

Large-scale Simulation on Nanocarbon Materials for Reducing Environmental Loads

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Abstract

Carbon nanotube-copper (CNT-Cu) composite has found to have extremely high ampacity which is approximately 100 times as high as that of common electrical conductors. This high ampacity, comparable with nano-carbons, indicates that the carbon nanotube play a significant role in this material. Despite some schematic descriptions of the structure and mechanism analysis are provided, we still need to go into the detail for the further understanding. For this, we first discuss the accurate atomic scale structure and its stability of this composite. The atomic coordination, structural stability, vibrational property, and the exchange of the electrons between CNT and Cu atoms are analyzed by use of the first-principles electron state calculations. Although stable structures are found, and some electrons are provided from the cluster to the CNT, the copper atoms act as a scattering factor and no increase of the conductance has been observed. Next, we focus on the current-induced force caused by each electron current in order to understand the origin of the extremely high ampacity. We have succeeded in obtaining a quantitative description of the current-induced force acting on CNT-Cu composites and found the force concentration around the interface between copper atoms and CNT. We believe that the competition between this force and the structural stability determines the ampacity. Finally, through analyzing the eigen-mode of CNT-Cu composites, it could be speculated that the vibrations of the copper atoms in CNT-Cu composite are suppressed compared to those in pure copper. This indicates that the temperature-dependence of the resistivity of CNT-Cu composite is weaker than that of pure copper, which is consistent with results observed in experiment.

Keywords: Carbon nanotube, Composite material, the First-principles density functional theory calculation, Non-equilibrium Green's function, current-induced force