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Heat conduction in coaxial nanocables of Au nanowire core and carbon nanotube shell: A molecular dynamics simulation

Liu Cui [a], Yanhui Feng [a, b, *], Jingjing Tang [a], Peng Tan [a], Xinxin Zhang [a, b]

[a] School of Mechanical Engineering, University of Science and Technology Beijing, Beijing 100083, China
[b] Beijing Key Laboratory of Energy Saving and Emission Reduction for Metallurgical Industry, University of Science and Technology Beijing, Beijing 100083, China

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ABSTRACT

Non-equilibrium molecular dynamics simulations have been employed to calculate the thermal conductivity of coaxial nanocables of Au nanowire core and carbon nanotube shell, i.e. nanotubes filled with nanowires. Our efforts are focused on how the thermal conductivity can be altered in nanocables. By performing analysis on the phonon vibrational density of states, we have revealed that the thermal conductivity of nanocables is 20-42% higher than the corresponding bare nanotubes, due to the interactions of C–C and C–Au and the mass transfer induced by nanowire axial motion. The dependences of thermal conductivity on the temperature, length, diameter, chirality and filling ratio have been investigated. It turns out that the tendencies of nanocable thermal conductivity changing with temperature, length and diameter are similar to bare nanotubes. In addition, the thermal conductivity of nanocables always goes up with the increasing filling ratio. For different chirality types, the zigzag (18, 0) nanocable has the largest thermal conductivity increments, followed by armchair (10, 10) and chiral (14, 7) nanocables.

1. Introduction

Since discovered in 1991 [1] carbon nanotubes (CNTs) have attracted a great deal of attention. Many investigations have indicated that CNTs possess various excellent properties including, for example, high Young's modulus [2], good field emission properties [3] and superior thermal conductivity [4]. CNTs are being considered as one promising candidate material for nanoscale device applications. Due to the unique quasi one-dimensional hollow structures, CNTs could be filled with other materials. In 1993, Ajayan and Iijima [5] firstly encapsulated Pt into CNTs. This immediately aroused widespread attention. Various studies have demonstrated that CNTs can be encapsulated with metals [6,7] and even fullerenes [8]. And the filled materials would have a great impact on CNT properties. Borowiak-Palen et al. [6] used a wet chemistry method to fill Fe into single-walled carbon nanotubes (SWCNTs) and found that Fe filled SWCNTs shown ferromagnetic behaviour even at room temperature. Kumar et al. [7] embedded tin into multi-walled carbon nanotubes (MWCNTs) through a catalytic decomposition method. They revealed that the reversible capacities of the tin filled CNTs were remarkably high, stabilizing in the 720–800 mAh/g region over the first 20 cycles. Jo et al. [9] investigated the electronic and magnetic properties of Fe, Co, and Ni nanowires (NWs) encapsulated in SWCNTs through the spin polarized *ab initio* calculation. Their results indicated that the reduction of magnetic moment for Fe NWs filled SWCNTs was relatively smaller than that for Co and Ni NWs.

However, there were few studies investigated the thermal conductivity of filled CNTs. The thermal conductivity of a material is a measure of how fast heat will flow in that material [10]. Vavro et al. [8] measured the thermal conductivity of buckypapers of carbon nanopeapods (CNTs embedded with fullerene C_{60} molecules). According to their experiments, there was little or no contribution by the C_{60} chains to the thermal conductivity of filled tubes. They pointed out three mechanisms and suggested that more accurate data and individual tube experiments were necessary to assess the relative importance of the various mechanisms. Noya et al. [11] and Kawamura et al. [12] computed the thermal conductivity of an individual carbon nanopeapod using molecular dynamics simulations. Both them indicated that thermal

* Corresponding author. School of Mechanical Engineering, University of Science and Technology Beijing, Beijing 100083, China. Tel./fax: +86 010 62334971.
E-mail address: yhfeng@me.ustb.edu.cn (Y. Feng).

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conductivity of the carbon nanopeapod was higher than CNT due to the motion of C_{60} molecules. Noya's results showed that the thermal conductivity of the carbon nanopeapod increased first and then decreased with rising temperature. However, Kawamura's results turned out just to the contrary. Toprak et al. [13] predicted that the thermal conductivity of Cu NWs filled SWCNTs was 24% higher than the corresponding SWCNTs and estimated to be 40% lower than pure copper NWs. The length dependence of thermal conductivity for the Cu NWs filled CNTs was similar to that of analogous bare SWCNTs and Cu NWs whereas the length increased, the thermal conductivity also increased.

The composite of CNT filled with NW can be named as coaxial nanocable [14], with the NW representing the conducting core and the CNT representing the insulating sheath. The coaxial nanocable of Au NW core and CNT shell was systematically investigated in this work, with the aim to reveal the dependence of thermal conductivity on temperatures, lengths, diameters, chiralities and filling ratios. Using the phonon vibrational density of states (VDOS), the heat transfer mechanisms for the change in the thermal conductivity of nanocables were also explored. This study is an attempt to explore possible structures and thermal properties to satisfy requirements of different nanoscale devices, such as thermoelectric devices requiring strongly suppressed thermal conductivity, whereas electronic or optoelectronic devices demanding efficient heat removal.

