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Mechanical properties of carbon nanotube by molecular dynamics simulation

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Abstract

The mechanical properties of single-walled carbon nanotube (SWCNT) are computed and simulated by using molecular dynamics (MD) in this paper. From the MD simulation for an armchair SWCNT whose diameter is 1.2 nm and length is 4.7 nm, we get that its Young modulus is 3.62 TPa, and tensile strength is 9.6 GPa. It is shown that the Young modulus and tensile strength of armchair SWCNTs are $1 \sim 2$ order higher than those of ordinary metal materials. Therefore we can draw a conclusion that carbon nanotubes (CNT) belong to a particular material with excellent mechanical properties.

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Keywords: Carbon nanotube; Molecular dynamics; Young modulus

1. Introduction

Since their initial discovery in 1991 by S. Iijima in NEC Corporation of Japan [1], the carbon nanotubes (CNTs) have got a lot of attention because of their unique optical, electronic and mechanical properties. Carbon is unique among the elements in its ability to create a wide-variety of network-like structures termed fullerene. From the present research status CNT materials have been expected to carry out the first wide-spreading industrial applications in the near future.

CNTs have a lot of potential applications including nanowires, nano-electronic devices and high-strength materials. The important problem in current research is the growth process of aligned CNT arrays. So the growth mechanism of CNT should be studied for solving growth process problem of various types of CNTs.

At present the single-walled CNT (SWCNT) and multi-walled CNT (MWCNT) have been successfully prepared and the process control to the radius, length, spirality and shell numbers of CNTs have achieved much progress. CNT has a lot of tempting properties, e.g., it has been approved by theory and experiments that CNT's Young modulus is very high [2], and the electrical property is varies with its diameter and helicity [3]. CNTs have been applied in many aspects, such as field emission, electronic switches, high-Tc superconductivity materials and so on.

Many properties of CNTs have not been satisfactorily explained by existing theories. We carried out computer simulation to CNTs by using

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molecular mechanics and molecular dynamics (MD) methods to give a quantitative analysis.

CNTs belong to mesoscopic material. We cannot get the reasonable results from the computer simulation if conventional continuum medium model is adopted. So atomic model should be used. In the computer simulation with atomic model, the involved objects can be considered as a congeries of invidious atoms, and each atom is an independent research unit. The atomic simulation method here we used is so called MD.

2. Molecular dynamics simulation method

MD method is employed to study atom motion in objective system, and Newton dynamics function is used to determine the variation of instantaneous location and velocity of each atom. The energy calculation and force analysis are then carried out to get the atom distribution at different thermodynamics state. In another words, the simulation process is setting up the properiate interatomics potential function and making the system to reach energy minimized state after calculation.

The principle of MD method is to calculate Hamilton dynamics equations applied to every atom:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \qquad \dot{q}_i = -\frac{\partial H}{\partial p_i}, \tag{1}$$

where q_i denotes component of coordinate, $\dot{q}_i$ denotes conjugate momentum, the dot denotes the derivative to time, and H denotes the classical Hamilton component which consists of kinetic energy and potentials. MD simulation is usually carried out in Cartesian coordinates, and this can simplify the calculation to a great extent. The initial conditions of MD simulation are the coordinates and momentum (velocity) of atoms. The atom locations are usually set to the equilibrium value, and the momentum is selected to satisfy the condition of initial temperature. The simulation process to CNTs using MD can be divided to four sections: the determination of initial locations and velocity of carbon atoms; the evolution of equilibrium state; the loop for adding new atoms and evolution; analysis and calculation.

3. Simulation of CNTs using MD method

The selection of potential function is a key factor which determinates the results' accuracy in MD simulation. The interaction between atoms in CNTs is bonding instead of van der Waals force, which is quite different from MD using in molecular biology. So we choose Brenner function to describe the bonding interaction of atoms in CNTs [4]. The Brenner function can exactly describe the bonding structure and properties of graphite, diamond and hydrocarbon molecular. What is more, it correctly reflects the construction and destruction of bonding interaction between atoms, and is favorable to study the growth of CNTs.

Since the determination of parameters in Brenner function for CNTs is very complicated, the multi-body potential function of embedded atom method (EAM) is employed to calculate CNTs which is put forward by Finnis. The potential function is described as follows:

$$U = \frac{1}{2}\sum_i \sum_j u(R_{ij}) - \sum_i f\left(\sum_j a\phi(R_{ij})\right), \tag{2}$$

where $u(R)$ denotes bi-body potential and f, ϕ denote multi-body potential.

The molecular interaction between different CNTs can be expressed by many kinds of force field functions, for example, Lennard-Jones (6, 12) function in which parameters are extracted from the experimental data of C60 and graphite [5]; Buckingham (exp + 6) plus electrostatic interactions in which parameters are extracted from energy and structure of benzene dimer [6]. We carried out the MD simulation to C60 and CNTs and testified whether these force field functions are correct or not. The values of minimized energy and C–C bond length are adopted from C60 and CNTs in Ref. [7].

