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Fracture and defect evolution in carbon nanocoil – A molecular dynamics study

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ABSTRACT

This paper investigates the mechanical properties of carbon nanocoils with use of the molecular dynamics method. Based on the positions of heptagon defects, the atomistic models of four carbon nanocoils, which are isomeric to each other, are established. The Brenner-II empirical potential is used to simulate the deformation and defect evolution processes of these carbon nanocoils under an uniaxial tensile load. It is found that the ductility of the carbon nanocoils is highly dependent on the position and direction of the defects. A specific kind of carbon nanocoil structure with higher ductility is also revealed through molecular dynamics simulations.

1. Introduction

Spiral structure is one of the basic structural forms of materials and exists extensively in nature such as grapevine, shell, protein and DNA. As one of the materials with spiral structures, carbon nanocoil (CNC) has found wide applications in numerous engineering fields, for example, super strong fibers, mass sensor, field emission device, nano-mechanical and electromagnetic devices, because of its excellent mechanical and electric properties arising from its distinctive spiral structural form [1–6].

CNC was first synthesized with use of the thermal chemical vapor deposition (CVD) technique in 1990 [7]. Since then its special structure and unique electric properties have attracted a lot of research attention. Motojima and his coworkers [8–11] discussed how to improve the yield of CNC through using the external electromagnetic field and bias voltage. Nakayama et al. revealed that metal catalyst such as Co, Fe, Ni or Sn–Fe alloy and Fe–Ni + TiO_2 alloy play a very important role in affecting the CNC production rate and yield [12–19]. Under lab production conditions, the CNC synthesis is controllable and its quality and output is satisfactory. Now, one can synthesize the CNC with diameters ranging from 10 nm to 100 nm in the lab environment [8].

Mechanical property is one of the important factors that must be considered for the engineering applications of nanostructures. There are numerous experimental studies on the mechanical properties of CNCs. Hayashida et al. [20] pointed out that the maximum nominal elongation rate of CNCs can reach 200% and it was estimated that the corresponding elastic spring constants and the Young's modulus are ranging from 0.01 N/m to 0.6 N/m and from 0.04 TPa to 0.13 TPa, respectively, prior to complete rupture. Moreover, based on the measurement data obtained from the force modulation microscopy (FMM), Volodin et al. [21–26] estimated that the Young modulus of the coiled multi-walled nanotube (MWNT) can reach a value of 0.7 TPa. Meanwhile, the mechanical properties of CNCs have also been investigated intensively by molecular dynamics (MD) simulations [27–33].

Compared with straight carbon nanotubes (CNTs), the distinctive feature of CNCs is that unavoidable natural topological defects always exist on CNCs. Previous researches showed that the existence of these defects and their evolutions under external loads may have a profound influence on the mechanical properties of nanostructures such as stiffness, tensile strength and ductility, just to name a few [34–45]. In CNC, heptagonal and pentagonal topological defects are prevalent. The existence of these defects on the one hand may trigger the concentration of stress on CNCs which may lead to the reduction of their strength, on the other hand the kink motion of the defects caused by the dislocation gliding and climbing will also improve the ductility of CNCs.

Although a lot of researches have been conducted on the mechanical properties of nanostructures with topological defects such as straight and Y-junction CNTs, relatively few studies can be found in the literature related to the influence of defects on the mechanical properties of CNCs. Moreover, it remains unclear how the evolution of the defects in CNC will affect its strength or ductility.

This paper aims at investigating the mechanical properties of CNCs with use of the molecular dynamics method based on four

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types of nanocoil models. The Brenner-II empirical potential [46] is used to simulate the deformation and defect evolution processes of these CNCs under an uniaxial tensile load. It is found that the ductility of the carbon nanocoils is highly dependent on the position and direction of the defects. A specific kind of CNC structure with higher ductility is also revealed through molecular dynamics simulations.

2. Computational model and method

The geometric sketch of a spring-like CNC is shown in Fig. 1. The inner and outer diameters of the CNC are defined as D_2 and D_1 respectively. The diameter of the CNC is d and pitch of the coil is H. In Fig. 1, L_c and L_t represent the axis of the coil and the axis of the tube, respectively.

Actually, a CNC can be viewed as a straight carbon nanotube with topological defects. Its negative curvature is induced by the heptagon defects on its inner side and the positive curvature is induced by the pentagon defects on its outer side. Based on the positions of heptagon defects relative to the axis of the coil, four types of atomistic models of CNCs, named as V-arm, V-zig, N-arm and N-zig, respectively, are established as shown in Fig. 2. The corresponding geometric parameters are listed in Table 1. To be more specific, in the so-called V-arm CNC, the corresponding heptagons above and below the tube axis are patterned in a V-shape and linked by a C–C bond. In the so-called V-zig CNC, the corresponding heptagons above and below the tube axis are also patterned in a V-shape and but linked by a hexagon. In the so-called N-arm and N-zig CNCs, however, the corresponding heptagons are all patterned in a N-shape but linked by a C–C bond and a hexagon, respectively. These four types of CNCs can be viewed as isomers.

