

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

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