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Temperature Dependent Thermal Properties in Single-Wall Carbon Nano Tubes Based on Phonon Scattering

Md. Alamgir Kabir[1], Rumelia Murshed[2], Ummul Husnaeen[3] & Zahid Hasan Mahmood[4]

[1,2,3]Dept. of Applied Physics, Electronics & Communication Engineering, Dhaka University, Bangladesh
[4]Professor, Dept. of Applied Physics, Electronics & Communication Engineering, Dhaka University, Bangladesh

ABSTRACT

Electronic devices and integrated systems are reduced to the size of micron and nanometer level and it becomes particularly important to predict the thermal transport properties of the components. Because of a unique structure and novel properties of carbon nanotubes (CNTs) have attracted significant attention. In this article, thermal transport properties of single wall CNTs (SWCNTs) are introduced. Combining equilibrium and non-equilibrium molecular dynamics with carbon potentials, we have studied the thermal conductivity of carbon nanotubes and its dependence on temperature. Phonon conduction depends on band gaps as well as thermal contact resistance of metallic CNTs, governed by phonon scattering and it shows evidence of 1-D quantization of the phonon band structure. We have studied here the thermal conductivity of single wall nanotubes dependence on chirality structure, dimensions of tubes, defects and vacancies in tubes. We found that the single wall carbon nanotubes have very high thermal conductivity comparable to diamond crystal and in-plane graphite sheet.

Key words: Thermal transport, Phonon, Green–Kubo method, Quantization, Umklapp scattering, Wiedemann-Franz law

1 INTRODUCTION

The pursuit for reducing the size of electronic devices and integrated Nano-Electro-Mechanical Systems (NEMS) provides the main driving force behind the research and technological advancement in nanotechnology. It is now broadly accepted that the thermal management issue in nano-sized devices becomes increasingly important as the size of the device reduces. Therefore, the thermal transport behaviors of nanomaterials plays substantially critical role in controlling the performance and stability of nano devices. Among various latent candidates for future nanoelectronics and various nanotechnology, carbon nanotubes (CNTs) have a unique position. Their remarkable properties, such as great strength, light weight, special electronic structures and properties and high stability, make carbon nanotubes the ideal material for a wide range of applications.

However, Single-wall carbon nanotubes (SWCNTs) have sparked great scientific and engineering interest because of their outstanding electrical and thermal properties. Consequently, they have been proposed for applications in integrated circuits (as transistors or interconnects) and in thermal management (as thermal interface materials) (Eric Pop 2006). The direct and quantitative measurement of thermal transport properties of individual nanotube is challenging, due to technological difficulties associated with nano-scale experimental measurements.

2 PHONON THERMAL TRANSPORT THEORY OF CNT

The transport of thermal energy in CNTs is assumed to be mainly related to a phonon conduction mechanism like to other metallic materials. The phonon conduction in nanotubes is influenced by several processes such as the number of phonon active modes, the boundary surface scattering, the length of the free path for the phonons and inelastic Umklapp-scattering (a harmonic phonon-phonon or electron-phonon scattering process). Thermal transport behaviors or conductivity of CNTs depends on an atomic arrangement, the diameter and length of the tubes, the number of structural defects and the morphology, as well as on the presence of impurities.

Since the mechanism of the thermal energy conduction by phonons or electrons depends profoundly on the band gaps of materials, the thermal transport mechanism of CNTs is much dependent on chirality of CNTs which determines the size of their band gaps. The largest band gap (order of 1.5 eV) is found in nanotubes with (n, m) indices satisfying the condition: $|n-m| \neq 3p$, where p is an integer. For other types of nanotubes, the band gap is considerably smaller in the case of armchair nanotubes ($n = m$). Thus, electronic contribution to the thermal conductivity will be significant in metallic CNTs with a small band gap (Dresselhaus 2010). On the other hand, thermal conductivity of chiral CNT is mainly governed by phonon. Unlike phonon thermal conductivity, electron thermal conductivity of CNTs for metallic CNTs is seldom reported. Thermal conductance of metallic CNTs may be profoundly dominated by phonons rather than electrons. Moreover, thermal contact resistance at high bias voltage is significant property in thermal conduction. However, this is happened due to the fact that, the theoretical treatment of CNTs as purely metallic, whereas only a small fraction of the crystalline ropes of CNTs in the experiment will be metallic and contribute to thermal transport.

