Dependence of Electrical & Thermal parameters of Carbon Nanotubes on their geometry

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ABSTRACT

Carbon nanotubes have shown great promise as a new class of electronic materials owing to the change in their properties with chirality and geometry of the nanotube. They are being considered for future VLSI applications due to their superior conductance and inductance properties which are important parameters while considering any material for an interconnect or via applications.

In this paper, we report the variation in electrical and thermal conductance of a CNT with its geometrical features using a diameter dependent model. Also the dependence of conductance of a CNT on the type of nanotubes, tube length and tube diameter has been studied.

As we know that at nanometre scale, the electrical and thermal transport properties of the components become extremely important with regard to the functioning of the device and it is very difficult to accurately measure these properties, therefore predictions using modeling and simulation play an important role in providing a guideline for design and fabrication of CNT interconnects and understanding the working of various CNT based devices.

Keywords: Carbon nanotubes, Electrical Conductance, Thermal Conductance

1 INTRODUCTION

Since the discovery of Carbon nanotubes, research in the area of nanotechnology has fuelled our quest to reduce the size of electronic devices and integrated micro and nano electro-mechanical systems (MEMS and NEMS).

In microelectronics, the scaling of devices has led to the desire to use nanowires in terms of vias, interconnects, field effect transistors (FETs) and memory elements. As the device size reduces, the power dissipation and thermal management in these nanosize devices become the key factors during the design process. Therefore, the electrical and thermal conduction properties of nanomaterials play a critical role in controlling the performance and stability of nano/micro devices. Among various potential candidates for future MEMS/NEMS applications, carbon nanotubes hold a unique position because of their remarkable properties like small size, great strength, light weight, special electronic structures, **huge current-carrying capacity** and high mechanical and thermal stability. Due to the technological difficulties of synthesizing high-quality and well-ordered nanotubes, it is very challenging to perform electrical and thermal conduction measurements on a specific type of tube. Thus, it is essential to observe theoretical predictions of the inductance and electrical and thermal conductance and the influence of the geometry of tubes on these values.

A single wall carbon nanotube (SWNT) has one shell while a multi wall carbon nanotube (MWNT) has several shells. Depending on the chirality (conformational variation), these shells demonstrate either metallic or semi-conducting properties. Thermal conductance also varies with chirality of the shell. Three types of nanotubes are known to exist, namely armchair, zigzag and chiral nanotubes, depending on the n and m parameters used to define a CNT. Armchair nanotubes are formed when $n = m$ and the chiral angle is 30°. Zigzag nanotubes are formed when either n or m is zero and the chiral angle is 0°. All other nanotubes, with chiral angles intermediate between 0° and 30° are known as chiral nanotubes [1,2].

1.1 Electrical Conductance of CNT

Most existing studies have shown that individual SWNTs have a high ballistic resistance (approximately 6.5kΩ) whereas CNT bundles (CNTs aligned parallely) provide high conductance [3]. Findings have also shown that all shells in a MWNT can conduct if they are properly connected to the end contacts [4], leading to a very low overall resistance.

CNTs show quantized conductance akin to nanowires. Therefore, conductance of a carbon nanotube can be evaluated using the two-terminal Landauer-Buttiker formula which states that for a 1-D system with N channels in parallel, the conductance $\boldsymbol{G=(Ne^2/h)T}$, where T is the transmission coefficient for electrons through the sample [5]. Due to spin degeneracy and sublattice degeneracy of electrons in graphene, each nanotube shell has four conducting channels in parallel ($N=4$). Hence the conductance of a single ballistic SWNT assuming perfect contacts ($T=1$), is given by $4e^2/h$ = 155 μS, which yields a resistance of 6.45 KΩ [5]. This is the fundamental resistance associated with a SWNT that cannot be avoided. The conductance per channel can be written as

$$G=G_0/(1+l/\lambda) \qquad \{1\}$$

where G_0 is quantum conductance, l is the length of CNTs and λ is the mean free path [3] but the ballistic conductance of the CNT should be a constant for any value of $l < \lambda$ [4]. Therefore, the model based on {1} was modified [6] to provide an accurate conductance analysis of the nanotubes.