In the present paper, the mechanical behavior and defect evolutions on different types of CNCs will be investigated. In one unit cell using for simulation, there are 10 heptagons and 10 pentagons. There are totally 360 carbon atoms in the unit cell of V-arm, V-zig and N-arm CNCs used for MD simulation. While for the N-zig CNC, we have 350 atoms in the unit cell.

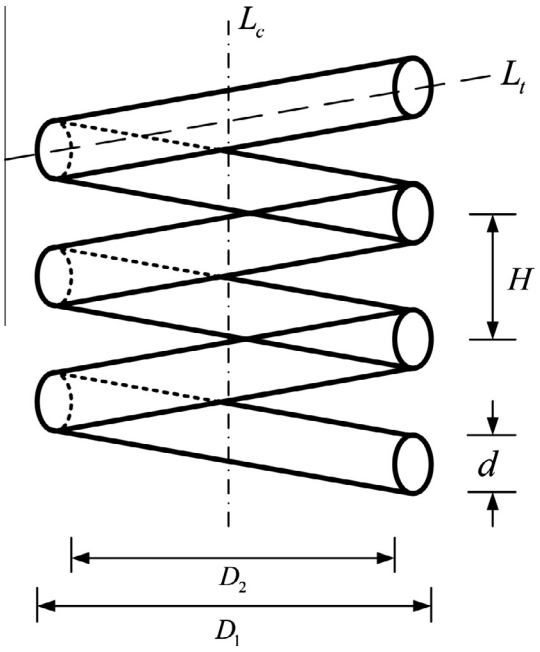

Fig. 1. A schematic illustration of a CNC.

In the present work, all MD simulations are performed using the GULP program in Material Studio package. First, MD simulations for a set of straight SWCNTs were carried out in order to calibrate the MD simulations results. Our simulation results indicate that the Young's modulus of SWCNTs is about 0.8 TPa, which is in reasonable agreement with the values reported in the literature [47–49].

Full geometry optimizations at 300 K without any constraints are first performed to obtain the totally relaxed initial configurations of CNCs. The lengths corresponding to the minimum energy configurations are adopted as the initial lengths of the simulated CNCs. Once the initial configurations are determined, axial tensile strains are gradually applied to one ends of CNCs by prescribing the displacements on the atoms at the end while keep the atoms at the other ends fixed. Under each prescribed tensile strain, the systems are fully relaxed and the corresponding potential energies of the CNC systems are calculated. The time step of all MD simulations is taken as 0.5 fs in order to represent a quasi-static loading process and the total simulation time is 50 ps for each simulated cases. In order to test the sensitivities of the obtained results with respect to the adopted simulation parameters, MD simulations are also performed with use of different loading rates and relaxation time, it is found that the corresponding simulation results are almost the same.

3. Simulation results and discussions

MD simulations are carried out under prescribed tensile strains for the afore-mentioned four types of CNCs, respectively, at 300 K. The average potential energy (per atom) of the system E_{ps} is calculated for comparison purpose. In the present study, the strain is measured as $\varepsilon = (l - l_0)/l_0$ with l_0 and l denoting the length of a CNC before and after the prescribed deformation, respectively.

3.1. Elastic deformation

MD simulations reveal that as in the case of straight SWCNTs and Y-junction SWCNTS [50–52], the deformation of a CNC typically undergo two distinct stages when the prescribed tensile strain is increased as shown in Fig. 3. The first stage is actually elastic in nature and is mainly mediated by C–C bonds elongations. There is no dislocation nucleation and structural transformation occurring at this stage. Accordingly, the potential energy E_{ps} exhibits approximately a quadratic dependence on the prescribed strain. When the prescribed strain is beyond a critical value ε_e, the deformation goes into the plastic stage. In this stage, some C–C bonds in the CNC break first (accompanied by potential energy releasing) and then reconstruct into some local stable structures. Once the local stable structures formed, the CNC system is stiffened again and begins to absorb the energy until the next bond breaking event occurs. This process will repeat again and again until ε reaches the value of ε_f at which the CNC breaks. This also explains the saw tooth behavior of the potential energy-strain curve in Fig. 3 when $\varepsilon > \varepsilon_e$. Table 2 gives the elastic limit strains (i.e., ε_e) and the elastic coefficients of four types of CNCs, respectively.

3.2. Plastic deformation and defect evolution

Fig. 3 shows the potential energy as a function of the tensile strain of V-arm CNC at 300 K. Herein and after, the number-marked points on the potential energy curve indicate the instants where topological changes of structure occur. From Fig. 3, it can be observed clearly that there are essentially four stages (identified as A, B, C and D, respectively) during the whole process of