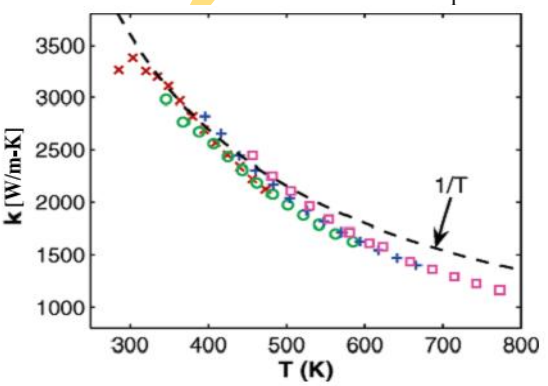


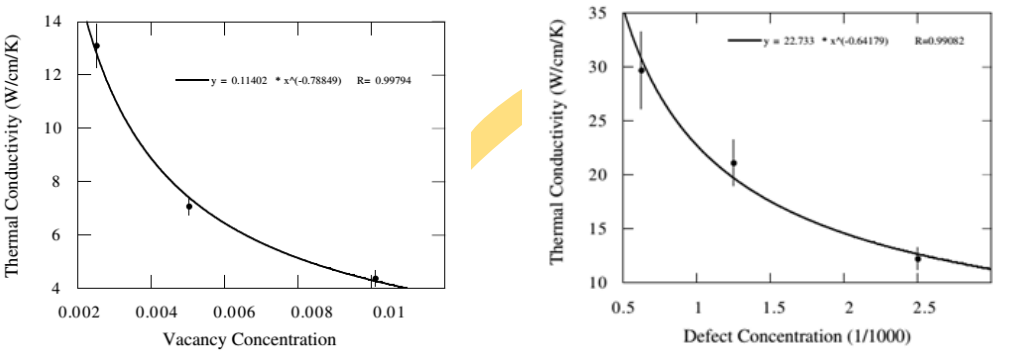
Figure 1. Extracted values of the thermal conductivity vs. average SWCNT temperature. Squares corresponding to data taken in 400 K ambient and so on. The dashed line indicates the 1/T trend expected due to Umklapp phonon scattering.

Thermal transport characteristics of single wall CNT under temperature variability is evaluated for phonon interaction. A plot of best-fit thermal conductivity at every bias point versus average temperature can be obtained, as shown in Fig. 1. It is carried out that the electrical characterization at various ambient temperatures from 250 to 400 K, the phonon thermal conductivity is therefore, deduced approximately from 300 to 800 K. This observed trend of the high-temperature thermal transport behavior in Fig. 1 is consistent with Umklapp phonon-phonon scattering, which gives an approximately 1/T temperature dependence.
However, more subtle effect should be noted at the upper end of the temperature range and that is a drop of the thermal conductivity at a higher rate than 1/T. This behavior is attributed to second-order three-phonon scattering processes, whose scattering rates are proportional to T, leading to a thermal conductivity that scales as 1/ (αT+βT2), Where, α and β are constants. But this has been observed in Si and Ge thermal transport behavior rather than CNT. The three phonon scattering process likely involves a harmonic interaction of two acoustic modes and one optical mode and the optical mode is raised significantly for metallic SWCNTs at high temperature. In this case phonon thermal conductivity suppresses electron thermal conductivity.

3 Thermal Transport Properties of Single Walled Carbon Nano Tubes

Vacancy and Defect concentration effect in thermal conductivity

The high value of thermal conductivity is for a pure and defect-free carbon nanotubes. However, nanotubes can have natural defects and vacancies where topological and vacancy defects are more severe in SWCNT. Topological defects like non-hexagonal carbon rings and vacancy-related defects can form during the nanotube growth process or after synthesis (JianweiChe 2000).



(a) (b)

Figure 2.(a) Thermal conductivity as a function of vacancy Concentration. (b) Thermal conductivity as a function of defect concentration [1].

