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Manoeuvering electrical & thermal parameters of carbon nanotubes

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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 of the nanotube. On one hand, they can rival the best metal and on the other, a semiconducting nanotube can work as a channel in a nano Field effect transistor. Carbon nanotube (CNT) bundles 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 as well as inductance of a CNT with its geometrical features using a diameter dependent model. Also the dependence of conductance and inductance 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.

INTRODUCTION

Since the discovery of Carbon nanotubes (CNTs)[1], 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). This is further aided by experimental breakthroughs that have led to realistic possibilities of using CNTs in a host of commercial applications like field emission based flat panel displays, semi-conducting devices, hydrogen storage and ultra-sensitive chemical and electromechanical sensors.

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[2-4].

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[5,6]. Findings have also shown that all shells in a MWNT can conduct if they are properly connected to the end contacts[7], leading to a very low overall resistance. In[8], a 25 µm long MWNT with an outer diameter of 100nm is shown to achieve an overall resistance of 35Ω. This is a significant improvement over the early experimental results of resistance values in KΩ/MΩ ranges where it was assumed that only one outer shell in a MWNT conducts.

As can be seen from the density of states (DOS) diagrams of various kinds of CNTs[9,10], they show quantized conductance akin to nanowires. Therefore, conductance of a carbon nanotube can be evaluated using the two-terminal Landauer-Buttiker formula. This formula states that, for a 1-D system with N channels in parallel, the conductance $G=(Ne^2/h)T$, where T is the transmission coefficient for electrons through the sample[11]. 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 $4e2/h$ = 155 µS, which yields a resistance of 6.45 KΩ[11]. This is the fundamental resistance associated with a SWNT that cannot be avoided[12]. This fundamental resistance is equally divided between the two contacts on either side of the nanotube.

An earlier conductance model expressed the conductance per channel as

$$G = G0/(1+l/\lambda) \quad (1)$$

where G0 is quantum conductance, l is the length of CNTs and » is the mean free path[6]. This equation led to different conductance values according to different l values below the mean free path of the CNT:

$$G = 0\ 0.667G0 \text{ for } l = 0.5\lambda \text{ and}$$

$$G = 0.556G0 \text{ for } l = 0.8\lambda.$$

These values are inconsistent with the ballistic properties of CNTs. The ballistic conductance of the CNT should be a constant for any value of l < », which has been demonstrate experimentally[6]. Therefore, the model based on (1) was modified[13] 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, *Douter* and *Dinner* are the maximum and minimum shell diameters respectively. Thus, the diameter of each shell is

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

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

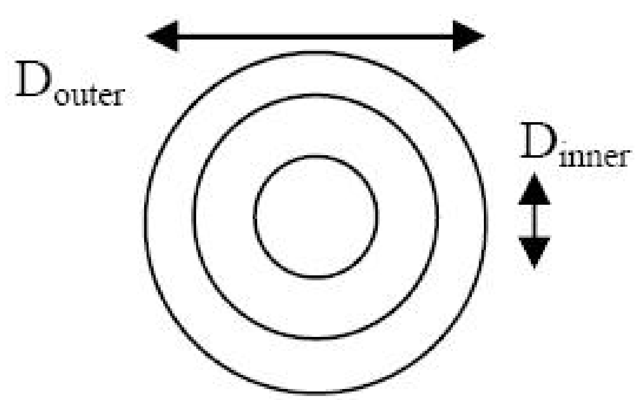

Figure 1 : Cross-section of MWNT

$N_{chan/shell} = (ad+b)r \; ; d>6$ nm

$= 2r \; ; d<6$ nm (4)

where $a = 0.1836$ nm^{-1} and $b = 1.275$[2]

Generally, we have $r = 1/3$ in MWNT or a CNT bundle then (8) becomes

$N_{chan/shell} = (ad+b)/3 \; ; d>6$ nm

$= 2/3 \; ; d<6$ nm

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

$$G_{shell}(d_i,l) = G_i N_{chan/shell} \; ; l<=\lambda$$

$$= G_o N_{chan/shell} \; ; l>\lambda \quad (5)$$

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 $Go= 2q^2 \lambda / h\, l$ is diameter dependent and the channel intrinsic conductance is a constant[13], i.e., $G_i = 2q^2/h = 1/12.9\text{k}\Omega$ (where h is Planck's constant, q the charge of an electron and l the tube length). Here, we consider the perfect contacts and neglect the contact resistance since recently developed fabrication techniques can provide contacts with very small resistance values[6].