2. Method

2.1. Model structures

The simulation models of coaxial nanocables are CNTs embedded by gold NWs. It is know that bulk gold crystallizes in face-centered cubic (fcc) lattices. However, the gold NWs filled in CNTs are found to have “weird” structures that differ from the crystalline bulk. They spontaneously exhibit multishell packs consisting of coaxial cylindrical shells [15]. Each shell consists of helical atom rows coiled round the wire axis and can be viewed as a triangular (1 1 1) lattice sheet that is folded on to itself to form a cylinder. KT-indices n–n'–n'' [16] were employed to describe a nanowire consisting of coaxial shells with n, n' and n'' helical atom rows ($n > n' > n''$), which can be counted at the cross section. For example, an SWCNT with the chirality of (10, 10) is filled with a same length gold NW, as shown in Fig. 1. The corresponding KT-index of the filled gold NW is 9-3. That is, the outer and inner gold shells are composed of 9 and 3 atom rows, respectively. Similar behaviour was also observed by Xiao et al. [17].

2.2. Thermal conductivity

Heat conduction actually results from the random motion of the carriers in the solid system transporting thermal energy from one location to another. The heat carriers include electrons, atoms and molecules in gases, liquids and solids. In dielectric solid materials like CNTs, heat is conducted through the vibration of atoms. The discrete units of vibrational energy that arises from oscillating atoms within a crystal can be defined as phonons [18]. That is, contributions to CNT thermal conductivity mostly come from phonons (i.e. phonon thermal conductivity, PTC). In metals such as Au NWs, the thermal conductivity is usually dominated by electrons (i.e. electronic thermal conductivity, ETC). In their composites, i.e. nanocables, both PTC and ETC should be taken into consideration.

2.2.1. Phonon thermal conductivity

Non-equilibrium molecular dynamics (NEMD) simulations have been proven to be a very useful technique to predict thermal transport properties of nanostructured materials [19–22]. In this work, NEMD simulations were used to calculate the PTC of CNTs and nanocables. The periodic boundary condition was used in the longitudinal direction of CNTs. The C–C bonding interactions among CNT atoms were determined by the Tersoff potential [23]. The embedded atom method (EAM) potential [24] was used to describe the Au–Au interactions. The C–Au interactions were assumed as the L–J potential, and L–J size and energy parameters are 0.29943 nm and 0.01273 eV [25], respectively.

In this work, the Muller-Plathe method [26] was used to establish a temperature gradient parallel to the tube axis. The CNTs and nanocables were axially partitioned into 40 slabs of equal length for temperature recording and control. As illustrated in Fig. 1, the first slab and the 21st slab were chosen as heat sink and heat source, respectively. A heat flux transferred between these two slabs through exchanging momentum between the ‘hottest’ atom in heat sink and the ‘coldest’ atom in the heat source. The

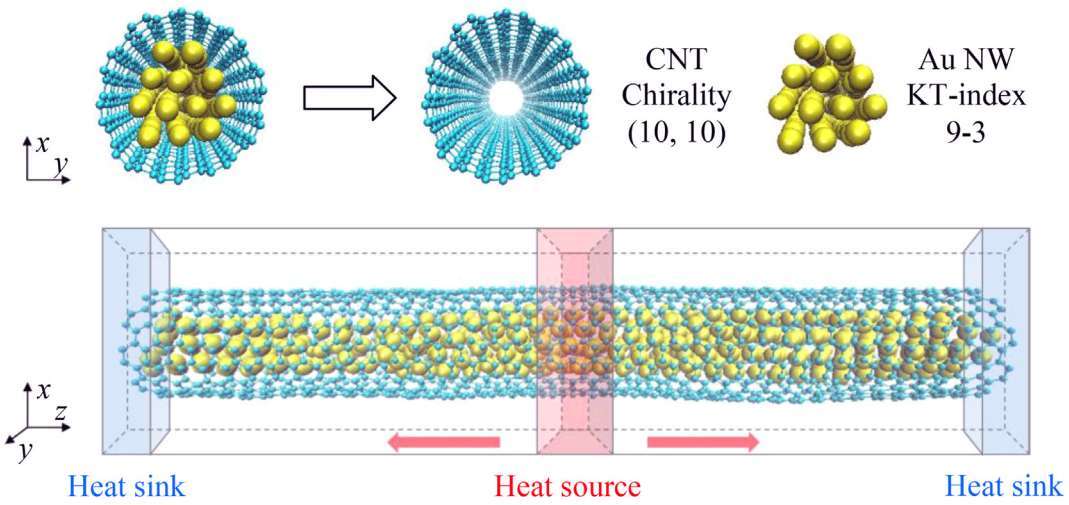

Fig. 1. Model of the coaxial nanocable of Au nanowire core and carbon nanotube shell.