The topography of SWCNT is denoted by two numbers (n, m) which describe how graphite sheets roll up to form CNTs. The SWCNT with $n \neq 0$

but $m = 0$ is named zigzag CNT, $n = m$ named armchair CNT, and the others are named chiral CNT. The electric properties of SWCNT are strongly dependent on its topography. The research shows that if $n - m$ is times of three then CNTs present metal conductivity, otherwise present semiconductor conductivity.

In classical mechanics the Young modulus is defined as:

$$Y = -\frac{1}{V_0}\frac{\partial^2 E}{\partial \epsilon^2}, \tag{3}$$

where V_0 is equilibrium volume, E is strain energy, and ϵ is axial strain. For a SWCNT, equilibrium volume can be defined as the volume of hollow cylinder:

$$V_0 = 2\pi LR\delta R, \tag{4}$$

where L stands for the length of CNT, R for radius, and δR for thickness. In previous research the thickness of CNT has lots of forms. We defined the thickness of CNT shell as follows in our research:

$$\delta R = 0.34 \text{ nm}.$$

For a MWCNT the thickness of CNT shell can be defined as the product of δR and shell layers.

The round cross-section armchair (n, n) SWCNT is studied. After putting some pressure on CNT in axial direction and calculating the variation of total potential and length, we can get the qualitative results of SWCNT's Young modulus. Here we suppose carbon atoms are randomly added to the whole CNT simulation system with random initial locations and velocities, then the whole system is in MD evolution, thus the CNT's growth process can be simulated.

The energy minimization is carried out for the armchair SWCNT, and MD simulation is carried out for energy optimized structure. Fourth-order prediction–correction algorithm is adopted for kinetic function, and the time step is 5 fs. The rotational momentum should be subtracted from atoms' momentum when determining thermodynamics temperature of CNT system. The calculation is carried out on a single-CPU PC.

4. Architecture of MDSim

The MD simulation software named MDSim is developed on Sun SPARC station 20/Solaris 2.6 system by ourselves, and has the characteristics of source level portability on Solaris/Linux/FreeBSD/Windows NT platforms. MDSim software consists of four modules: forend data generation (DataGen), simulation and evolution (SimEvol), backend statistics and processing (DataStat) and data inspection (Inspect). From the simulation results of Young modulus for SWCNTs, it can be seen that MDSim can satisfy the requirement of CNT simulation. Now MDSim software is under further development.

The dataflow chart of MDSim is presented in Fig. 1.

The format of the simulated object's topography parameter file and coordinate parameter file are the same among four modules of MDSim for convenience of data exchange. The function of DataGen is to generate the topography structure and force field parameters of CNT according to the given structure parameters; the function of DataStat is to calculate the variation of structures during simulation process, and to calculate thermodynamics parameters according to the output data by SimEvol when the simulation process was finished; the function of Inspect is to visualize the simulated objects according to the topography structures and coordinate parameters in every modules.

The core module in MDSim is SimEvol. Its main function is to do simulation and evolution work according to the topography structures, coordinate parameters and force field parameters. The flowchart of SimEvol is given in Fig. 2.

The thermodynamics parameters, such as total energy of system, temperature or pressure etc., should be monitored in simulation process.

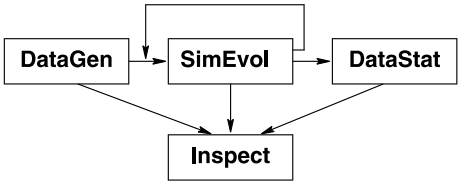

Fig. 1. Dataflow chart of MDSim.

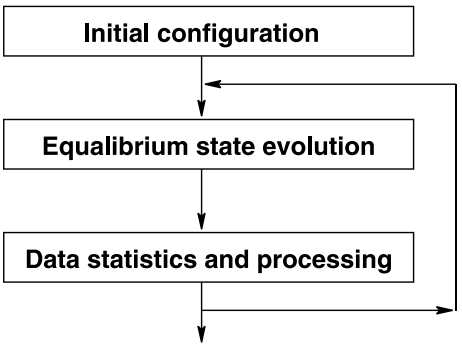

Fig. 2. Main process flowchart of SimEvol.

In development of MDSim, several techniques were adopted to ensure the maximum portability between different platforms. C/C++ languages were used as they have implementations at a lot of hardware and OS platforms. We use GNU's Gtk + 1.2 to do 2D graph and graphical interface design because it is free for use and its easier portability. OpenGL/MesaGL was used for 3D graph and MPI 1.1 was adopted for parallel programming.

5. Results

We do a MD simulation to the armchair SWCNT and compute its Young modulus. The simulated object is illustrated in Fig. 3.