In Fig. 2 (a), the thermal conductivities are calculated for various vacancy concentrations. It is shown that, the thermal conductivity decreases as the vacancy concentration increases. The vacancies should have much severe effects in one-dimensional (1-D) materials (carbon nanotubes can be thought of as a quasi 1-D wire) than in 3-D ones. The 1-D material like CNT get this vacancy effect probably for that, it has no strong valence

double bond providing effective additional channels for phonons to bypass the vacancy sites. This probable bypassing could be present in 3-D materials.

Similarly, conformational defects can also reduce the thermal conductivity significantly. One of the common conformation defects in nanotubes is where four hexagons change into two pentagons and two hexagons. Fig. 2 (b) shows how this conformational defect affects the overall thermal conductivity of single wall CNTs. However, compared with vacancies, the conformational defect is a major form of point defect. Besides phonons are scattered more as defect effects dominate which leads to less thermal transport in ambient temperature.

3.1 Temperature dependent intrinsic thermal transport

Fig. 3 represents the measured thermal conductivity k of a SWCNT sample as a function of temperature from 350 K to 8 K. From 350 K to 40 K, k decreases smoothly with decreasing temperature with very little curvature. The inset to Fig. 3 shows the low-temperature behavior. Thermal transport parameter, k (T) changes slope Near 30 K where below this temperature, k (T) is strictly linear with temperature rising and extrapolates to zero at T=5K. This behavior is identical in all types of carbon nanotube samples but the intrinsic nature in thermal transport in nanotube bundles is significant. Moreover, the practical temperature dependent thermal conduction is deviated from the theoretical value due to irregular geometry of nanotube.

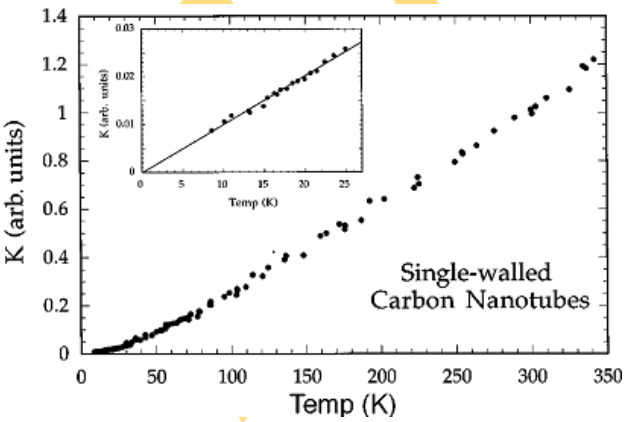


Figure 3. Temperature-dependent intrinsic thermal conductivity of single walled carbon nanotube. The inset shows the low-temperature behavior in greater detail [18].

3.2 Thermal conductivity in various chirality of CNT

The phonon thermal conductivity of a CNT was found to have dependence on its chirality. Using the homogeneous non-equilibrium Green–Kubo method, the temperature dependences of the thermal conductivities of (11, 11), (20, 0), (10, 13) nanotubes with nearly equal radii were calculated.

As shown in Fig. 4, the thermal conductivities of three types of nanotube according to chirality are counted to have similar temperature dependence. In the range from 100 to 400 K, the conductivity of the (11, 11) nanotube was lower than that of the (20, 0) nanotube, while the (10, 13) nanotube showed lower values of thermal conductivity compared with other types of nanotubes

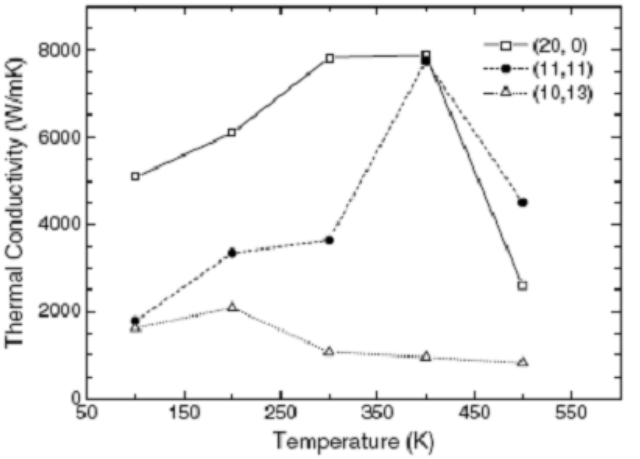


Figure 4. Thermal conductivities of (20, 0)-open squares, (11, 11)-solid circles, and (10, 13)-open triangles, single wall nanotubes [10].

