Molecular simulation of the influence of nickel coating on the interfacial bonding strength of carbon nanotube/magnesium composites

***X. Zhou, S. Y. Song, L. Li, and J. Y. Wu**

State Key Laboratory of Structural Analysis for Industrial Equipment, Department of Engineering Mechanics, Faculty of Vehicle Engineering and Mechanics, Dalian University of Technology, Dalian 116024, China.

*Corresponding author: zhouxia@dlut.edu.cn

Abstract

The mechanical behaviors of Ni-coated single-walled carbon nanotubes (SWCNTs) reinforced magnesium matrix composites are investigated using molecular dynamics (MD) simulation method. The results show that the Young's modulus of the Ni-coated SWCNT/Mg composite is obviously larger than that of the uncoated SWCNT/Mg composite. The results also show that the interfacial bonding of SWCNT/Mg composite can be drastically increased by addition of Ni coating to provide an effective channel for load transfer between the nanotube and Mg matrix. Furthermore, the influences of Ni coating number on the interfacial bonding characteristics of SWCNT/Mg composites also are studied. For three types of Ni coating number, i.e., without Ni coating, with one layer of Ni and two-layer of Ni, the final pullout interfacial bonding strength of the Ni-coated SWCNT from Mg matrix about are 3.9 and 11.9 times larger, respectively, than that of the uncoated SWCNT.

Keywords: Magnesium matrix composites, Mechanical properties, Molecular dynamics simulation, Carbon nanotube.

Introduction

Metal matrix nanocomposites reinforced with carbon nanotubes have good mechanical properties, high shear strength, high temperature resistance and excellent abrasion resistance, so they are widely used in automobile, aerospace and other high-tech areas. Usually studies on carbon nanotube reinforced metal matrix composite are focused on its macro-mechanical properties; however, it is less involved in the microscopic behavior caused by heterogeneity.

Accurate methods of interface tests are difficult to be conducted and the description theory is not yet complete, so molecular dynamics simulation has been widely used in the study of interfacial behavior. The tensile properties of nickel-coated armchair single-walled carbon nanotube reinforced gold matrix composite were studied by Song (2010) with molecular dynamics. A modified embedded atom method was used by Uddin (2010) to predict mechanical properties of single-walled and multi-walled nanotubes reinforced nickel monocrystal composites. They found that large volume fraction and large diameter carbon nanotubes with modified coating can be effective in improving mechanical properties of the composites.

Carbon nanotubes reinforced magnesium alloy composites have excellent mechanical properties than other metal alloys, so it had become a research focus in the field of nano-composite mechanics. Some scholars studied effects of the volume fraction, distribution, interface characteristics and fabrication process of carbon nanotube on its mechanical properties. The interfacial bonding problem of carbon nanotube and matrix is still a challenge and carbon nanotubes reinforced magnesium matrix composite's interfacial behavior studied by molecular dynamics have not been reported. In this paper, using self-compiled molecular dynamics simulation program, we studied the tensile properties of carbon nanotubes reinforced nano-crystal magnesium composites without Ni

coating, with one-layer of Ni and with two-layer of Ni, respectively, and found some laws of Ni-coated carbon nanotubes affecting the mechanical properties of the composite. These laws provided some references in the design of nanotubes reinforced magnesium matrix composite.

Potential Function and Calculation Model

In order to simulate the single-walled carbon nanotubes (SWCNTs) reinforced nano-monocrystal magnesium composite accurately, we chose EAM/FS potential proposed by Finnis and Sinclair (1984) and EAM potential shown in the work by Daw and Baskes (1984) to describe the interaction of HCP magnesium atoms and nickel atoms, respectively. According to the rule of mixture, we chose Lennard-Jone potential to describe the interaction of magnesium, nickel and carbon atoms as well as magnesium and nickel metal. Describing the interaction of carbon atoms in SWCNTs, we chose AIREBO potential used in the work by Stuart and Tutein (2000).

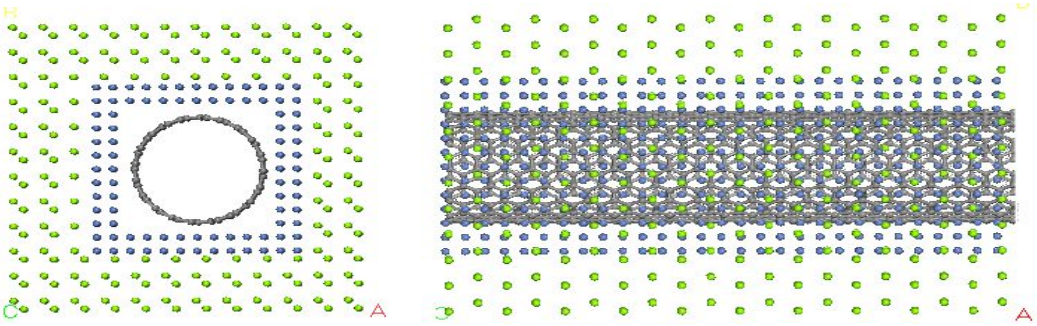

Figure 1. Top and side view of composite model embedded by SWCNT with two-layer of Ni

