Deformation and Fracture Mechanisms in Single-walled Carbon Nanotube/silicon Nanocomposites Based on Molecular Dynamics Analysis

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Abstract
To understand deformation and fracture mechanisms of nanocomposites, nano-tensile/compressive test, nano-bending and nano-cutting of nanotube/silicon nanocomposites are investigated by molecular dynamics (MD) simulation. As a result of these analyses, it has been found that mechanical properties such as Young's modulus and fracture strength are sensitive to the orientation of nanotubes in the matrix. On the other hand, shearing deformation is insensitive to the orientation of nanotubes, Therefore, more stable ductile-mode machining is observed in cutting of the nanocomposite than that of silicon.

1 Introduction

Carbon nanotube is considered to be an ideal reinforcing fiber of nanocomposite materials because of its excellent mechanical properties. However, the microscopic reinforcement mechanism has not been fully understood yet. The reason is that the strength of nanocomposites depends on the orientation and the location of nanotubes in a matrix and on the bonding strength between nanotubes and the matrix. In this paper, to understand deformation and fracture mechanisms of nanocomposites under different loading conditions, nano-tensile/compressive test, nano-bending and nano-cutting of nanotube/silicon nanocomposites are investigated by molecular dynamics.

2 Molecular Dynamics Simulation

To analyze the effect of reinforcement on transition mechanism from brittle to ductile modes in fracture behaviors of nanocomposite materials, MD simulations were carried out with three-dimensional models as shown in Figures 1, 2 and 3. Defect-free mono-crystalline silicon, which is a typical brittle material, and armchair single-walled carbon nanotubes with the smallest diameter are employed as the dominant brittle matrix and the reinforcing fibers, respectively. Although a Tersoff-

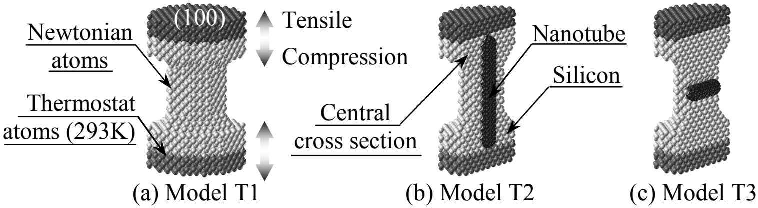


Figure 1: Initial models for tensile and compression test

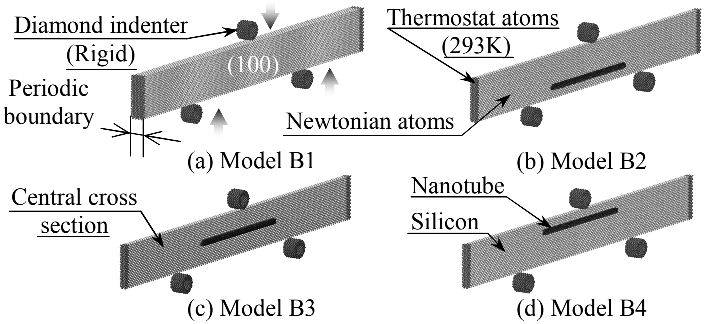


Figure 2: Initial models for three-point bending

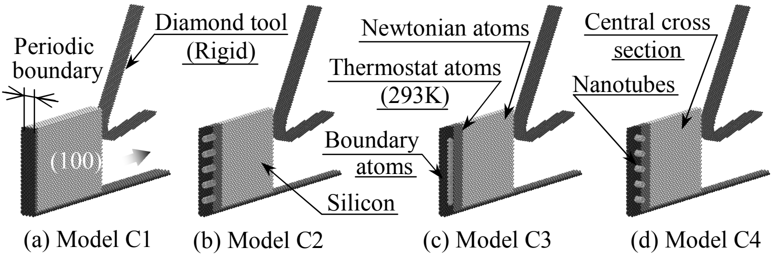
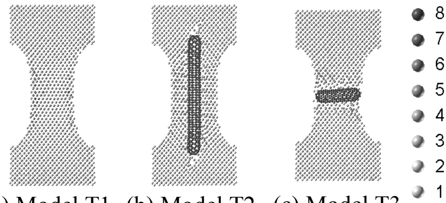


Figure 3: Initial models for cutting

type three-body potential [1] is applied for the MD analyses of nanotube/silicon nanocomposite structure, a Morse-type two-body potential [2] is employed to express the interaction between nanocomposite and indenter/tool atoms. Specimens consist of Newtonian, thermostat, and fixed boundary atoms. The equivalent average temperature of the thermostat atoms is adjusted at 293K. Stress analyses [2] are carried out to investigate the distributions of stresses in the models. The number of nearest neighbours, which is indicated as N_n, is used as an index of crystallinity of silicon atoms. For tensile/compression test, gravity centers of the both ends of the thermostat atoms move at 10m/s in opposite directions, respectively. Three-point bending is performed by an upward movement of the supporting indenters and a downward movement of the central indenter with a speed of 50m/s. For cutting, a moving control volume is applied with a cutting speed of 200m/s. Periodic boundaries are applied for bending and cutting.

