

## INVESTIGATION OF THERMAL CONDUCTIVITY OF SINGLE-WALL CARBON NANOTUBES

by

**Mahmoud Jafari<sup>\*</sup>, Majid Vaezzadeh, Mohamad Mansouri,  
and Abazar Hajnorouzi**

Department of Physics, Faculty of Science, K. N. Toosi University of Technology, Tehran, Iran

Short paper

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*In this paper, the thermal conductivity of single-wall carbon nanotubes is determined by lattice vibrations (phonons) and free elections. The thermal conductivity is modeled up to 8-300 K and the observed deviations in K-T figures are explained in terms of phonon vibrations models. An suitable theoretical model is shown for thermal conductivity behavior with respect to temperature and is generalized for experimental results. This model enables us to calculate the thermal conductivity and the thermal potential energy of single-wall carbon nanotubes.*

*Key word: single-wall carbon nanotube, thermal conductivity, specific heat capacity, thermal potential energy*

### Introduction

Graphite structures in nano scale, the carbon nanotubes are studied not only for their electronic and mechanical properties, but also for their thermal properties. Single-wall nanotubes (SWCNT) have thermal conductivity equal or more than that of diamond and graphite [1].

As diamond and graphite display the highest thermal conductivity at moderate temperatures, is likely that be greater and more outstanding in this regard. Indeed recent theoretical work [2] predicts that the thermal conductivity of nanotubes is as high as 6600 W/mk. Thus, SWCNT could be used as cooler in micro and nano electrical devices, particularly, in ultra-large scale integration (ULSI) (so complex circuits) [3]. In addition, at low temperature, the thermal conductivity should show effects of 1-D quantization in thermal capacity.

The thermal conductivity of SWCNT has been investigated both experimentally and theoretically. Experimental results were investigated by Hone *et al.*, on crystal ropes of SWCNT from 350 K to 8 K [4].

Hone *et al.* experimentally demonstrated the temperature-dependent of thermal conductivity of bundles of SWCNT. From 8 K to 350 K, the thermal conductivity is decreased smoothly by decreasing as well and displayed linear temperature dependence below 30-8 K. The absence of a maximum in  $k(T)$  prevents phonon convert scattering processes.

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\* Corresponding author; e-mail: jafari@kntu.ac.ir

The ratio of the thermal and electrical conductivity indicates that the thermal conductivity is dominated by phonons at all temperatures.

In this study, by using the experimental results, the thermal conductivity temperature dependence is studied theoretically. We use electrical and thermal conductivity similarities and after calculating thermal potential energy (TPE) of nanotube systems, these parameters will obtain by mathematical model and presents information about carriers and thermal conductivity mechanisms.

### Theory and model

According the basic concepts of solid state physics, the heat can be transported through solid materials by means of electric and thermal currents, and it can also be considered as a factor for thermal current within a good approximation. The difference lies in the fact that in the former case, the electrical power is:

$$P_{(\text{watt})} = \frac{dW}{dt} = IV = nevA \frac{U}{e} = nvAU \quad (1)$$

where  $V$ ,  $n$ ,  $v$ ,  $u$ , and  $A$  are electrical potential, electrons per unit volume, velocity, and cross-sectional area, respectively.

Similarly, for heat conduction we have:

$$H_{(\text{watt})} = \frac{dQ}{dt} = kA \frac{\Delta T}{\Delta x} \quad (2)$$

where  $k$  and  $\Delta T/\Delta x$  are thermal conductivity and temperature variation with respect to the displacement.

According to eqs. (1) and (2), electrical power and heat conduction have similar dimension. In this paper based on similarity between electric and thermal conductivity properties, we will obtain for eq. (2), similar formularization as eq. (1).

Suppose the TPE is noted  $U$ . This parameter can play the role of electrical potential energy for the case of heat conduction.

As we know from the basic concepts of solid state physics, the heat can be flowed in solid materials by means of electric and thermal currents, it can also be considered as a factor for thermal current within a good approximation. The difference lies in the fact that in the former case, the electrical potential energy leads to electron transport and in the later case thermal potential energy,  $U$ . Dependence of thermal conductivity to phonon vibration is encoded in the thermal potential energy which is formulated in a straightforward manner and will be discussed in the next sections.

By implementing the Newton's second law, one can attain the electron velocity ( $V$ ):

$$m \left| \frac{dv}{dt} \right| = eE = \frac{\Delta u}{\Delta x} \quad (3)$$

where  $m$ ,  $v$ ,  $t$ ,  $e$ ,  $E$ ,  $\Delta u/\Delta x$  are electron mass, electron velocity, time, electric charge, electrical field, potential energy variation with respect to displacement, respectively.