3.3 Effect of different diameter of CNT in thermal transport

It is well known to account that CNTs are characterized by a large aspect ratio and a huge surface area. Structure size of CNTs is particularly important because the phonon mean free paths in nanotubes are thought to be relatively long. At low temperature, SWCNT samples exhibit a linear thermal conductivity, K (T), strongly suggesting quantization effects. Measuring the K (T) of SWCNT samples with varying diameters: the phonon sub-band splitting is higher in smaller-diameter tubes, so that the linear K (T) behavior should extend to the higher temperature.

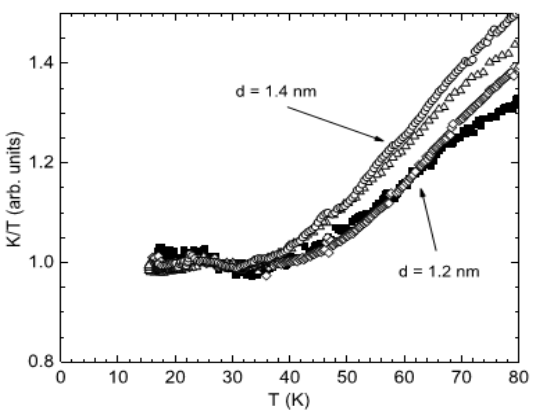


Figure 5. Thermal conductivity divided by temperature for SWCNT samples with average diameters of 1.2 nm and 1.4 nm [11, 21].

Fig. 5 shows the thermal conductivity divided by temperature (K/T) of two nanotube samples with diameter of 1.2 nm and 1.4 nm. In both samples, K/T approaches a constant value at low T (temperature), just as is expected for 1-D channels. At higher temperatures, K/T increases like somewhat expotentially, as more phonon modes introduce.

In the 1.2-nm diameter sample, the upturn in K/T occurs almost 5 K higher than in the 1.4-nm diameter sample.

3.4 Effect of different length of CNT in thermal transport

The dependence on sample size (L) is also eliminated at high temperatures, when the thermal conductivity is limited by phonon-phonon scattering rather than by scattering with the sample boundaries. Fig. 6 depicts the estimated thermal conductivity versus temperature for SWCNTs of various lengths, demonstrating sensible agreement with thermal transport behavior. However, this study shows empirical findings of the SWCNT thermal conductivity in the 0.5-10 μm length range and the 100-800 K temperature range. These phenomena can be explained by the variable ratio between the phonon mean free path and the CNT length.

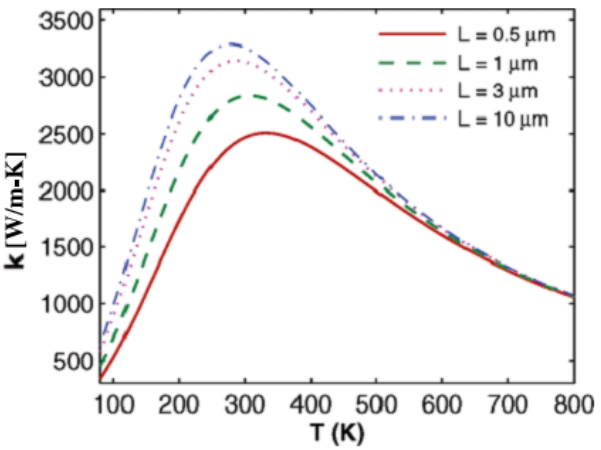


Figure 6. Analytic plot of the intrinsic thermal conductivity over the 100-800 K temperature range for various length of SWCNT. The length dependence is included heuristically with a simple scaling argument.

Based on these results, the thermal transport behavior is expected to become constant when the tube length is much longer than the mean free path of energy-carrying phonon and also the different behaviors at low and high temperatures.