Using (5), the conductance of a metallic SWNT with ($N_{chan/shell} = 2$), a given diameter d (0.4nm < d< 4nm) and a length l, can be written as

$$G_{shell}(d,l) = 2\,G_i \; ; l <= \lambda$$

$$= 2\,G_o \; ; l > \lambda$$

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 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. We have considered the conductance at T = 300K (room temperature) in the tube direction and the impact of inter-shell interaction is not included.

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[4]. 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[14], 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}[14].

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

$K_{th} = \pi^2 k_B^2 T / 3h = 9.46\text{X}10^{-13}\,T$; where 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

$$N_{ph} = 12\,(n^2+mn+m^2)/\,d_R \;\text{[14]} \quad (8)$$

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 "3 b_0 and b_0 = 0.142 nm is the equilibrium interatomic distance[15]. 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 the TABLE.

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

$$K_s = K_{ballistic}; l<=l_{mfp} \tag{11}$$

TABLE 1 : CNT parameters associated with thermal conductance

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 hexa - gons (unit cell)	14	14	158
Atoms in unit cell	28	28	316
Number of phonon channels	84	84	948
Ballistic thermal conductance (W/K) At T=300 K	2.38×10^{-8}	2.38×10^{-8}	2.69×10^{-7}

$$= K_{ballistic} * l_{mfp} /l; l>l_{mfp}$$

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.

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

For a single wall nanotube, N_{sh} is 1.

Therefore, for (7,0) SWNT,

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

which is consistent with the recent findings[17].

For MWNT, number of shells (N_{sh}) would vary with the inner and outer diameters of the tube as given by (2).

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[3-14].

INDUCTANCE OF CNT

CNT has two kinds of inductances: magnetic inductance and kinetic inductance.

Kinetic inductance

The kinetic inductance represents the kinetic energy of electrons, which is a per unit length quantity for each conduction channel in a CNT shell[19]. One conduction channel consists of spin-up and spin-down electrons and its kinetic inductance[20] is

$$L_{K,Chan} = h/4e^2 v_F = 8\ nH/\mu m \tag{13}$$

where h is Planck's constant, e is the charge of a single electron and v_F is the Fermi velocity in graphite.

The kinetic inductance value of an individual SWCNT/MWCNT is in the range of nH/μm, which is several orders larger than the corresponding magnetic inductance (in the range of pH/μm). One can neglect the magnetic inductance in such analysis[20].

As is the case with conductance, the kinetic inductance of a nanotube will also depend on the total number of shells, N_{sh} and the number of conduction channels of each shell.

The metallic shells/tubes inside a CNT bundle contribute to the number of conduction channels and so do the semiconducting shells with large diameters ($d_i > 4$ nm). For SWCNTs ($d < 4$nm), only metallic tube has energy levels to cross its Fermi level, providing conduction channels. Semiconducting tube does not provide any conduction channels. However, for MWCNT $N_{chan/shell}(d_i)$,

Using $N_{chan/shell}(d_i)$, the MWNT kinetic inductance is calculated

$$L_{k,MW} = L_{k,chan} / \sum_{N_{sh}} N_{chan/shell}(d_i) \quad nH/\mu m \tag{14}$$

Here, only room temperature $T = 300$K is considered and the inter-shell interaction is not included. When the MWNT diameter gets larger, the number of the conduction channels increases and the kinetic inductance of the MWNT decreases. (14) can estimate the kinetic inductance of a SWNT as a special case: a metallic SWNT consists of 2 conduction channels, leading to an inductance of 4nH/μm.

Magnetic inductance

The magnetic inductance depends on the magnetic fields inside and between the tubes. It involves partial self-inductance of each tube and the mutual inductance amongst tubes. From (14) we can see that larger bundles consist of more CNTs and conduction channels, reducing the kinetic inductance values but for a single CNT and a small bundle, the kinetic inductance is several orders higher than the magnetic inductance. When the bundle width increases, the kinetic part decreases more rapidly than the magnetic part. Therefore, the inductance estimation of a large CNT bundle needs to consider both kinetic and magnetic inductances.

