A STUDY ON HEAT TRANSFER IN NANO TUBES

N. SRIDHAR
Research Scholar
Email:nandipatisridhar@gmail.com

Dr. S. CHAKRADHAR GOUD
Principal, Sri Sarada Institute of Science and Technology
Email:cgsakki@yahoo.com

Dr. B. DURGA PRASAD
Professor, JNTUA

ABSTRACT

Interfacial thermal transport between offset parallel 10, 10 single-wall carbon NANO tubes is investigated by molecular dynamics simulation and analytical thermal modelling as a function of NANO tube spacing, overlap, and length. A four order of magnitude reduction in interfacial thermal resistance is found as the NANO tubes are brought into intimate contact. A reduction is also found for longer NANO tubes and for NANO tubes with increased overlap area. This paper presents the unique atomic structure and properties of carbon NANO tube (CNT). The electronic band structure of carbon NANO tube along with their small size and low dimension are responsible for their unique electrical, mechanical, and thermal properties. The thermal properties of carbon nanotubes are directly related to their unique structure and small size. Because of these properties, nanotubes may prove to be an ideal material for the study of low-dimensional phonon physics, and for thermal management, both on the macro- and the micro-scale.

Keywords: *Heat Transfer, Nano Tubes, Thermal Properties*

INTRODUCTION

Due to their superior thermal conductivity, single-wall carbon nanotubes SWNTs have elicited great interest as potential thermal management materials, for example, as fillers in polymer composites and as thermal interface materials. Recent measurements on carbon nanotube suspensions and composites indicate that their effective thermal conductivities are lower than expected based on the high nanotube thermal conductivity and that thermal resistance between the nanotube and the surrounding medium may be a key factor limiting heat flow. Another important but little-studied factor impacting the effective thermal conductivity of carbon nanotube-polymer composite materials is interfacial thermal resistance between carbon nanotubes. These composites are well known to exhibit percolation behaviour and correspondingly display an interconnected network structure in which individual nanotubes are in contact with other nanotubes as well as with the surrounding host material. Nanotube-nanotube thermal resistances will also be important in Bucky paper-based materials. Additionally, phonons in suspended carbon nanotubes play an important role in mediating electron tunnelling transport, and it is expected that thermal/vibration coupling between neighbouring nanotubes in nanotube arrays will have a significant effect on the performance of devices based on these structures. Few studies to date have discussed the interfacial resistance at the contacts between carbon nanotubes. Molecular dynamics simulations reveal that heat transport in aligned nanotube bundles is dominated by tube-tube interfacial resistance.11 This may explain why the thermal conductivity of nanotube bundles is much lower than that of a single carbon nanotube.17 No studies have yet been reported that investigate the dependence of nanotube-nanotube interfacial resistance on nanotube length or on overlap and spacing at the tube-tube

junctions. These parameters can be varied experimentally; in particular, nanotube length can be controlled by chemical vapor deposition processing conditions,18 and nanotube spacing and size can be controlled by the placement of catalyst.19 It is critically important to understand how length, spacing, and overlap influence energy transport so that enhancement in nanotube composite thermal conductivity beyond current levels can be achieved and so that a fundamental understanding of thermal and vibrational coupling between isolated, arbitrarily spaced carbon nanotubes can be attained. In addition, carbon nanotubes are of great interest as oscillators in mass detection and radio frequency signal processing. Their mechanical properties will strongly impact quality factor and performance in these applications. Although such properties have been investigated by a number of groups for individual nanotubes see for a review, few systematic studies of size effects on mechanical properties have been performed. Such effects, particularly those related to aspect ratio, will become important design parameters as advances in synthesis and processing enable ever-improving control of nanotube structure and dimensions. Existing studies in this area have so far been limited to examination of the influence of diameter and wall thickness. Little is known about the length dependence of carbon nanotube mechanical properties. In this paper classical thermal modelling results that show the effect of nanotube length, overlap, and spacing on thermal interfacial resistance between two carbon nanotubes are presented.