According to this model, the conductance of a MWNT or a SWNT is determined by two factors namely the conducting channels per shell and the number of shells. A SWNT consists of 1 shell and for an MWNT, the number of shells is diameter-dependant, i.e.

$$N_{shell} = 1+[(D_{outer} - D_{inner})/2\delta] \quad \{2\}$$

where δ=0.34nm is the Vander Waals distance, D_{outer} and D_{inner} are the maximum and minimum shell diameters respectively. Thus, the diameter of each shell is

$$d_i = D_{inner} + i\times 2\delta \text{ , where i =0,1,.., Nshell -1} \quad \{3\}$$

Assuming the metallic tube ratio is r, the approximate number of conducting channels per shell is given by

$$N_{chan/shell} = \begin{cases} (ad+b)r & ; \ d>6 \text{ nm} \\ 2r & ; \ d<6 \text{ nm} \end{cases} \quad \{4\}$$

where a = 0.1836 nm^{-1} and b = 1.275 [3]. Generally, we have r = 1/ 3 in MWNT or a CNT bundle.

One conducting channel will provide either intrinsic conductance (Gi) or Ohmic conductance (Go) according to the tube length l. For the low bias situation V_b<≈ 0.1V, the diameter-dependent channel conductance for one shell is

$$G_{shell}(d_i,l) = \begin{cases} G_i \, N_{chan/shell} & ; \ l <= \lambda \\ G_o \, N_{chan/shell} & ; \ l > \lambda \end{cases} \quad \{5\}$$

where the mean free path $\lambda = v_F \, d / \alpha T$ is diameter-dependent (α is the total scattering rate, T is temperature and v_F is the fermi velocity of graphene).

Ohmic conductance $G_o = 2q^2\lambda/hl$ is diameter dependent and the channel intrinsic conductance is a constant [6], i.e., $G_i = 2q^2/h$ = 1/12.9kΩ (where h is Planck's constant, q the charge of an electron and l the tube length).

The number of shells in MWNT is determined by D_{outer} based on {2}. Each shell has its own d_i, λ and $N_{chan/shell}$, which can be derived from D_{outer}. Hence, the total conductance is the summation of conductance of all these shells and can be written as

$$G_{MW}(D_{outer},l) = \sum_{D_{inner}}^{D_{outer}} G_{shell}(d_i,l) = \sum_{N_{shell}} G_{shell}(d_i,l) \quad \{6\}$$

It can be seen from {6} that when the outer diameter of a MWNT increases and the number of shells remains the same, the conductance will gradually increase. Then, when the outer diameter reaches a certain value, this MWNT will have one more shell and its conductance will increase dramatically. In case of CNTs with length larger than λ, the conductance starts to decrease due to the effect of Ohmic resistance.

1.2 Thermal Conductance of CNT

As in the case of electrical conductance, the thermal conductance values of the shells of a CNT depends upon the length and diameter of the particular shell [2]. If the length of the shell is less than the phonon mean free path, l_{mfp}, the phonons in the CNT shell will transport without scattering, i.e., the CNT shell has ballistic thermal conductance $K_{ballistic}$ which is the product of number of phonon channels N_{ph} and the thermal conductance per phonon channel K_{th} [7].

$$K_{ballistic} = K_{th} \times N_{ph} \quad \{7\}$$

where $K_{th} = \pi^2 \, k_B^2 \, T / 3h = 9.46X10^{-13}$ T ; h is Planck's constant, k_B is Boltzmann constant and T is the temperature. N_{ph} can be calculated for each CNT shell using the chiral vector indices n and m as

$$N_{ph} = 12\,(n^2+mn+m^2)/\, d_R \ \ [7] \quad \{8\}$$

where d_R is the greatest common divisor of (2n+m) and (2m+n). The diameter of the shell can also be determined by n and m using the following expression

$$d_i = a_0/\pi * (n^2+mn+m^2)^{1/2} \quad \{9\}$$

where a_0 is the length of unit chiral vector and is equal to $\sqrt{3}\ b_0$ and b_0 = 0.142 nm is the equilibrium interatomic distance [8]. Therefore,

$$N_{ph} = 12\,\pi^2\, d_i^{\,2} / \, a_0^{\,2}\, d_R \quad \{10\}$$

We can infer from this expression that number of phonon channels is diameter dependant and increases with diameter of the shell. Also, there may exist many chiral vectors (different n,m) for the same diameter shells which in turn would lead to different number of phonon channels. That means a zigzag, an armchair and a chiral CNT of the same diameter may have different number of phonon channels. Also, the armchair and zigzag tubes having vastly different diameters can have the same number of phonon channels if their n parameter is same as shown in table 1. It can be seen that chirality of the tube affects its thermal conductance to a great extent. Among (7,0) and (7,3) CNTs, the number of phonon channels is much larger in the chiral CNT (7,3). Now, considering the length of the CNT, when the shell length reaches l_{mfp}, the thermal conductance will achieve saturation and become a constant, at $l=l_{mfp}$ the thermal conductance $K=K_{ballistic}$. After that, the thermal conductance will decrease linearly with the increase in its length and $K= K_{ballistic} * l_{mfp} / l$. The thermal conductance of a shell can now be written as

$$K_s = \begin{cases} K_{ballistic} & ; \ l<=l_{mfp} \\ K_{ballistic} * l_{mfp}/l & ; \ l>l_{mfp} \end{cases} \quad \{11\}$$

The total thermal conductance of a CNT (K_{CNT}) can now be calculated if we know the number of shells, N_{sh} in the nanotube.