Then by integrating eq. (3) and using eqs. (1) and (2) we obtain:

$$v = \frac{\tau \Delta u}{m \Delta x} \quad \rightarrow \quad H = \frac{dQ}{dt} = nvAU = \frac{n\tau U \Delta u}{m \Delta x} \quad (4)$$

where  $\tau$  is the relaxation time. Using eqs. (2) and (4), we obtain the thermal conductivity ( $k$ ) as follow:

$$kA \frac{\Delta T}{\Delta x} = \frac{nU\tau}{m} \frac{\Delta u}{\Delta x} \rightarrow k = \frac{nU\tau}{m} \frac{\Delta u}{\Delta T} \quad (5)$$

On the other hand the specific heat capacity is  $C_v = \Delta u / \Delta T$  [ $\text{mJg}^{-1}\text{K}^{-1}$ ]:

$$k = \frac{nU\tau}{m} C_v \quad (6)$$

and the electrical conductance ( $\sigma$ ) [5] is:

$$\sigma = \frac{ne^2\tau}{m} \quad (7)$$

Consequently, we obtain the thermal conductivity as a function of the TPE, specific heat capacity, and electrical resistance ( $\rho$ ):

$$k = \frac{nU\tau C_v}{m} = \frac{ne^2U\tau C_v}{me^2} = \frac{UC_v}{\rho e^2} \quad (8)$$

An important parameter in eq. 8 is the thermal potential energy ( $U$ ). In order to obtain  $U$ , values for  $\rho$  and  $C_v$  are required. These parameters can easily be determined. By using experimental data and normalized theoretical equations  $\rho$  and  $C_v$  would be determined at temperature of 300 K.

According to theoretical data and comparing them with obtained experimental results from fig. 1 [6], it is drawn for electrical resistance and allows us to draw out the following equation for electrical resistance:

$$\frac{\rho}{\rho_{300}} = \exp\left(\frac{T_0}{T}\right)^{\frac{1}{n+1}} \quad (9)$$

Figure 1, shows the direct current electrical resistance for SWCNT sample as a temperature function from 300-4.2 K.

By taking advantage of experimental data, thermal conductivity a SWCNT sample dependent to temperature, and using “creation function” of the theory model  $Y(T)$ , “destruction function”  $X(T)$ , “creation and destruction function”  $Z(T)$  on different temperature spans, fig. 2, we can draw thermal conductivity.

The experimental result [4], fig. 2, shows that thermal conductivity curve has two critical temperatures, at 30 K and 225 K. At low temperature, thermal conductivity behavior as a function of temperature depends on free electrons and has linear temperature dependence. This linearity will continue up to 30 K and can be formulated by destruction function  $X(T)$  [7]:

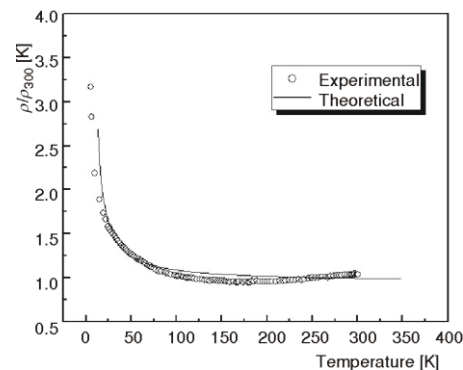


Figure 1. Resistance temperature dependence of SWCNT sample [6]

$$k_1 = ATX(T) \rightarrow X(T) = \frac{1}{1 + e^{\gamma(T/T_c - 1)}} \quad (10)$$

$X(T)$  in eq. (10) is called destruction function because it has a minus sign in its exponential term for  $T < T_c = 30$  and for plus sign, the function will be strictly falling.  $\gamma$  is the sharpness parameter, and  $T_c$  is the critical temperature. After 30 K, some of phonon modes begins to appear and will continue to 225 K. Thermal conductivity is expressed as a destruction function of  $T^{5/4}$  and formulated by creation and destruction function  $Z(T)$ .

$$k_2 = BT^{5/4}Z(T) \rightarrow Z(T) = \frac{1}{1 + e^{\gamma(T/(T_c + \delta T) - 1)}} + \frac{1}{1 + e^{\gamma T/(T_c - 1)}} \quad (11)$$

$\delta T$  is relevant to second critical point in thermal conductivity curve.

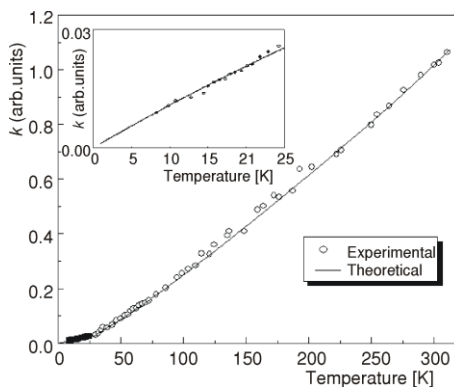
Finally, increasing the temperature from 225 K to 300 K, causes activating other phonon mode ( $TA$ ) and change thermal conductivity as  $T^{3/2}$  functions, and formulated by creation function  $Y(T)$ , and as a result of thermal conductivity it is:

$$k_3 = CT^{3/2}Y(T) \rightarrow Y(T) = 1 - X(T) \quad (12)$$

$Y(T)$  is called creation function for  $T > 225$  K and eq. (12) will be strictly rising for positive values of  $\gamma$ . Therefore, thermal conductivity ( $k$ ) for temperature span 8-300 K is as follow:

$$k = \sum k_i = k_1 + k_2 + k_3 = \left\{ \begin{array}{l} ATX(T) \longrightarrow T \leq 30 \text{ K} \\ BT^{5/4}Z(T) \longrightarrow 30 \text{ K} \leq T \leq 225 \text{ K} \\ CT^{3/2}Y(T) \longrightarrow 225 \text{ K} \leq T \leq 300 \text{ K} \end{array} \right\} \quad (13)$$

where  $A$ ,  $B$ , and  $C$  are constant confidents.



