demonstrate that the non-linear elastic deformation happens after the structure buckles.

Our simulation results also show that the CNTs exhibit super-elastic characteristic up to axial strain as large as 20% at zero temperature without any defects or plastic deformations are produced during the simulation processes. But with the temperature increasing, the axial deformation of the CNTs is not elastic and some structure transformations appear in the severely distorted region, as shown in Fig.3.

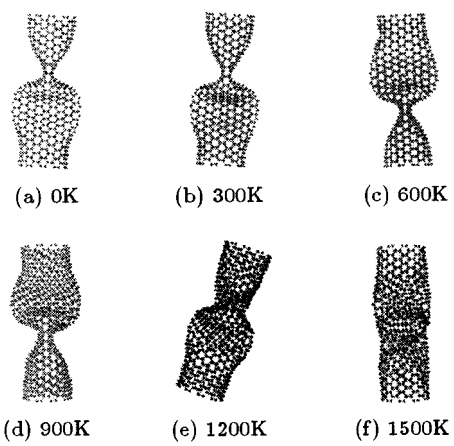



**Fig.3.** Deformation configurations of 12% axially compressed CNTs at different temperature.

The deformed configurations of the CNTs at different temperature are plotted in Fig.3, when the axial strain is 12%. As can be seen, "fins" structure is formed to release strain energy when the CNTs buckle. With the strain increasing, the arrangements of micro structures are different at each temperature. The micro structures at 0, 300 and 600K are more symmetric than those at 1200 and 1500K. The configuration details show that there is no any defects at low temperature, while some $sp^3$ bonds can be found at high temperature, as shown in Fig.4. The variation of structure happened in the largest collapse region at high temperature. The hexagonal micro-unit has been transformed to diamond-like structure.

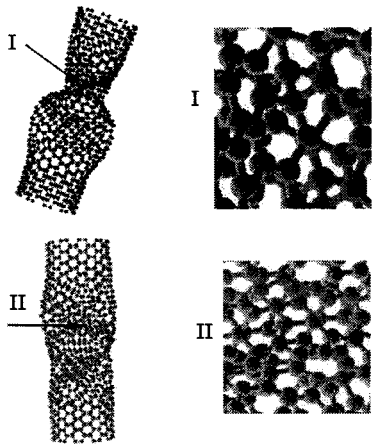



**Fig.4.** Deformation details of 12% axially compressed CNTs, at 1200K (I) and 1500K (II).

The research on the various forms of carbon materials by Saito[12] shows that there is $sp^2$ hybridization of C—C bonds in the structures of graphite and the CNTs. The length of C—C bonds in equilibrium position is 0.140–0.144nm, while in diamond-like structure, the atomic orbit of the C—C bond is in $sp^3$ hybridization and the length of C—C bonds is 0.150–0.160nm. The RDF (radial distribution function) of the CNTs at different temperatures is depicted in Fig.5, when the axial strain is 12%. We can see that there is a peak between 0.150 and 0.160nm at 1200 and 1500K. These distributions show that there is a structure transformation in the axially strained CNTs at high temperatures. From the Figs 4 and 5, we can conclude that the original $sp^2$ bonds transform to $sp^3$ bonds in severely deformed regions and unrecoverable deformations are produced in the collapse regions.

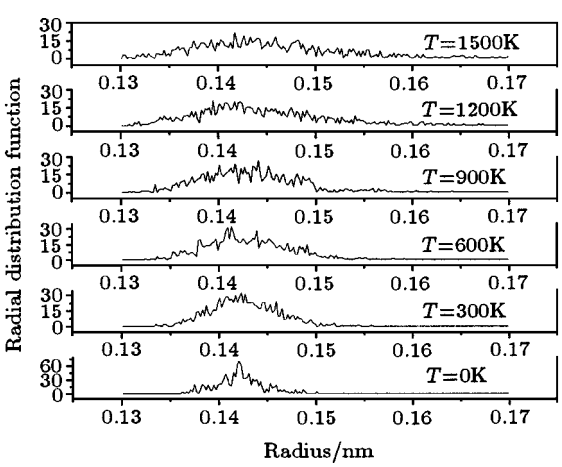



**Fig.5.** The RDF when the axial strain is 12% at different temperature.

According to the theory of statistical mechanics, the temperature leads to the atoms fluctuating around their equilibrium positions. At low temperature, the thermal fluctuation is slight. Even if the structure buckles violently and large non-linear elastic deformation is produced, the atoms cannot overcome the local energy barrier to produce the defects or plastic deformations. At high temperature, the effect of the thermal motion increases significantly, the thermal motion induces the atoms energy to increase so much that the atoms overcome the local energy barrier and the transformation of the local structure leads to the unrecoverable deformation.

Zhang *et al* [13] studied the stability of the CNTs at high temperature under high pressure by experiment, the results show that there was a structure transformation during the process. It also indicates that the thermal motion or temperature have a great effect on the stability and mechanical properties of the CNTs.

# 4. Summary

In this work, we use classical molecular dynamics to study the effect of temperature on the mechanical properties of CNTs under axial compression. At low temperature, the non-linear elastic deformation persists even at the axial strain of 20%. At high temperature, the thermal fluctuation becomes more remarkable and the atoms may have enough energy to overcome the local energy barrier. The $sp^3$ C—C bonds appear in the severely distorted region and the unrecoverable deformation is produced. The results demonstrate that there is a great effect of the temperature on the mechanical properties of CNTs, which is important for the design of nano-reinforced composite materials.

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