CNT (n,m)	CNT (7,7)	CNT (7,0)	CNT (7,3)
Type of CNT	Armchair	Zigzag	Chiral
Nanotube diameter (nm)	0.949	0.548	0.696
Chiral angle (degrees)	30.0	0.0	17.0
Number of phonon channels	84	84	948
Ballistic Thermal Conductance (W/K)	2.38X 10^{-8}	2.38X 10^{-8}	2.69X 10^{-7}

Table 1 : CNT Thermal Conductance

$$K_{CNT} = \sum_{N_{sh}} K_{sh} \qquad \{12\}$$

For a single wall nanotube, N_{sh} is 1. Therefore, for (7,0) SWNT,

$$K_{ballistic} = K_{th} \text{ X } N_{ph} = 84 \text{ X } 9.46 \text{ X } 10^{-13} \text{ T}$$
$$= 2.38 \text{ X } 10^{-8} \text{ W/K (T=300K)}$$

which is consistent with the recent findings.

Here also, we consider that all the shells of the MWNT are in contact with the metal electrodes at both ends, hence contributing to the total thermal conductance of the tube. When the outer diameter of MWNT increases, the number of shells increase giving rise to a substantial increase in thermal conductance of the tube. The inter shell coupling effect can be ignored for the purpose of calculation of thermal conductance since this effect is very weak [1,7].

1.3 Results and Discussion

ELECTRICAL CONDUCTANCE

The mean free path of electrons in SWNT is typically 1-2 μm. For CNT lengths less than this, electron transport is essentially ballistic within the nanotube and the electrical conductance is independent of length.

However, for lengths greater than the mean free path, conductance decreases (resistance increases) with length of the CNT (figure 2) which has also been confirmed by experimental observations [9]. Figure 3 shows increase in conductance with diameter of SWNT. Figure 4 shows variation in conductance of an MWNT with its length which follows the same pattern as SWNT. However, in case of MWNT, the mean free path is found to be more than that of SWNTs. The D_{inner}/D_{outer} ratio impacts the conductance through changing the number of shells of MWNTs. A smaller value leads to more shells and hence more number of conducting channels leading to a higher conductance. It is seen that for short tube lengths ($l < \lambda$), the conductance increases dramatically with diameter (figure 5). When $l > \lambda$, there is a modest effect on conductance improvement with diameter since the CNT shows Ohmic resistance for the length beyond several micrometers.

THERMAL CONDUCTANCE

Table 1 shows the effect of chirality on the thermal conductance of a CNT. The increase in diameter gives rise to more number of phonon channels hence increasing its thermal conductance (figure 6) .

MWNTs possess high thermal conductance varying with tube diameter, length and number of shells in the tube. When D_{outer} increases, the number of thermal conductance channels increase and in case of an end contact (where it can be reasonably assumed that all the shells are connected to the two electrodes on either end with the metal electrodes), each shell of the CNT would contribute to the thermal conductance of the tube according to its own geometrical parameters leading to a high total conductance.

Now, considering the length of the CNT, when the CNT length is less than the L_{mfp}, the thermal conductance is maximum and is equal to the ballistic conductance, ($K=K_{ballistic}$). After that, the thermal conductance will decrease with the increase in tube length in accordance with {11} (figure 7&8).

1.4 Conclusion

The above results provide an estimation of electrical and thermal conductance for different geometries of both MWNT as well as SWNT. In practice, the observed d.c. resistance of a CNT (at low bias) may be much higher than the resistance derived due to the presence of imperfect metal-nanotube contacts which give rise to an additional contact resistance. It is also to be noted that the thermal conductance depends largely on the tube geometry, mainly its chirality, diameter and length. Therefore, It can be deduced that if we have control on the diameter and length of the CNT while synthesizing them [4,10], it is possible to achieve the desired electrical and thermal parameters of the CNTs to be used in a nano scale device or as an interconnect.

This study would aid in observation of the change in conductance and inductance of nanotubes under different conditions and while using these nanotubes in practical devices.

