Computational Materials Science 151 (2018) 273–277

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Tensile responses of carbon nanotubes-reinforced copper nanocomposites: Molecular dynamics simulation

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ARTICLE INFO

Keywords:
Molecule dynamics simulation
Tensile responses
Young's modulus
Carbon nanotubes

ABSTRACT

The uniaxial tensile responses of carbon nanotubes (CNTs) reinforced copper nanocomposites was studied with molecular dynamics (MD) simulations. The interaction force between atoms is modeled using Tersoff potential, embedded-atoms method (EAM) and Lennard-Jones (LJ) potential. We obtained the stress–strain curves to describe the tensile behaviors of CNTs/copper systems. The effects of nanotubes number, diameter and layers number were investigated. The results show that the carbon nanotubes strongly improve the Young's modulus and yield strength of CNTs/copper nanocomposites. The increasing nanotubes number, diameter and layers number significantly enhances the Young's modulus of CNTs/copper. There are noticeable effects on the yield strengths of CNTs/copper nanocomposites with different tubes number, diameter and layers number.

1. Introduction

Carbon nanotubes (CNTs), discovered by Iijima and Ichihashi [1], have attracted tremendous attention in their synthesis, characterization and nanoscale applications. The recent experimental and theoretical results show that the Young's Modulus of SWNTs can be up to 1TPa [2–5]. Due to their excellent mechanical and physical properties [6–8], carbon nanotubes can be used as reinforcement filler in composites materials. Owing to their improved mechanical, physical, electrical and electronic properties, carbon nanotube have become an attractive reinforcement in composite materials, such as nanotube/polymer, nanotube/ceramic and nanotube/metal composites.

In recent years, many researchers have endeavored to fabricate advanced composites to exploit the unique properties of CNTs. CNTs-reinforced Zr, fabricated by Bian et al. [9], displays high fracture strength, strong ultrasonic attenuation characteristics and excellent wave-absorption ability. Kuzunaki et al. [10] characterized the processing and the mechanical properties of carbon nanotubes-reinforced aluminum composites, pointed out the strength of the composites is slightly affected by the annealing time at 873 K. Ma et al. [11] found that the CNTs played a strengthening and toughening role in the ceramic matrix composites by study the nano-SiC ceramic-based CNTs composites. The CNTs/metal composites prepared by electrodeposition have high hardness, excellent wear resistance and good resistance to corrosion [12,13]. Shaffer and Windle [14] disclosed the tensile elastic moduli of the nanotube/polymer composites were assessed as a function of nanotube loading and temperature. Qian et al. [15,16] studied the mechanical properties of nanotube/polystyrene composites, they found that the changes in the mechanical properties of the composites were more pronounce at higher nanotube concentrations.

Pure copper and copper alloys are widely used in the electronics industry due to their excellent electrical and thermal conductivities [17]. Ladani et al. fabricated the carbon nanotube/copper and carbon nanofiber/copper composites and investigated their electrical performance [18]. Superaligned carbon nanotubes reinforced copper matrix laminar composites had been fabricated by Jin et al. [19,20]. Zheng et al. [21] and Muhsan et al. [22] fabricated carbon nanotubes reinforced copper composites by using different fabrication processes. It is found that copper-CNTs composites exhibited increased mechanical properties [23]. The copper alloys reinforced by CNTs have great potential for electrical contact applications [24]. The experimental investigations in the mechanical properties of copper-CNTs composites are expensive and difficult task, while the computational methods are efficient approach for parametric studies of the influence of composite and geometry on the material properties [25]. Awad et al. [26–28] studied the interfacial strength between carbon nanotubes and copper with molecular dynamics simulations. Duan et al. [29,30] found that Ni-coating can enhance the interfacial strength and damping characteristic of carbon nanotube/copper nanocomposites. This letter aims at reporting the tensile responses of carbon nanotubes-reinforced copper composites by molecular dynamic simulations. The realistic models of copper matrix and carbon nanotubes were established. Our