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). This has also been confirmed by experimental observations[16]. 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. Figure 5 shows variation in conductance with diameter of MWNT. The

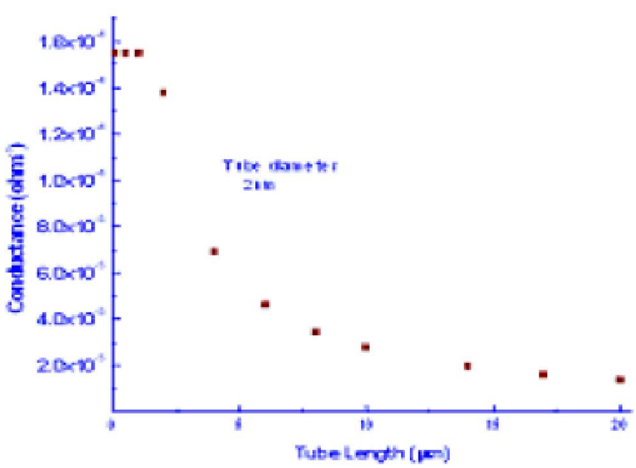

Figure 2 : Conductance v/s. tube length (Metallic SWNT - diameter 2 nm)

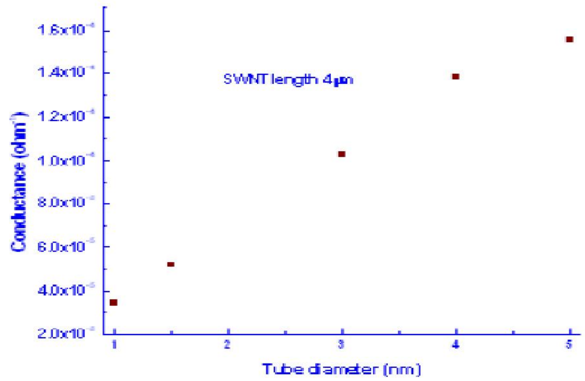

Figure 3 : Conductance v/s. tube diameter (Metallic SWNT - length 4µm)

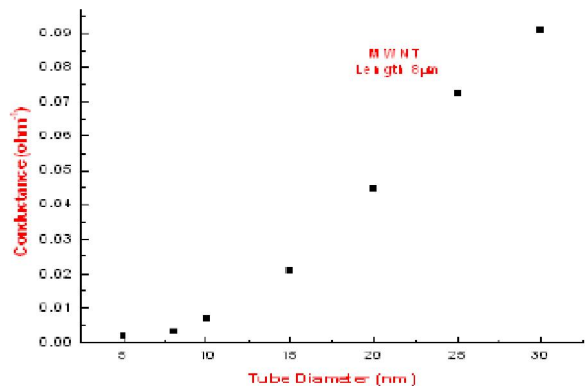

Figure 4 : Conductance v/s. tube diameter (MWNT - length 8 µm)

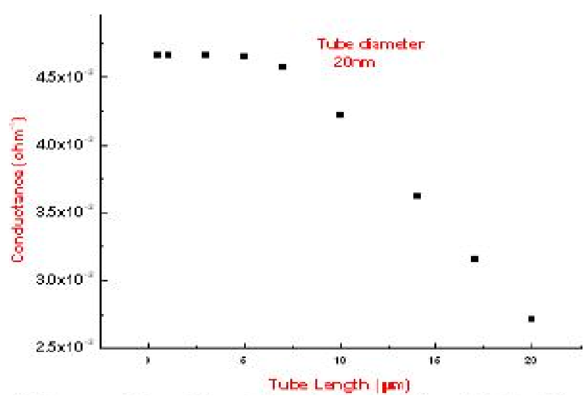

Figure 5 : Conductance v/s. tube length (MWNT - diameter 20 nm)

D_{inner}/D_{outer} ratio impacts the conductance through changing the number of shells of MWCNTs. 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. 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).

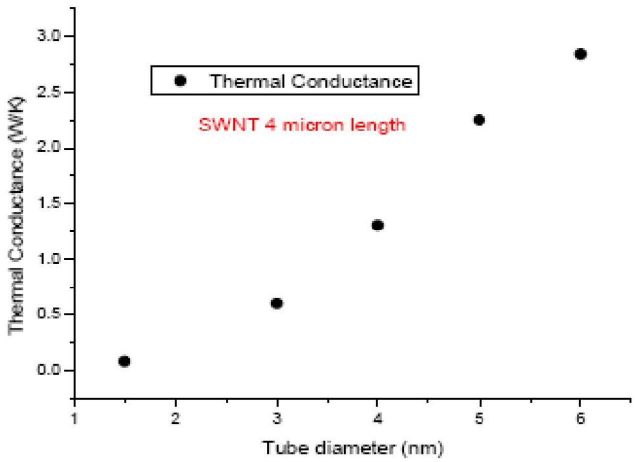

Figure 6 : Thermal conductance v/s. tube diameter (SWNT - length 4μm)

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 (figure 9).