We have begun to explore the thermal properties of nanotubes by measuring the specific heat and thermal conductivity of bulk SWNT samples. In addition, we have synthesized nanotube-based composite materials and measured their thermal conductivity. The measured specific heat of single-walled nanotubes differs from that of both 2D graphene and 3D graphite, especially at low temperatures, where 1D quantization of the phonon bandstructure is observed. The measured specific heat shows only weak effects of intertube coupling in nanotube bundling, suggesting that this coupling is weaker than expected. The thermal conductivity of nanotubes is large, even in bulk samples: aligned bundles of SWNTs show a thermal conductivity of > 200 W/m K at room temperature. A linear K(T) up to approximately 40 K may be due to 1D quantization; measurement of K(T) of samples with different average nanotube diameters supports this interpretation.

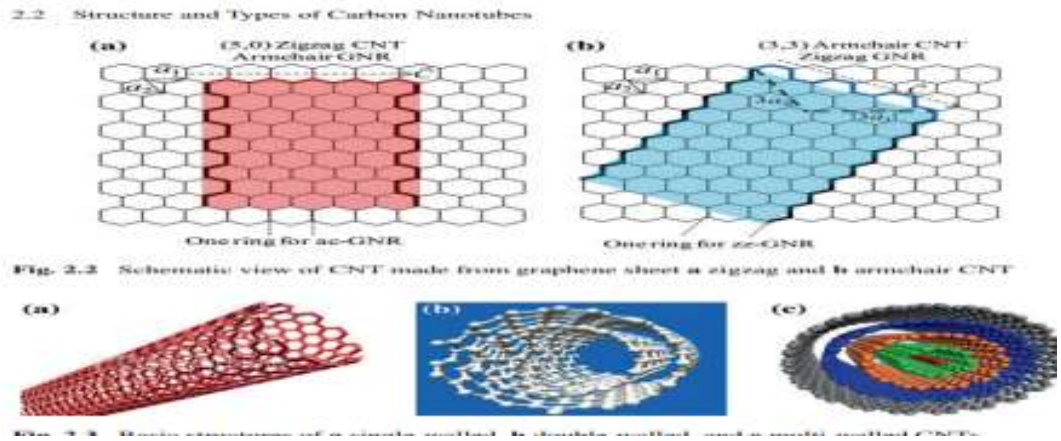
LITERATURE REVIEW

A carbon atom can form various types of allotropes. In 3D structures, diamond and graphite are the allotropes of carbon. Carbon also forms low-dimensional (2D, 1D or 0D) allotropes collectively known as carbon nanomaterials. Examples of such nanomaterials are 1D carbon nanotubes (CNTs) and 0D fullerenes. In the list of carbon nanomaterials, graphene is known as 2D single layer of graphite. The sp2 bonds in graphene is stronger than sp3 bonds in diamond that makes graphene the strongest material (Sarkar et al. 2011). The lattice structure of graphene in real space consists of hexagonal arrangement of carbon atoms as shown in Fig. 2.1a. An isolated carbon atoms have four valence electrons in its 2s, and 2p atomic orbitals. While forming into graphene, three atomic orbitals of the carbon atom, 2s, 2px, and

2py, are hybridized into three sp2 orbitals. These sp2 orbitals are in the same plane while the remaining 2pz is perpendicular to other orbitals as shown in Fig. 2.1b (Sarkar et al. 2011). The σ bonds between the adjacent carbon atoms are formed by the sp2 hybridized orbitals, whereas the 2pz orbitals form the π bonds that are out of the plane of graphene (Javey and Kong, 2009). Carbon nanotubes (CNTs) are made by rolling up of sheet of graphene into a cylinder. These nanostructures are constructed with length-to-diameter ratio of up to (1.32 × 108):1 (Wang 2009) that is significantly larger than any other material. As their name suggests, the diameter of nanotube is in the order of few nanometers, while they can be up to 18 centimeters in length (Javey and Kong, 2009). CNTs are most promising candidates in the field of nanoelectronics, especially for interconnect applications. Metallic CNTs have aroused a lot of research interest for their applicability as VLSI interconnects due to high thermal stability, high thermal conductivity, and large current carrying capability. A CNT can carry current density in excess of 103 MA/cm2, which can enhance the electrical performance as well as eliminate electromigration reliability concerns that plagues current nanoscale Cu interconnects (Wei et al., 2001). Recent modeling works have revealed that CNT bundle interconnects can potentially offer added advantages over Cu. Moreover, recent experiments have demonstrated that the resistance values as small as 200 Ω can be achieved in CNT bundles.