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https://doi.org/10.1016/j.commatsci.2018.05.012
Received 26 December 2017; Received in revised form 14 April 2018; Accepted 4 May 2018

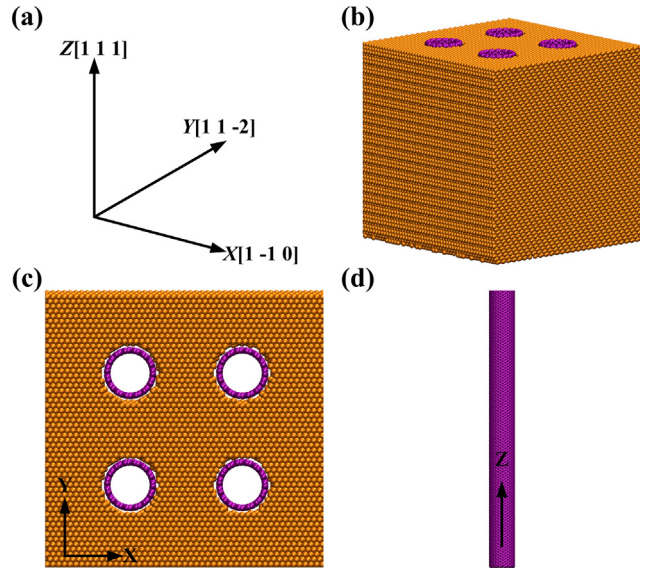

Fig. 1. (a) The coordinates of the model and the crystallographic orientations of the copper matrix. (b) Unit cell model for CNTs/Copper composites. (c) The overhead view of model. (d) Model for single-walled carbon nanotube. Orange is Cu atom and purple is C atom. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

simulations employed the empirical interaction potential between copper atoms, carbon atoms and copper-carbon atoms. The effects of nanotube number, nanotube diameter and nanotube layers number were investigated.

2. Modeling and method

In our simulations, models with carbon nanotubes regularly arranging in face-centered cubic (fcc) copper matrix along the Z axis as shown in Fig. 1. The cubic cell models was used to simulate the microstructure of CNTs/copper composites. The carbon nanotubes were built with Material Studio. Then the superaligned carbon nanotubes were embed in the copper matrix with large-scale atomic/molecular massively parallel similar (LAMMPS) code [31]. The LAMMPS package was employed to investigate the tensile responses of carbon nanotubes reinforced copper nanocomposites. The specimen used for the copper matrix is a nanofilm of 34a × 34a × 34a long, where a is the lattice constant. The carbon nanotubes regularly arrange in the copper matrix. The diameters of carbon nanotubes are set as 8.14 Å, 16.27 Å, 20.34 Å, 24.41 Å and 27.12 Å respectively. The number of carbon nanotubes vary from one to nine. The single-walled carbon nanotubes (SWCNTs), double-walled carbon nanotubes (DWCNTs) and triple-walled carbon nanotubes (TWCNTs) were employed. In order to assess carbon nanotubes' reinforcing potential, analogous tensile responses of a pure copper matrix are also performed.

The accuracy of the potential function determines the reliability of Molecular dynamics simulations. The carbon-carbon interaction in inner layer of carbon nanotubes were described by Tersoff potential [32,33], while the empirical bond order potential formulated by Brenner [34,35]. The potential function is given by Eq. (1). The interactions between copper atoms are described with embedded-atoms method (EAM) developed by Bai et al. [36], which is presented as Eq. (2). Here, we adopted the classical Lennard-Jones (LJ) potential to describe the nonbonded interactions, which is presented as Eq. (3). For the CNTs/Cu systems, the total energy can be expressed as Eq. (4).