1.5 Figures

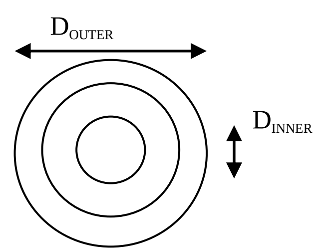

Figure 1 – Cross section of MWNT

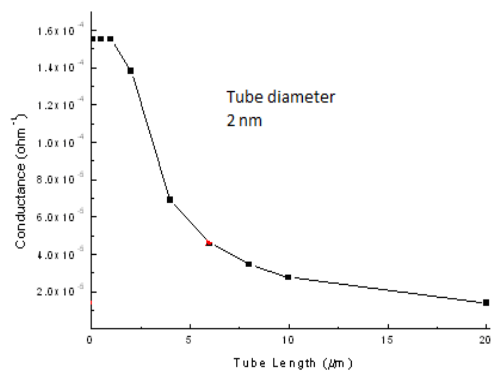

Figure 2 – Conductance v/s. Tube Length (Metallic SWNT - diameter 2 nm)

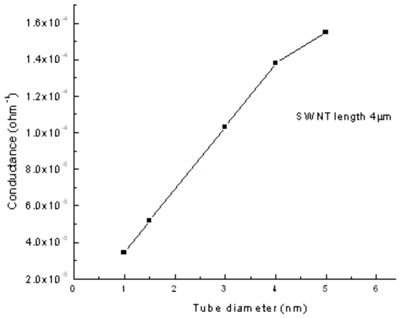

Figure 3 – Conductance v/s. Tube Diameter (Metallic SWNT - length 4µm)

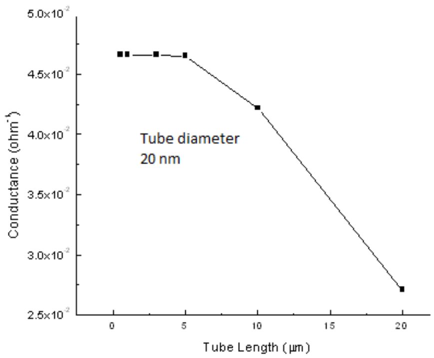

Figure 4 – Conductance v/s. Tube Length (MWNT - diameter 20 nm)

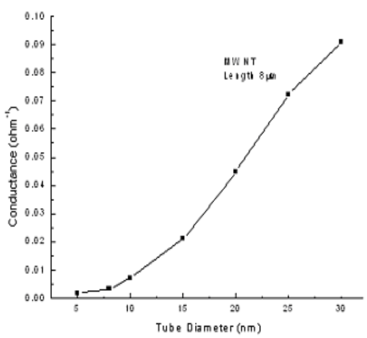

Figure 5 – Conductance v/s. Tube Diameter (MWNT - length 8 µm)

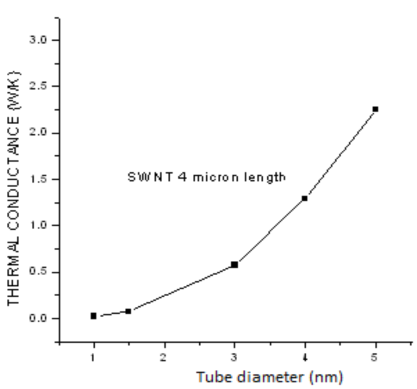

Figure 6 – Thermal Conductance v/s. Tube Diameter (SWNT - length 4µm)

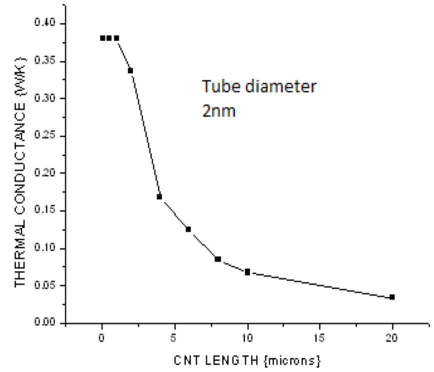

Figure 7 – Thermal Conductance v/s. Tube Length (SWNT – diameter 2 nm)

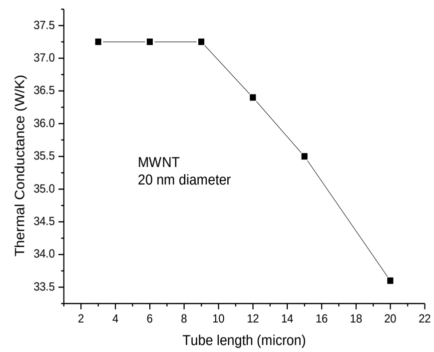

Figure 8 – Thermal Conductance v/s. Tube Length (MWNT – diameter 20 nm)

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