**Figure 2. Temperature dependent on thermal conductivity of SWNT sample [4, 8]**

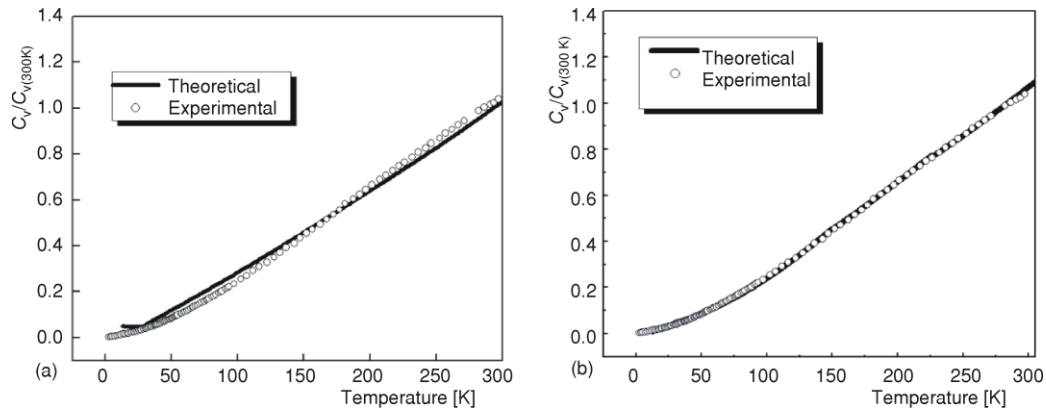
Figure 2, correspond of proposed model with experimental data of thermal conductivity a SWCNT sample dependent to temperature [4].

So represent the correspondence between the theoretical and measured experimental thermal conductivity ( $k$ ) in the range of 350 to 8 K for the SWCNT sample. The inside fig. 2 shows the low-temperature behavior. Near 30 K and 225 K,  $k(T)$  slope changes; below 30 K temperature,  $k(T)$  is strictly linear in temperature and extrapolates to zero at  $T = 0$ .

### Thermal potential energy

The specific heat capacity refers to 300 K by using eq. 8 is directly related to  $\rho$ ,  $k$ , and inversely to  $U$ .

In fig. 3 we observe difference between  $C_v$  experimental [8] and theoretical (eq. 8) after normalized to 300 K. Figure 3(a) shows temperature dependence of capacity specific for single-wall nanotubes for the mean value of  $U \sim 1.056$  (continued line), and fig. 3(b) shows



**Figure 3.** Difference between  $C_v$  experimental [8] and theoretical (eq. 8) after normalized to 300 K (a) when apply average value for  $U = 1.056$  and (b) for the case using eq. 14

the thermal capacity of single-wall nanotubes experimentally for the case using eq. 14 (straight line).

Figure 3(a) obviously shows that TPE varies smoothly in the range of 8-300 K. For this reason, the average value has been utilized. In temperature range of  $30\text{ K} < T < 150\text{ K}$ , the interaction of, electron-phonon has less effect than in the temperature range of  $225 < T < 300$ . Thus TPE is supposed to be less than its mean value at low temperatures. In addition in the temperature range of  $225\text{ K} < T < 300\text{ K}$ , the TPE is greater than the mean value.  $U$  is the temperature function and shows that does not vary extensively by temperature. Its temperature dependence is mostly due to the quantities  $C_v$  and  $\rho$  from eqs. (8) and (9), respectively:

$$U(T) = \alpha T^\beta \quad (14)$$

where  $\alpha$  and  $\beta$  are the parameters of fitting data are given in tab. 1.

**Table 1.** The parameters of fitting data

$\alpha$	$\beta$	$T$ [K]
0.00185	1.75	30
0.06	0.5	30-150
0.15	0.3	150-225
0.43	0.1	225-300

## Conclusion

The thermal conductivity of SWCNT was investigated for free electrons and phonon modes vibrations. The thermal conductivity was also simulated as a function of  $T$  (free electrons),  $T^{5/4}$  and  $T^{3/2}$  (phonon modes). The contribution of phonons modes play a dominant role in the thermal conductivity of SWCNT up to 300 K. So we use  $U(T)$ , this was carried out by fitting three experimental curves;  $k$ ,  $\rho$ , and  $C_v$ . Moreover,  $U(T)$  is smoothness function of  $T$ , which can be changed, according to the amount of interactions between electron and phonon.

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