Fracture of Vacancy-defected Carbon Nanotubes and Their Embedded Composites

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ABSTRACT

In this paper, we investigate effects of vacancy defects on fracture of carbon nanotubes and carbon nanotube/aluminum composites. Our studies show that even a one-atom vacancy defect can dramatically reduce the failure stresses and strains of carbon nanotubes. Consequently, nanocomposites, in which vacancy-defected nanotubes are embedded, exhibits different characteristics from those, in which pristine nanotubes are embedded. It has been found that defected nanotubes with a small volume fraction cannot reinforce but instead weaken nanocomposite materials. Although a large volume fraction of defected nanotubes can slightly increase the failure stresses of nanocomposites, the failure strains of nanocomposites are always decreased. At last, we investigate the effects of randomly distributed vacancy defects on fracture of nanotubes. A spatial Poisson point process is employed to randomly locate vacancy defects on nanotubes.

Keywords: carbon nanotubes, nanocomposites, fracture, vacancy, random

1 INTRODUCTION

It is known that carbon nanotubes (CNTs) have large tensile modulus [1] and high thermal conductivity [3]. The Young's moduli of CNTs are around 1 Tpa and their thermal conductivity can be 6600 W/m K. On the other hand, CNTs are expected to have high strength. Previous theoretical analyses and numerical simulations predicted failure strengths of up to 300 Gpa for CNTs [3]. Consequently, they have been proposed as ideal fibers for the manufacture of the next generation of composite materials with mechanical and thermal management applications [4]. However, low failure stresses, which are in the range of 21 Gpa to 63 Gpa, were observed in the experiments [5]. Such observation conflicted with theoretical and numerical analyses outcomes.

Some researchers have pointed out the significant effects of vacancy defects on nanotube fracture. Vacancy defects, i.e., defects resulting from missing carbon atoms, are likely candidates to severely reduce the strength of CNTs. Such defects could be caused by ion irradiation, absorption of electrons, or CNT fabrication processes. At the nanoscale, the number and locations of vacancy defects, and even the type of the defects, are not deterministic variables, and their randomness is induced by CNT growth procedures, oxidative purification process, or surrounding temperatures. In this paper, we employ molecular dynamics to study mechanics of vacancy-defected nanotubes and their embedded nanocomposites. CNTs with randomly-located vacancy defects will be also considered.

2 MECHANICS OF VACANCY-DEFECTED NANOTUBES

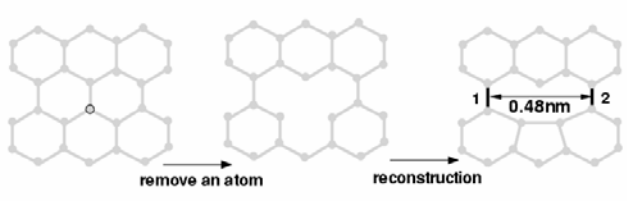

Figure 1. One-atom vacancy defect in a zigzag nanotube

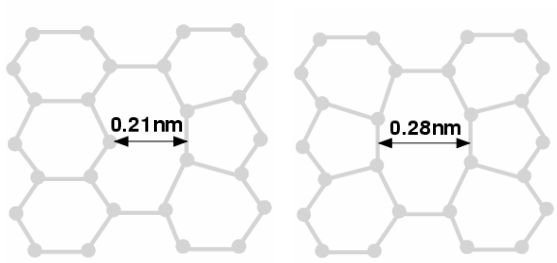

Figure 2. One-atom (left) and two-atom (right) vacancy defects in an armchair nanotube

In this section, we assume that vacancy defects are present in the middle of CNTs. The vacancy defects are modeled by taking out atoms and then reconstructing bonds. If a single atom is removed from a zigzag tube, a 12-membered ring exists. Such a ring can be reconstructed to a pentagon and an enneagon as shown in Figure 1. This configuration is identical to the symmetric configuration defined in [6]. Although there are other possible configurations, the asymmetric configurations, during the reconstruction, we use the symmetric one because it results in a lower potential. The one-atom vacancy-defected nanotube, shown in Figure 1, can be viewed as the nanotube containing an initial crack. The crack length, which is the distance between bonds 1 and 2, is 0.48nm. Here, we neglect the curvature effect of nanotubes.

Similarly, longer crack with more missing atoms can be defined. Initial cracks due to vacancy defects in armchair nanotubes are shown in Figure 2.