Composite models with two-layer of Ni-coated interface are shown in Fig.1. The model's actual size is 3.851×3.851×5.211nm. In the simulation, displacement loading was applied along the Z-axis direction. The simulation process was as follows: the unconstrained relaxation was conducted on the initial configuration so that the system reached a steady free state; fixed one end of the model and applied 0.001 tensile strain along the Z-direction on the atom of the other end. Then did a relaxation of 2400～3000 steps in 10~170ps so that system returned to equilibrium state. Added the same displacement load and repeated the above-mentioned process.

Simulation Results and Analysis

Relaxation Process

Before molecular dynamics simulation, we balanced the simulation system. At 0.01 K, we minimized the energy of nano-monocrystal magnesium composite with carbon nanotubes without Ni coating and with one layer of Ni embedded in. The step-length of simulation is 5fs with a relaxation of 30000 steps. Fig. 2 (a) and (b) respectively show the potential energy variation curves of magnesium composites reinforced by (6, 6) SWCNTs without Ni coating and with two-layer of Ni during the balance process. As can be seen from Fig.2, the system without Ni coating reached equilibrium substantially at 7ps, but for that with tow-layer of Ni, the time of equilibrium was more than 150ps.

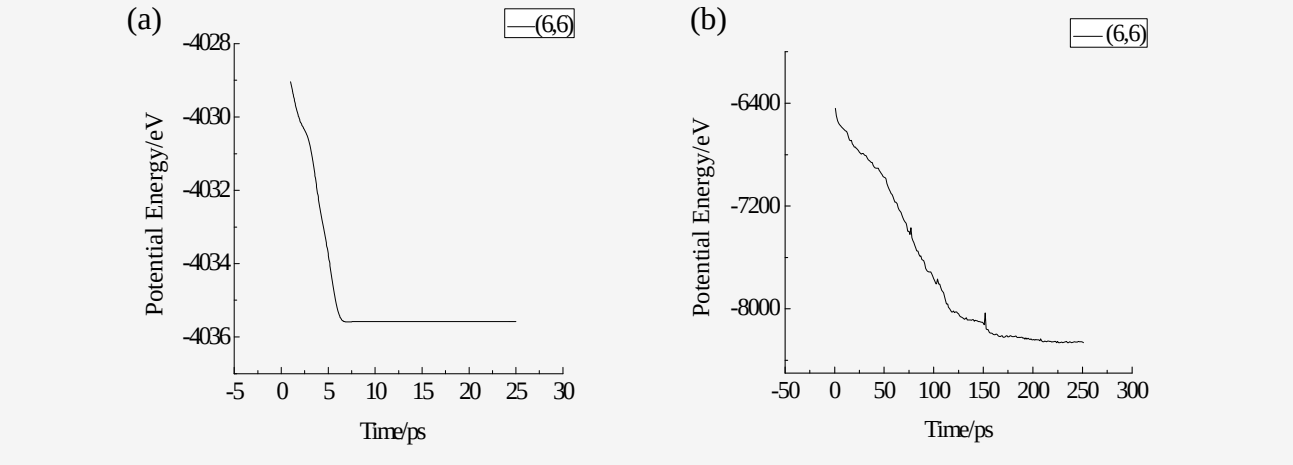

Figure 2. Potential energy variation curves of magnesium composites reinforced by (6, 6) SWCNT: (a) without Ni and (b) with two-layer of Ni

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Mechanical Properties of CNT/Mg composite

The stress-strain curves of (6, 6) CNTs reinforced magnesium matrix composite are shown in Fig.3. It can be seen that the strength of the interface with Ni coating is higher than that without Ni coating and the strength of the two-layer is higher than the one-layer.