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).

Inductance

The total inductance of a CNT is obtained by adding the kinetic and magnetic parts together. In case of a single shell as in SWNT, Magnetic inductance is negligible as compared to the Kinetic inductance (figure 10) so it can be ignored.

In case of a MWNT, the D_{inner}/D_{outer} ratio impacts the inductance through changing the number of shells and hence number of conduction channels (both metallic and

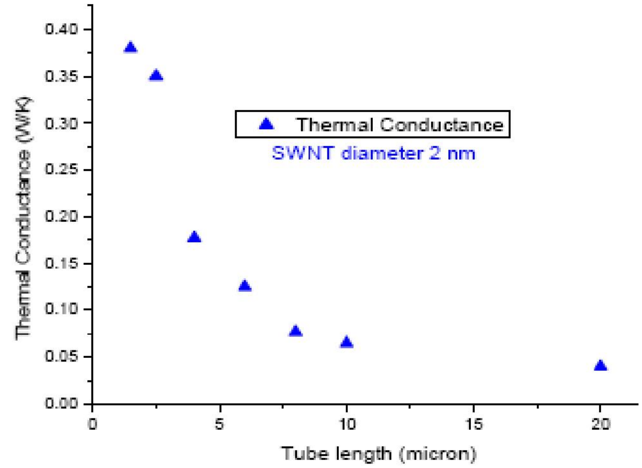

Figure 7 : Thermal conductance v/s. tube length (SWNT – diameter 2 nm)

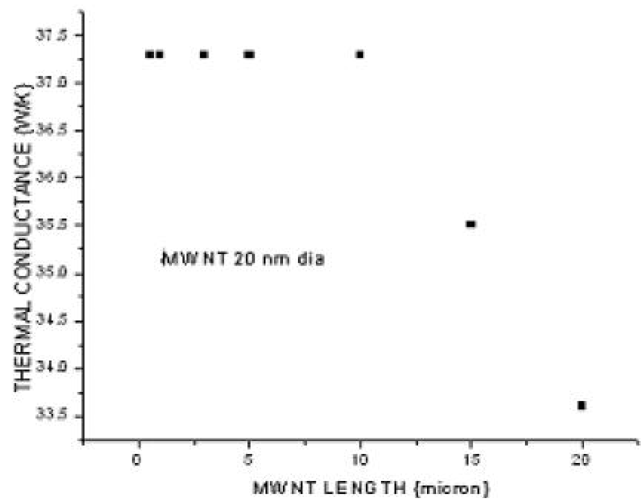

Figure 8 : Thermal conductance v/s. tube length (MWNT – diameter 20 nm)