We study size effect of vacancy defects on nanotube fracture at the room temperature of 300K. Initial cracks with various lengths up to 2nm are considered. Figure 3 compares failure stresses of (40,0) vacancy-defected zigzag nanotubes and those of (23,23) vacancy-defected armchair nanotubes. Both (40,0) zigzag nanotubes and (23,23) armchair nanotubes have the similar length and diameter. We can see that the pristine armchair nanotube has a higher failure stress than the pristine zigzag nanotube. Belytschko and his co-workers [7] also gave the same conclusion. Furthermore, vacancy-defected armchair nanotubes have higher failure stresses than vacancy-defected zigzag nanotubes if the initial crack lengths are the same. The exception is that when the initial crack length is 0.48nm, failure stresses are the same for both armchair and zigzag tubes. Such phenomenon can be observed at various temperatures. This is because fracture of zigzag nanotubes is mode I fracture while most of armchairs have mixed mode I/II fracture. However, when the initial crack length is 0.48nm there is mode I fracture observed on the armchair tube.

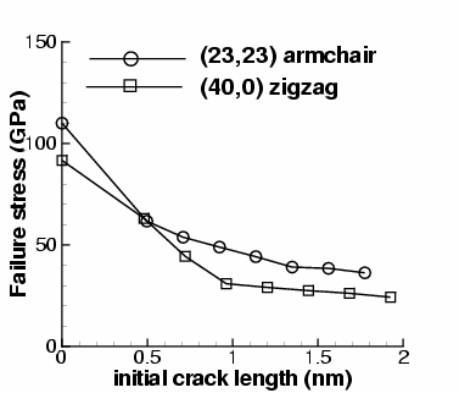

Figure 3. Failure stresses of defected nanotubes at 300K

3 MECHANICS OF NANOTUBE-BASED COMPOSITES

In this paper, we also investigate aluminum-based nanocomposites in that long continuous CNTs are embedded with uniform alignment and homogeneous distribution. A unit cell model of aluminum nanocomposites with periodic boundary conditions is studied. The volume fraction of a carbon nanotube in the nanocomposite is 20%. The prescribed displacement is applied along the axial direction of the nanotube to investigate fracture of nanocomposites. Both the pristine tube and the defected tube with a two-atom vacancy are considered. Nonbonded interaction is between CNTs and the aluminum matrix.

Figure 4 shows the failure stresses/strain of nanocomposites compared with those of aluminum (Al) crystalline at various temperatures. High temperatures result in low strengths. It also can be seen that the pristine nanotube can enhance the strength of nanocomposites to 200% of that of Al crystalline. However, if the defected tubes with a two-atom vacancy are employed as inclusions, the enhancement of nanocomposite strength is only 25%, as illustrated in Figure 4(a). The above phenomenon is due to the fact that defected nanotubes have much lower strengths than pristine nanotubes. Consequently, the enhancement of vacancy-defected tubes as inclusions on the reinforcement of nanocomposites is not as significant as those of pristine tubes.

An interesting phenomenon can be observed in Figure 4(b), which compares failure strains of Al crystalline and CNT/Al nanocomposites. It can be seen that pristine CNTs can improve failure strains of nanocomposites but the defected CNTs decrease failure strains of nanocomposites even though the strengths are improved. Such phenomenon occurs because Al crystalline has a failure strain lower than a pristine CNT but higher than a defected tube.

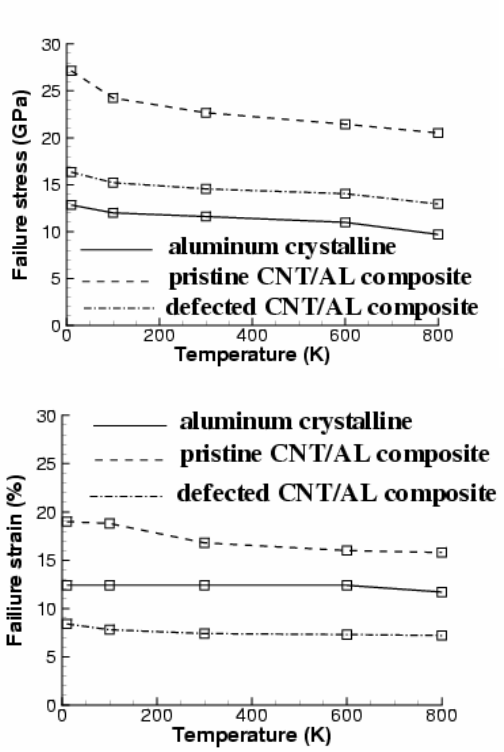

Figure 4. Comparison of failure stresses (top) and failure strains (bottom)

If various volume fractions of nanotubes are considered, defected nanotubes will result in different characteristics. The effects of volume fraction of embedded nanotubes on strength of CNT/Al nanocomposites are illustrated in Figure 5. If pristine nanotubes are embedded, lower strength of CNT/AL is calculated for smaller volume fraction of nanotubes. The nanocomposite strength is similar to the strength of aluminum crystalline when the volume fraction is less than 5%. As well, an interesting

phenomenon when defected nanotubes are embedded is observed. When the volume fraction of defected nanotubes is less than 15%, it can be seen that nanotubes cannot reinforce but instead weaken CNT/Al composites. We think this phenomenon is due to the different roles of failure stress and strain of defected nanotubes in nanocomposites.