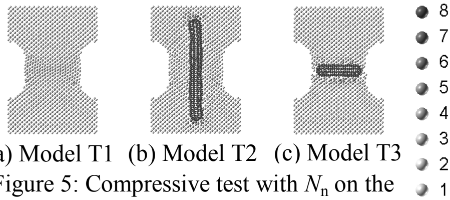
3 Results of the simulations

Figures 4 and 5 show snapshots obtained in the tensile and compressive tests on the central cross section at the fracture strength and at the compressive strain of 14%, respectively. Although nanotubes have excellent mechanical properties in the axial direction, relatively small loads flatten them in the radial direction. The results of the tests show that the Young's modulus and the fracture strength of Model T2 increase by 28% and 19%, respectively, comparing with those of pure silicon. Moreover, the compressive strength of Model T2 increases by 41% at the strain of 14%. On the other hand, the Young's modulus and the fracture strength of Model T3 decrease by 13% and 28%, respectively. Furthermore, the compressive strength of Model T3 equals to that of pure silicon. In addition, in spite of the nanotube slippage in the matrix of Model T2 under the tensile stress, the bonding strength between the nanotube and the matrix remains at the same level.



(a) Model T1 (b) Model T2 (c) Model T3
(ε=26.8%) (ε=26.3%) (ε=19.1%)

Figure 4: Tensile test with N_n on the central cross section at the fracture strength

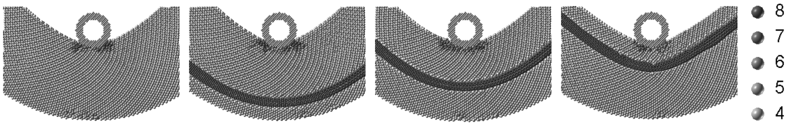


(a) Model T1 (b) Model T2 (c) Model T3

Figure 5: Compressive test with N_n on the central cross section at the strain of 14.0%

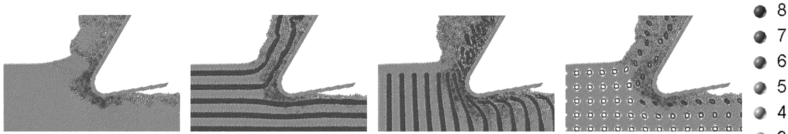
Figure 6 shows snapshots obtained in the bending tests at the fracture strength. The matrix fracture takes place on the tensile-stressed side and the nanotubes prevent the increase of tensile stress in the matrix around them. Therefore, the fracture strength of Model B2 increases by 40% comparing with that of pure silicon. On the other hand, the fracture strength of Model B4 decreases by 17% when the nanotube is located under the compressive-stressed side. As a result, it has been found that the fracture strength is sensitive to the location of nanotubes in the matrix.

Figure 7 shows the snapshots in the cutting tests after the cutting distance of 50nm. In the results, more stable ductile-mode machining of the nanocomposite materials is



(a) Model B1 (b) Model B2 (c) Model B3 (d) Model B4

Figure 6: Bending test with N_n on the central cross section at the fracture strength



(a) Model C1 (b) Model C2 (c) Model C3 (d) Model C4

Figure 7: Cutting test with N_n on the central cross section after cutting 50nm

observed than that of pure silicon for the following reason. For ductile-mode machining of silicon, amorphous phase transformation and stable shearing in the amorphous region are inevitable. When the depth of cut becomes large, a thin amorphous layer intermittently extends upward from the cutting edge to free surface to be cut so a periodic shearing takes place in the amorphous layer. However, in the nanocomposite, a nanotube acts as an obstacle for the extension of amorphous layer. Therefore, the amorphous region grows enough for continuous shearing deformation. This phenomenon is insensitive to the orientation of nanotubes in terms of the cutting direction.

4 Conclusions

As a result of these analyses, mechanical properties such as Young's modulus, tensile and fracture strength are sensitive to the orientation and the location of nanotubes in the matrix. On the other hand, shearing deformation is insensitive to the orientation of nanotubes. Therefore, more stable ductile-mode machining is observed in cutting of nanocomposite than that of silicon. The transition from brittle to ductile modes was also in good agreement with the observation results of micromachining experiments of nanotube/epoxy nanocomposites reported by R.G. Jasinevicius, et al. [3].

References:

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[3] R.G. Jasinevicius, et al.: Proc. of the euspen Int. Conf. I (2009) 25-28.