$$E_{CNTs} = \frac{1}{2}\sum_{i}\sum_{j\neq i} f_C(r_{ij})[f_R(r_{ij}) + b_{ij}f_A(r_{ij})] \tag{1}$$

where E_{CNTs} in the potential energy between the atoms, f_C is a cutoff function to ensure the nearest-neighbor interactions, f_A and f_R are the attractive and repulsive pairwise terms, b_{ij} is a bond-order parameter, r_{ij} is the distance between atoms I and j.

$$E_{Cu} = F_\alpha\left(\sum_{j\neq i}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\varnothing_{\alpha\beta}(r_{ij}) \tag{2}$$

where E_{Cu} is the embedding energy which is a fuction of the atomic electron density. ρ and ∅ are a pair potential interaction, α and β are the element types of atoms i and j.

$$E_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{3}$$

where E_{LJ} is the potential energy between a pair of atoms, r the separation distance between the pair of atoms, ε the potential well depth, and σ is the van der Waals separation distance. The parameters of the LJ potentials in our model are listed as follows: $\varepsilon_{C-Cu} = 11.7$ eV, $\sigma_{C-Cu} = 3.00$ Å [37] and $\varepsilon_{C-C} = 2.84$ eV and $\sigma_{C-C} = 3.4$ Å [38].

$$E_{total} = E_{CNTs} + E_{Cu} + E_{LJ} \tag{4}$$

where E_{total} is the total potential energy of CNTs/Cu systems, E_{CNTs} and E_{Cu} are the potential energies of the copper matrix and CNTs, respectively. E_{LJ} is the Lennard – Jones potential.

We employed the periodic boundary conditions in all the three directions. An energy minimization process was carried out to avoid overlaps in the positions of the atoms after models established. The time increment is set as 1.0 fs. The sample is then relaxed with a Nose/Hoover thermostat at NPT ensemble for 15 ps to maintain the temperature of 300 K. Then the uniaxial tension deformation with constant strain rate is applied on the models at a constant temperature, and the virial stresses are calculated at each strain level to obtain the stress-strain curves. Then the CNTs/Cu systems were stretched uniformly along the longitudinal direction with a same constant strain loading rate of $5 \times 10^{-3}\,ps^{-1}$ to minimize the effect of loading rate. It should be noted that compared to the typical strain rates used in real tensile test, the strain rate used in this MD simulations is very high due to the intrinsic limitation of the MD method. The stresses of the bare copper and the CNTs/copper systems during deformation were calculated by the virial theorem [39,40]. The calculated stress was the average of all atomistic stresses, and the stress of individual atoms was calculated by using the following equations [39,41].

$$\sigma_{\alpha\beta} = \sigma^{kin}_{\alpha\beta} + \sigma^{int}_{\alpha\beta} \tag{5}$$

$$\sigma^{int}_{\alpha\beta} = \frac{1}{2V}\left(\sum_{i\in V}\sum_{j} f^{\alpha}_{ij}\cdot r^{\beta}_{ij}\right) \tag{6}$$

where $\sigma_{\alpha\beta}$ is the total virial stress, $\sigma^{kin}_{\alpha\beta}$ and $\sigma^{int}_{\alpha\beta}$ are the kinetic and internal contribution to the virial stress, respectively, V is the volume, f^{α}_{ij} is the force acting on atom I because of its interaction with atom j in the α direction, r^{β}_{ij} is the distance between atoms i and j in the β direction, where α and β denote indices in a Cartesian coordinate system. Then the stress-strain curve can be obtained by averaging all the atoms in the system. The Young's modulus (Y) of the bare copper and CNTs/copper systems can be calculates as follows [30,39]

$$Y = \frac{d\sigma^*}{d\varepsilon^*} \tag{7}$$

where σ^* and ε^* are the stress and strain of the systems, respectively. The initial linear elastic region (strain < 2%) was used in the computation of the elastic modulus. The value of the yield strength was defined as the maximum stress.

3. Results and discussions

The SWNTs consists of hexangular carbon rings, which makes the