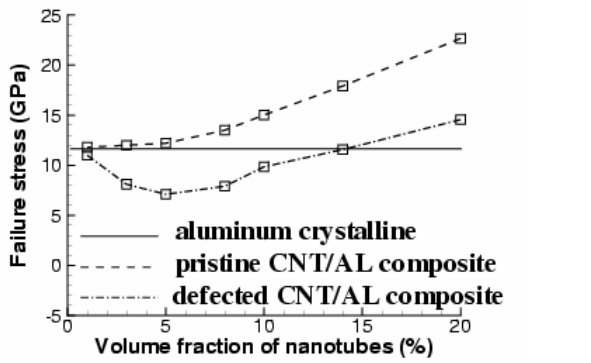

Figure 5. Effects of volume fraction on strength of CNT/Al composites

4 MECHANCIS OF NANOTUBES WITH RANDOMLY LOCATED VACANCIES

In this paper, we consider two uncertainties associated with vacancy defects on nanotubes. One is the number of missing atoms and the other is the location of a vacancy defect. Due to the unique structures of single-walled carbon nanotubes, they can be mapped onto two-dimensional (2D) graphene planes with a thickness of 0.34nm. Consequently, a 3D model can be simplified as a 2D surface problem when considering vacancy defects on nanotubes. On the other hand, since vacancy defects occur on carbon nanotubes in a completely random manner, we employ a homogeneous Poisson point process to determine the occurrence probability of a specified number of Poisson points, i.e. missing atoms in this paper, via

$$P\left(N(A)=k\right)=\frac{e^{-\lambda A}(\lambda A)^k}{k!},\ k=1,2,3\ldots \qquad (1)$$

where A is the plane area; $N(A)$ is the number of Poisson points (missing atoms) on this area A; and λ is the Poisson point density (missing atom density) per area.

For a given number of Poisson points, they are deposed on a two-dimensional graphene sheet, to which the considered nanotube can be mapped, at random positions. We mark the carbon atoms, which are the nearest ones to the Poisson points, as the missing atoms. After taking out the missing atoms, we perform bond reconstruction to generate one-atom, two-atom, and/or cluster-atom vacancy defects. Even for the same number of missing atoms, the numbers and locations of vacancy defects can be various from case to case. For example, a vacancy-defected nanotube in Figure 6 contains two one-atom vacancies, one two-atom vacancies and one cluster-atom vacancy on one side.

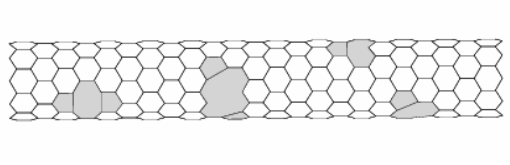

Figure 6. A (10,0) nanotube with randomly-located vacancy defects

The relations between the failure stress and the missing atom density are illustrated in Figure 7 for both (10,0) nanotubes and (6,6) nanotubes. For any given missing atom density, 100 simulations are conducted to calculate the mean value and stand deviation of failure stresses. Since the missing atom density determines the average volume fraction of vacancy defects, Figure 7 also indicates the effect of volume fraction of vacancy defects on nanotube fracture. It has been predicted that pristine zigzag nanotubes have a failure stress of 90 GPa while pristine armchair nanotubes have a failure stress of 110GPa [7]. Figure 7 shows that even a small average volume fraction of 0.2% (the missing atom density is 0.08 nm^{-2}) can dramatically reduce nanotube failure stresses: the average failure stresses of 60 GPa and 70 GPa for zigzag nanotubes and armchair nanotubes, respectively. Some researchers [6] pointed out that larger defect sizes results in lower failure stresses. The similar conclusion can be obtained from Figure 7. However, due to the uncertainties of vacancy defects, it is possible that zigzag nanotubes have higher failure stresses than armchair nanotubes at the same missing atom density.

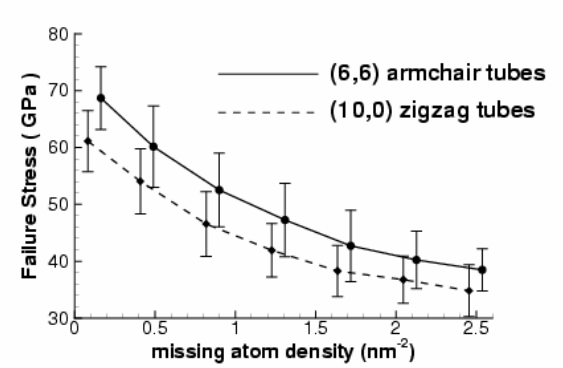

Figure 7. Failure stresses of vacancy-defected nanotubes.

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