3.5 Thermal conductivity of SWCNT compared to 2-D graphene sheet and 3-D graphite

The observed thermal conductivity of SWCNT displays a temperature dependence that is different from that of graphite with noticeable manner, even though both materials are composed of graphitic sheets. Fig. 7 shows three types of carbon device: Comparison of calculated thermal conductivity of nanotubes, single plane of graphene and 3-D graphite.
In graphite, when graphene layers are stacked in graphite, the interlayer interactions quench the thermal transport magnitude by nearly 1 order of magnitude. It is likely that the same process occurs in nanotube bundles. Thus, it is significant that the coupling between tubes in bundles is weaker than expected and it may be an advantage for thermal applications. In high-quality graphite, thermal conductivity, which is dominated by acoustic phonons, varies up to 150 K, at which point phonon-phonon Umklapp scattering causes k to decrease rapidly with increasing T. pure graphite samples can have a thermal conductivity near 6000 W/m-K at the peak and 2000 W/m-K at room temperature.

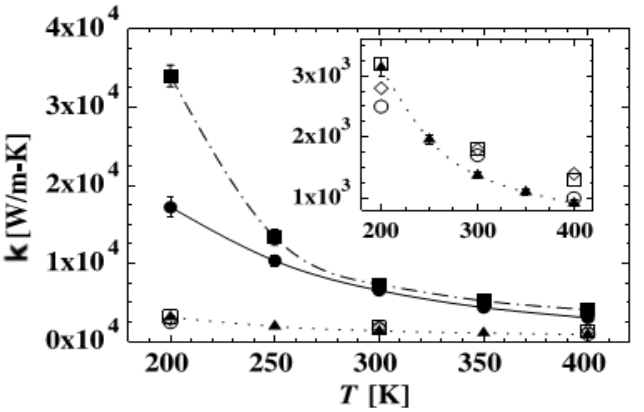


Figure 7. Calculated nanotube thermal conductivity (solid line) compared to the thermal conductivity of a 2-D graphene sheet (dot–dashed line) and a 3-D graphite sample (dotted line)

3.6 Thermal conductivity of SWCNT according to thermal contact resistance

The electrical contact resistance of SWCNT is the order of 10-100 kΩ with adjustable parameter Rc. It is assumed that, Rc is temperature dependent and used Pt electrode is isothermal. This mainly affect the slope of I-V curve at low bias. And quantum contact resistance is adjusted in series connection. It is usually happened due to intrinsic photon-limited resistance of SWCNT. The thermal contact resistance is the order of 5–10× 106K/W by introducing Neumann boundary conditions in the heat conduction equation:

$$k_L A (dT_L / dx) = (T_L - T_0) / R_{C, Th} \quad (1)$$

Where, the subscript 'L' denotes the nearest point at the left electrode contact and 'T0' is the room temperature of the electrode (e.g. 300K). The aforementioned boundary condition introduces a little temperature drop at electrode junction, which is proportional to the thermal contact resistance and heat flux. Thenumericalvalueofthethermal contact resistance,asmentioned above, isconsistent with theareaofthethermalcontactand with thetypicalsolid-solid thermal resistance perunitarea. Also, in heat transport, relative contribution of electrons and phonons along the single wall nanotube can be estimated by Wiedemann-Franz law. Electron thermal conductivity can be expressed as:

$$Ke = L_0 T\sigma = L_0 T (L / RA) \quad (2)$$

Where, Lorenzconstant, L0= 2.45× 10-8WΩK-2. Eq. 2can also be expressed with respect to thelength'L',cross-sectionalarea 'A',and theelectrical resistance 'R'.Fig.8 compares the thermal conductivity due to electrons (solidlines) estimated from Eq. 2 under electrical resistanceat low and highbiasconditions. The phonon thermal conductivity (dashed lines) is sufficiently high than electron thermal conductivity under same biasing condition. The Wiedemann-FranzLawis best applied when transport is dominated byelasticscattering.

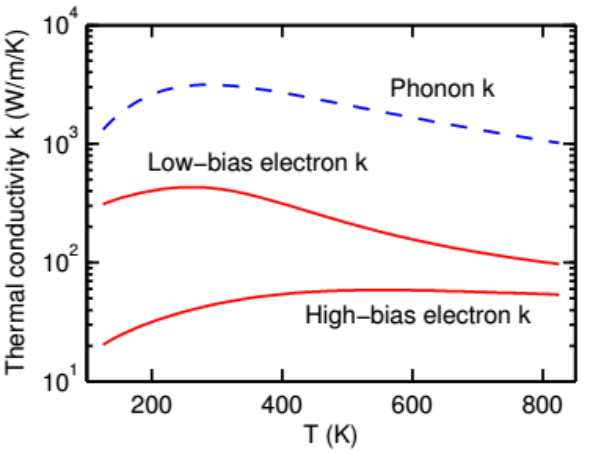


Figure 8. Thermal conductivity due to phonons as well as electrons estimated from the Wiedemann-Franz law. The low bias (~ 60 mV) and high bias (~ 6 V) electron thermal conductivity across 3 μm long tube