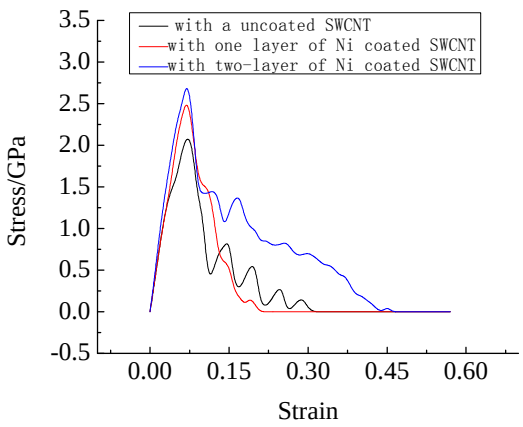

Figure 3. The stress and strain curve of SWCNT/Mg composites with different Ni atom layers

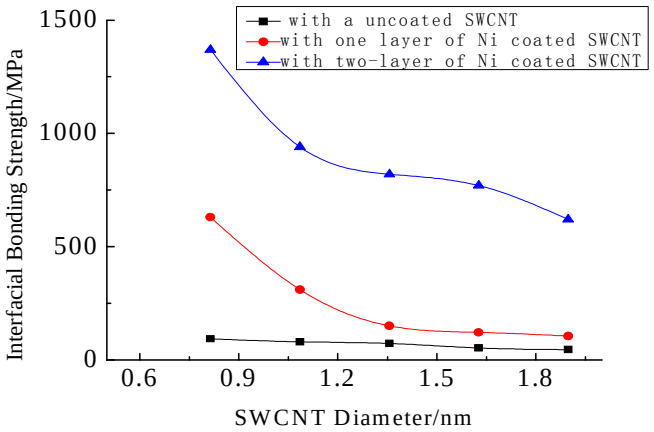

Figure 4. The influence of SWCNT diameter and Ni layer number on interface bonding strength

Interface Bonding Strength of CNTs/Mg composite

Diameters and interfacial characteristics of single-walled carbon nanotubes have an important impact on the interface strength of the CNTs / Mg composite. The change trend of interface

bonding strength is shown in Fig.4. It can be seen that CNT's diameter and Ni layer greatly influenced the interfacial strength of composite. Whether there existed Ni layer on the interface or not, the interface bonding strength between carbon nanotubes and magnesium decreased as CNT's diameter increased. Ni layer on the interface improved the strength of carbon nanotubes reinforced composite greatly and the more the nickel atom was, the higher the interfacial strength was. The interfacial strength of the CNTs reinforced composite increased more than 200 percent with every increase of Ni layer. Fig.5 shows the morphology of the carbon nanotube pulled out from the magnesium matrix completely. It can be seen that there existed a strong interaction between Ni and Mg atoms.

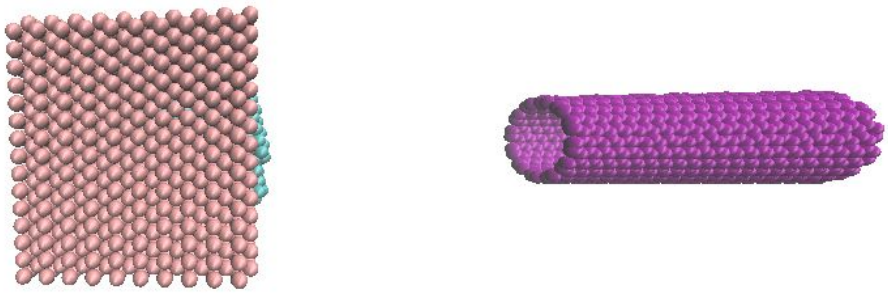

Fig. 5 The model of SWCNT after being pulled-out

Conclusions

This study investigated effects of Ni layer on mechanical properties of the modified SWCNT reinforced magnesium matrix composite. The calculation results indicate that with a fixed diameter of CNTs, the Ni-coated CNT/Mg composite had a higher elastic modulus, yield strength and interfacial strength than that without Ni layer. And the more the Ni layer was, the higher the elastic modulus, yield strength and interfacial strength was. Besides, when the diameter of CNTs was smaller, its coupling with interfacial Ni layer was better. CNTs/Mg composites with smaller diameters and more nickel layers had better mechanical properties. This conclusion has an important guiding significance for the design of high-performance CNTs / Mg composite.

Acknowledgments

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References

Song, H. Y. and Zha, X. W. (2010), Mechanical properties of nickel-coated single-walled carbon nanotubes and their embedded gold matrix composites. *Phys Lett A. 374*, pp. 1068–1072.

Uddin, J. and Baskes, M. I. (2010), Modified embedded atom method study of the mechanical properties of carbon nanotube reinforced nickel composites. *Phys Rev B.* 81, pp. 104103.

Finnis, M. W. and Sinclair, J. E. (1984), A simple empirical N-body potential for transition metals. *Phil Mag A.* 50, pp. 45-55.

Daw, M. S. and Baskes, M. I. (1984), Embedded-atom method: derivation and application to impurities, surfaces, and other defects in metals. *Phys Rev B.* 29, pp. 6443-6453.

Stuart, S. J., Tutein, A. B. and Harrison, J. A. (2000), A reactive potential for hydrocarbons with intermolecular interactions. *J Chem Phys.* 112, pp. 6472–6486.