The simulated CNT's diameter is 1.204 nm and length is 4.747 nm. Simulation process is carried out on Redhat 6.2 system with single Intel Celeron 566 CPU. The simulation time step is 5×10^{-3} ps, and total simulation time is 5 ps, the actual CPU time is 576.86 s.

The variation of total energy and temperature is presented in Figs. 4 and 5.

The simulation results show that the simulated CNT's Young modulus is 3.62 TPa and tensile strength is 9.6 GPa. These numerical results are larger than the experimental data in [8] (Young modulus is 0.45 TPa, and tensile strength is 3.6 GPa), we think the difference can be explained by the following reasons:

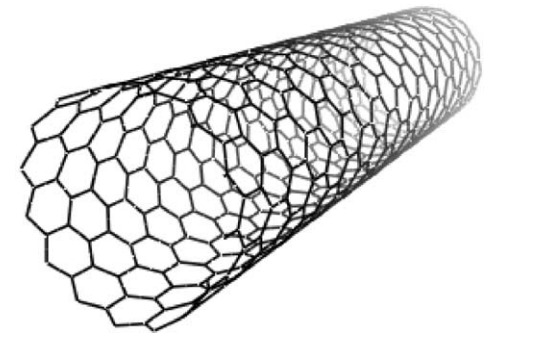

Fig. 3. Topography of the simulated single-walled CNT.

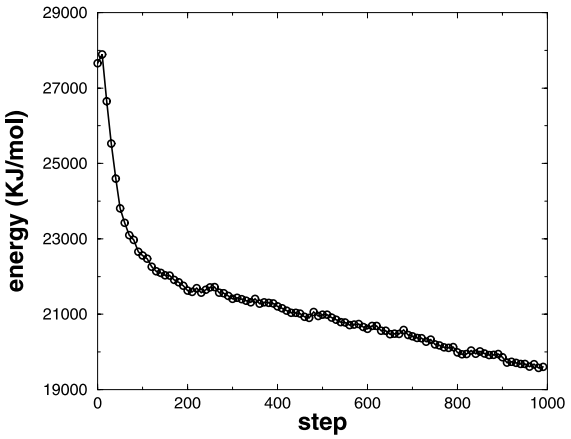

Fig. 4. Total energy variation in simulation process.

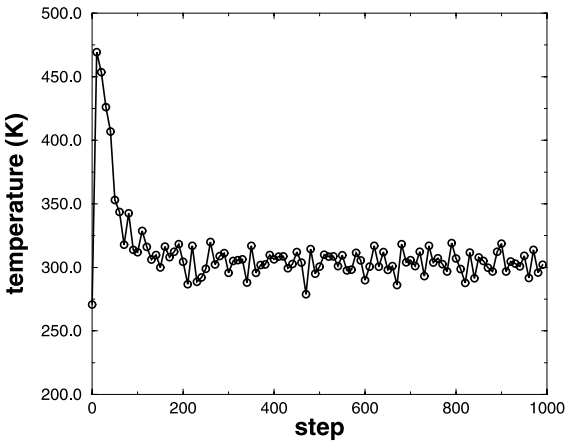

Fig. 5. Temperature variation in simulation process.

- Difference of structure: the CNT in [8] is MWCNT.
- Difference of size: the CNT in [8] is 20 μm in diameter and 1.95 mm in total length, the free length is 0.92 mm.
- The system error of force field physical model.

6. Summary

In this paper the mechanical properties of single-walled nanotubes are analyzed and computed using MD method. The interatomic potential function is Brenner function and improved EAM function. After the MD simulation to an armchair SWCNT with diameter 1.2 nm and length 4.7 nm, the results show that Young modulus is 3.62 TPa and tensile strength is 9.6 GPa. These values are larger than experimental data presented in reference. The authors considered that the difference is mainly made by structure difference and the system error of force field model. The simulation results show that the Young's modulus and tensile strength of the armchair SWCNT is $1 \sim 2$ order higher than those of ordinary metal materials. Therefore CNT's mechanical properties are very good and it is expected that CNTs can be widely used in the future.

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References

[1] S. Iijima, Nature 354 (1991) 56–58.
[2] A. Thess, R. Lee, et al., Science 273 (2000) 483–487.
[3] Thomas W. Ebbesen, Phys. Today, June 27, 1996.
[4] D.W. Brenner, Phys. Rev. B 42 (1990) 9458.
[5] L.A. Girifalco, Phys. Chem. 96 (1992) 858.
[6] G.D. Smith, R. Jaffe, Phys. Chem. 100 (1996) 9624.
[7] D.W. Brenner, J.W. Mintmire, Phys. Rev. B 45 (1992) 12592.
[8] S.S. Xi, W.Z. Li, et al., J. Phys. Chem. Solids 61 (2000) 1153–1158.