4 Conclusion & Future Perspective

The thermal transport properties of single wall nanotube are dominated by phonon scattering for specific band gap and extensively dependent on temperature. Moreover, electron conduction is suppressed by phonon conduction in thermal contact resistance property. Considering chirality and structure size of tubes, the low temperature transport behavior is almost linear and at the end of high temperature, second order three phonon scattering process is introduced. Also, thermal transport behavior is dominant in graphene sheet rather than pure graphite sample. This remarkable factor is very important since it promises efficient thermal management in nanotube-based NEMS devices. In addition, more accurate phonon interaction in thermal transport could be developed by quantitatively studying the various types of nanotubes.

Future research would be conducted on Multi wall carbon nanotubes as well as other nanostructures. Also, electronic conductivity for both electrical and thermal transport would be a great importance as nano device in nano-emerged technology.

References

JianweiChe, Tahir Çagin and William A Goddard III (2000), "Thermal conductivity of carbon nanotubes", Nanotechnology, vol. 11, no. 2, pp. 65-69.

Yoshiyuki Miyamoto, Steven G. Louie, and Marvin L. Cohen (1996),"Chiral Conductivities of Nanotubes", Phys. Rev. Lett., vol. 76, no. 12, pp. 2121–2124.

Ali Javey, Ryan Tu, Damon Farmer, Jing Guo,Roy Gordon, and Hongjie Dai (2005),"High Performance n-Type Carbon Nanotube Field-Effect Transistors with Chemically Doped Contacts", Nano Lett., vol. *5, no.* 2, pp. 345–348.

Baratunde A. Cola, Jun Xu, Timothy S. Fisher (2009),"Contact mechanics and thermal conductance of carbon nanotube array interfaces" Int. J. of Heat and Mass Transfer, vol. 52, no. 15–16, pp. 3490–3503.

E. Faizabadi and F. Heidaripour (2011), "Effects of the central armchair nanotube size on the conductance of carbon nanotube quantum dots", Proc. SPIE 8101, Carbon Nanotubes, Graphene, and Associated Devices IV, San Diego, California, doi:10.1117/12.892925.

N R Pradhan, H Duan, J Liang and G S Iannacchione (2009), "The specific heat and effective thermal conductivity of composites containing single-wall and multi-wall carbon nanotubes", Nanotechnology, vol. 20, no. 24,doi:10.1088/0957.

Eric Pop, David Mann, Qian Wang, Kenneth Goodson, and Hongjie Dai (2006),"Thermal Conductance of an Individual Single-Wall Carbon Nanotube above Room Temperature", Nano Lett., vol. 6, No. 1, pp. **96-100.**

Vasili Perebeinos, J. Tersoff, and Phaedon Avouris (2005), "Electron-phonon interaction and transport in semiconducting carbon nanotubes," Phys. Rev. Lett., vol. 94, no. 08, pp. 6802.

Yunfeng Gu and Yunfei Chen (2007), "Thermal conductivities of single-walled carbon nanotubes calculated from the complete phonon dispersion relations", Phys. Rev. B, vol. 76, no. 13, pp. 4110.

Z. Han and A. Fina (2007), "Thermal conductivity of carbon nanotubes and their polymer nanocomposites: A review", vol. 36, no. 7, pp. 914-944.

J. Hone (2007), "Carbon Nanotubes: Thermal Properties", New York, Taylor & Francis, pp. 603-610.

M. S. Dresselhaus and P. C. Eklund (2010), "Phonons in carbon nanotubes", Adv. in Phy., vol. 49, no. 6, pp. 705-814.

T. J. Singh and G. S. Verma (1982), "Resonance effects in three-phonon processes", Phys. Rev. B, vol.25, no. 6, pp. 4106-4109.