STRUCTURE AND TYPES OF CARBON NANOTUBES

To understand the crystal structure of CNTs, it is necessary to understand their atomic structure. Both CNTs and GNRs (graphene nanoribbons) can be understood as structures derived from a graphene sheet, shown in Fig. 2.2. A graphene sheet is a single layer of carbon atoms packed into 2D honeycomb lattice structure. CNT, considered as rolled-up graphene sheet, have the edges of the sheet joint together to form a seamless cylinder. The dashed arrows in Fig. 2.2a, b show the circumferential vector C , which indicates the rolling up direction for CNT. The vector is defined as C = n1aˆ1 + n2aˆ2 where a1 and a2 are the lattice vectors of graphene and n1 and n2 are the chiral indices. The chiral indices (n1, n2) uniquely defines the chirality, or the rolled-up direction of graphene sheet. Depending on the chiral indices (n1, n2), CNTs can be classified to zigzag and armchair structures as shown in Fig. 2.2a, b, respectively. For armchair CNTs, the chiral indices n1 and n2 are equal while for zigzag CNTs, n1 or n2 = 0 (Li et al., 2009b). For other values of indices, CNTs are known as chiral. Depending upon their different structures, CNTs can exhibit metallic or semiconducting properties. By satisfying the condition n1 − n2 = 3i (where i is an integer), the armchair CNTs are always metallic, whereas zigzag CNTs are either metallic or semiconducting in nature (Javey and Kong 2009; Li et al. 2009b). Statistically, a natural mix of CNTs will have 1/3rd metallic and 2/3rd semiconducting chiralities



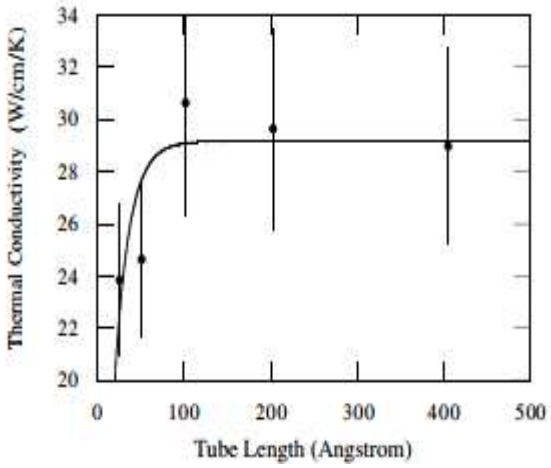
THERMAL CONDUCTIVITY

As diamond and graphite display the highest known thermal conductivity at moderate temperatures, it is likely that nanotubes should be outstanding in this regard as well. Indeed, recent theoretical work has predicted that the room temperature thermal conductivity of nanotubes is as high as 6600 W/m K. In addition, at low temperature, the thermal conductivity should show the effects of 1D quantization just as is seen in the specific heat. The thermal conductivity in a highly anisotropic material is most sensitive to the high velocity and high-scattering-length phonons. Therefore, it is likely that even in nanotube bundles, the thermal conductivity should directly probe on-tube phonons and be insensitive to inter-tube coupling. Figure 7 shows the measured temperature-dependent thermal conductivity of bulk samples of SWNTs that have been aligned by filtration in a high magnetic field. In the alignment direction, the room-temperature thermal conductivity is greater than 200 W/m K, which is comparable to a good metal and within an order of magnitude of that of highly crystalline graphite or diamond. The thermal conductivity of unaligned samples is about one order of magnitude smaller. However, the temperature dependence of the thermal conductivity is roughly the same in both types of sample. Also, in both types of sample, simultaneous measurement of the electrical and thermal conductivity shows that the electronic contribution to K (T) is negligible at all temperatures.