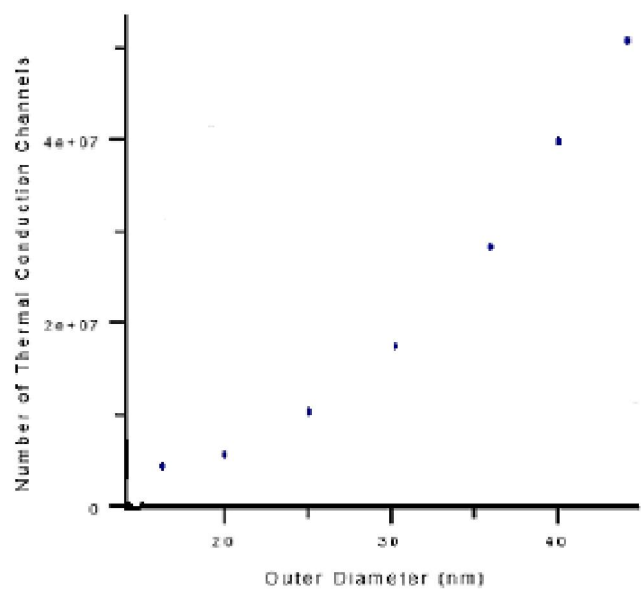

Figure 9 : No. of TC channels v/s. MWNT diameter

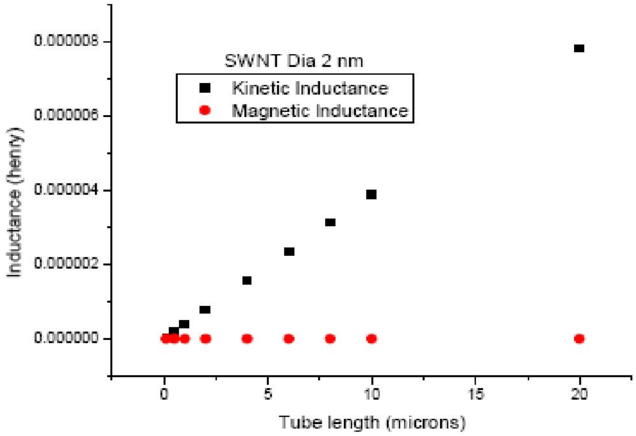

Figure 10 : Inductance v/s. tube length (SWNT – diameter 2 nm)

semiconducting shells contribute to the conduction channels[6] decreasing the kinetic inductance and making it comparable to the magnetic part inductance (figure 11 & 12).

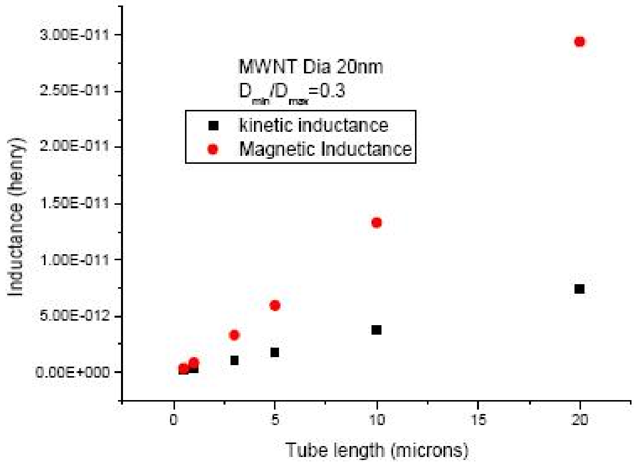

Figure 11 : Inductance v/s. tube length (MWNT – diameter 20 nm)

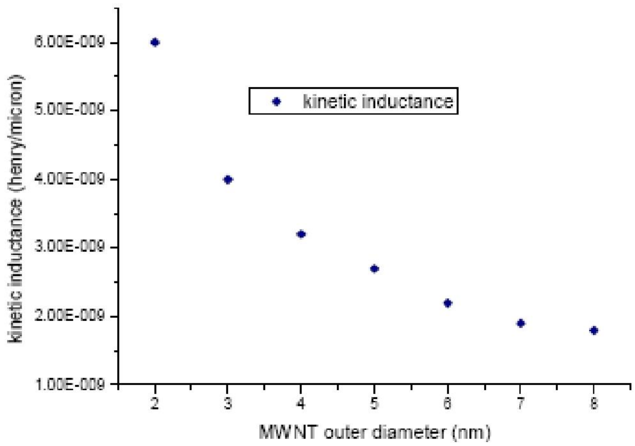

Figure 12 : Kinetic inductance v/s. outer diameter (MWNT per unit length)

Diameter and length are important factors in determining both magnetic and kinetic inductances. When the diameter increases, kinetic and magnetic inductances will reduce as number of conduction channels increases whereas the increase in length will have an opposite effect, increasing inductances.

CONCLUSION

The above results provide an estimation of electrical and thermal conductance and inductance 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. The total resistance of a CNT is then expressed as the sum of resistances arising from three aspects : the fundamental CNT resistance, scattering resistance and the imperfect metal-nanotube contact resistance. The total resistance therefore becomes so high that it masks the observation of intrinsic transport properties of a CNT. The observed resistance for CNTs has typically been in the range of 100 KΩ although few people have reported the resistance to be <10 KΩ (the lowest observed resistance being ~7 KΩ approaching the theoretical limit)[7].

It is also to be noted that the thermal conductance depends largely on the tube geometry, mainly its chirality, diameter and length. Similarly inductance is also highly dependent on length and diameter of a CNT. Therefore, It can be deduced that if we have control on the diameter and length of the CNT while synthesizing them[7-18], 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.

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