D. J. Ecsedy and P. G. Klemens (1977), Thermal resistivity of dielectric crystals due to four-phonon processes and optical modes, Phys. Rev. B, vol.15, no. 5, pp. 957.

C. J. Glassbrenner and Glen A. Slack (1964), "Thermal Conductivity of Silicon and Germanium from 3°K to the Melting Point", Phys. Rev. 134, no. 4A, pp. 1058.

David Mann, Eric Pop, Jien Cao, Qian Wang, Kenneth Goodson, and Hongjie Dai (2006), "Thermally and Molecularly Stimulated Relaxation of Hot Phonons in Suspended Carbon Nanotubes", J. Phys. Chem. *B*, vol. 110, no. 4, pp. 1502–1505.

T. Yamamoto (2004), "Universal Features of Quantized Thermal Conductance of Carbon Nanotubes", Phys. Rev. Lett., vol. 92, no. 07, doi: 10.1103.

J. Hone, M. Whitney, C. Piskoti, and A. Zettl (1999),"Thermal conductivity of single-walled carbon nanotubes", Phy. Rev. B, vol. 59, no. 4, pp. 2514–2516.

J. Hone, M. C. Llaguno, N. M. Nemes, A. T. Johnson, J. E. Fischer, D. A. Walters, M. J. Casavant, J. Schmidt and R. E. Smalley (2000), "Electrical and thermal transport

Properties of magnetically aligned single wall carbon nanotube films", Appl. Phys. Lett., vol-77, no. 5, pp. 666– 668.

J. E. Fischer, H. Dai, A. Thess, R. Lee, N. M. Hanjani, D. L. Dehaas, and R. E. Smalley (1997),"Metallic resistivity in crystalline ropes of single-wall carbon nanotubes", Phys. Rev. B, vol. 55, no. 8, pp. R4921-24.

J. Hone, M.C. Llaguno, M.J. Biercuk, A.T. Johnson, B. Batlogg, Z. Benes, J.E. Fischer (2002), "Thermal properties of carbon nanotubes and nanotube-based materials", Appl. Phy. A, vol. 74, no. 3, pp. 339-343.

Eric Pop, David A. Mann, Kenneth E. Goodson and Hongjie Dai (2007),"Electrical and thermal transport in metallic single-wall carbon nanotubes on insulating substrates", J. Appl. Phys.,vol. 101, no. 9, doi: 10.1063.

Maune Hareem , Chiu Hsin-Ying , Bockrath Marc (2006) "Thermal resistance of the nanoscale constrictions between carbon nanotubes and solid substrates," Appl. Phys. Lett., vol. 89, no. 1, pp. 3109.

M. Grujicic, G. Cao, Walter N. Roy (2005),"Computational analysis of the lattice contribution to thermal conductivity of single-walled carbon nanotubes", J. of Mat. Sci., vol. 40, no. 08, pp.1943-1952.

Choongho Yu ,Li Shi ,Zhen Yao , Deyu Li ,and Arunava Majumdar (2005),"Thermal Conductance and Thermopower of an Individual Single-Wall Carbon Nanotube", Nano Lett., vol. 5, no. 9, pp. 1842-1846.

Savas Berber, Young-Kyun Kwon, and David Tománek (2000), "Unusually High Thermal Conductivity of Carbon Nanotubes", Phy. Rev. Lett, vol. 84, no. 20, pp. 4613-4616.

Eric Pop, David A. Mann, J. Reifenberg, K. Goodson, Hongjie Dai (2005) "Electro-thermal transport in metallic single-wall carbon nanotubes for interconnect applications," in IEEE Intl. Electron Devices Meeting (IEDM), pp. 253-256.

David G. Cahill, Wayne K. Ford, Kenneth E. Goodson, Gerald D. Mahan, Arun Majumdar, Humphrey J. Maris, Roberto Merlin and Simon R. Phillpot (2003) "Nanoscale thermal transport," J. Appl. Phys., vol. 93, no. 2, pp. 793-818.

Ji-Yong Park , Sami Rosenblatt , Yuval Yaish , Vera Sazonova , Hande Üstünel , Stephan Braig , T. A. Arias , Piet W. Brouwer , and Paul L. McEuen (2004), "Electron-phonon scattering in metallic single-walled carbon nanotubes," Nano Lett., vol. 4, no. 3, pp. 517.

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