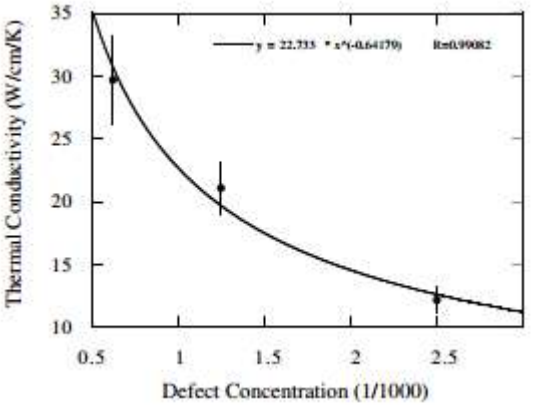
NUMERICAL CALCULATIONS

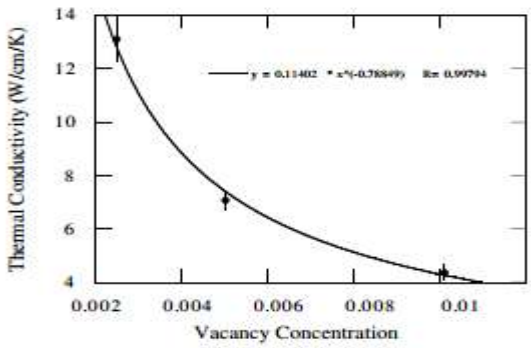
The empirical interatomic interaction used in our calculations is the Brenner-type of bond order dependent potential. The Brenner potential is parametrized for hydrocarbon systems, and is widely used in modelling carbon based systems, such as diamond, graphite sheet, fullerenes and carbon nanotubes. In all MD simulations, 1 fs time step is employed, and 40 ps initial MD is used to equilibrate the systems. After equilibration, 400 ps constant energy (NVE) simulation is carried out, and the heat current is calculated every time step. The average temperature in all simulations is 300 K. One main concern of using MD to calculate the thermal conductivity is the size effect of the simulation box due to periodic boundary conditions. When the simulation is conducted in a small box, phonons will get scattered more frequently because they re-enter the simulation box before they can be dissipated. In other words, the mean free path of phonons is

limited to the order of the simulation box. This artifact usually underestimates the thermal conductivity. In order to obtain the correct thermal conductivity, we test the convergence of MD simulations on thermal conductivity by using different size systems and early time correlation function analysis. For a (10,10) single-walled nanotube, four different systems are investigated.



They contain 400, 800, 1600, 3200 and 6400 atoms, respectively. As we expected, the phonon mean free path is the limiting factor to obtain accurate results. For a small simulation system, the calculated thermal conductivity is smaller than the correct value because of the overestimation of phonon scattering. As the simulation system size gets larger, the theoretical value converges to a constant which is independent of simulation size. The convergence behaviour can be seen in figure 1. The theoretical predicted value approaches 29.8 W cm−1 K−1 along the tube axis, which is very high in comparison with conventional materials. We also mention here that the thermal conductivity for an isolated single-wall carbon nanotube is not a well defined quantity, since the cross section of heat conduction can be chosen in various ways. In this paper, we choose a 1 Å thickness cylinder as the geometric configuration. Other choices can also be made such as choosing the van de Waals thickness. The choice of the cross section is not important here since we will make comparison under consistent conditions. Later in this section, we will show the thermal conductivity for nanotube bundles where the cross section is uniquely defined, and the results can be used to compare with experiments and other materials.





CONCLUSIONS

The implication is very important since it promises efficient thermal management in nanotube-based MEMS/NEMS devices. The defect influence on the thermal conductivity of carbon nanotube reveals an interesting phenomenon that has not been noted before. More detailed analysis is needed to understand the origin of this behaviour. In addition, more accurate interaction potentials will be developed to

quantitatively study the nanotubes and other nanostructures.

REFERENCES

[1] Chico L, Crespi V H and Benedict L X 1996 Phys. Rev. Lett. 76 971
[2] Langer L, Bayot V and Grivei E 1996 Phys. Rev. Lett. 76 479
[3] Ebbesen T W, Lezec H J, Hiura H, Bennett J W, Ghaemi H F and Thio T 1996 Nature 382 54
[4] Pichler T, Knupfer M and Golden M S 1998 Phys. Rev. Lett. 80 4729
[5] Iijima S 1991 Nature 354 56
[6] Iijima S and Ichihashi T 1993 Nature 363 603
[7] Bethunes D S, Kiang C H, Devries M S, Gorman G, Savoy R, Vazquez J and Beyers R 1993 Nature 363 605
[8] Che J, Ca¸ g˘ın T and Goddard W A III 2000 J. Chem. Phys. Submitted
[9] Kubo R, Toda M and Hashitsume N 1985 Statistical Physics vol 2 (Berlin: Springer)
[10] Brenner D W 1990 Phys. Rev. B 42 9458
[11] Che J, Ca¸ g˘ın T and Goddard W A III 1999 Theor. Chem. Acct. 102 346