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Concept of Conductivity of Bent Carbon Nanotube

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Abstract—*The present paper reports the 'the concept of conductivity of bent carbon nanotubes. Bent carbon nanotube can be considered by as a graphitic one atom thick can be rolled into a tube whose radius be less than 1nm and diameter be 1.4nm[1]. The bending phenomena in carbon nanotubes have been indicated and study experimentally and had indicated that under sever bending the buckling is usual way for nanotubes to reduce its strain. The usual approach to the theoretical modeling, the buckling phenomena has so far made use of classical potential. Even for calculation of thermal conductivity of bent carbon nanotubes, which make use of the relatively more sophisticated quantum tight binding Hamiltonian [2]. Here we discuss the thermal conductivity of carbon nanotubes.*

As the size of electronic and mechanical devices are decreased to the micron and nanometer levels, it becomes particularly important to predict the thermal transport properties of components. Using molecular level theories, then such discussions are particularly important for modeling nano electric devices, nano electronic devices where scaling laws may change particularly, but it is most difficult to accurately measure the properties of substances. Here we using the empirical bond order dependent force field and here we study the thermal conductivity of nanotubes that dependent on structure, defects and vacancies. The graphite crystals having anisotropic character those reflected in bent carbon nano tubes. It is found that the bent carbon nanotubes (BCNTs) having very high thermal conductivity with respect to diamond crystal and plane graphite sheet [3].

The theoretical obtained results will be compared with previous obtained theoretical and experimental results.

Keywords*:-Thermal conductivity, carbon nanotubes, molecular dynamics, tight binding approach.*

1. INTRODUCTION

As reduce the size of electronic devices and integrated micro nano electromechanical system provides the main driving force behind the scientific research and technological advancement in nanotechnology. It is widely accepted in thermal management in nanosize devices becomes increasingly important as the size of device reduces [3].

Nanotechnology-Nanotechnology is a relatively new branch of science which involves manipulation of properties of matter at nanoscales. The premise of nanotechnology lies in the fact that the properties of an element or compound can be manipulated easily when it exists its nanoform (diameter of 1-100nm). Nanotechnology is a branch of applied science and technology, and its journals are a huge curios of nanotechnology related information; they highlight cutting edge developments in nanotechnology and its application such as micro fabrication, nanomedicines, nanoelectronics, molecular biology and nano engineering. Nano technology mostly uses the carbon nanotubes as nanomaterials for fabrication of different nano devices [4].

Thermal conductive properties -Carbon nanotubes having extra ordinary thermal conductive properties. The record setting anisotropic thermal conductivity of carbon nanotubes is enabling applications where heat needs to move from one place to another. Such an application is electronics, particularly advanced computing, where uncooled chips now routinely reach over 100°C. Before carbon nanotubes the best thermal conductor was diamond. But after that carbon nanotubes have a thermal conductivity twice that of diamond [5].

Carbon nanotubes –Carbon nanotubes are allotropes of carbon with a cylindrical nano structure. These cylindrical carbon molecules have unusual properties, which are valuable for nanotechnology, electronics, optics and other fields of materials science and technology. Owing to the materials exceptional strength and stiffness, nanotubes have been constructed with length to diameter ratio up to 132,000,000:1, significantly larger than for any other materials.

In addition, owing to their extra ordinary thermal conductivity that is thermal conductivity, mechanical and electrical properties, carbon nanotubes find applications as additive to various structural materials. For instance, nanotubes form a tiny position of materials in some base ball, bats, golf, car ,parts of Damascus steel[6].For their bright future, a great deal of effort has been devoted to understanding and characterizing their properties[7-10]. Multiwall carbon nanotubes was discovered in 1991 by Ijima [11]. Single walled carbon

nanotube was discovered by et-al[12] and Bethune et-al in 1993[13].

Carbon nanotubes having unique electronic properties. They are either metallic or semiconducting depending upon on their chirality (configurationally variations).A number of experiments and theoretical investigation have focused on electronic structure, characterizing their mechanical properties. In this paper we focus on understanding the lattice thermal transport properties of carbon nanotubes. Due to technological difficulties of synthesizing high quality and well ordered nanotubes, it is still challenging to perform thermal conducting measurements. Hence it is essential to observe thermal prediction of thermal conductivity and the influence of various defects. As we know that there are two approaches to calculate the transport properties of materials that is, one is based on the Boltzmann equation based on experiment, second is based on the fluctuation dissipation relation from linear response theory that can be produced by first principle. For novel materials, no experimental results are available hence here BE cannot be used to predict transport properties. Hence here MD (molecular dynamics) simulation, the fluctuation dissipation relation can be applied. In this paper we use equilibrium MD simulations to calculate carbon nanotube thermal conductivity and its dependence on vacancies and defects. Here we can go over the theoretical background for thermal conductivity relation [14]

RESULTS AND DISCUSSION-

For this discussion we consider the macroscopic thermal conductivity that is Fourier`s law of heat flow under uniform temperature is considered. Here we make use of the harmonic mapping method, which is exact only for harmonic system. In this harmonic systems each normal mode is decupled from others. Therefore the only contribution to thermal conductivity for a macroscopic system from photon modes that having wavelength equal to or longer than the macroscopic length scale. As discussed in our previous work. This is very similar to vibrational relaxation of harmonic system bilinearly coupled to harmonic path, where both the full quantum relaxation rate and full classical relaxation rate are the same [15].

For a (10,10) singled walled nanotube, four different systems are investigated. These contain 500, 1000, 2000, 4000, and 8000 atoms respectively. We know that the phonon mean free path is limiting factor for obtaining the accurate value results. As the simulation system size gets larger, the theoretical value convergence to constant which is independent of simulation size. The convergence behavior is demonstrated in fig.1.

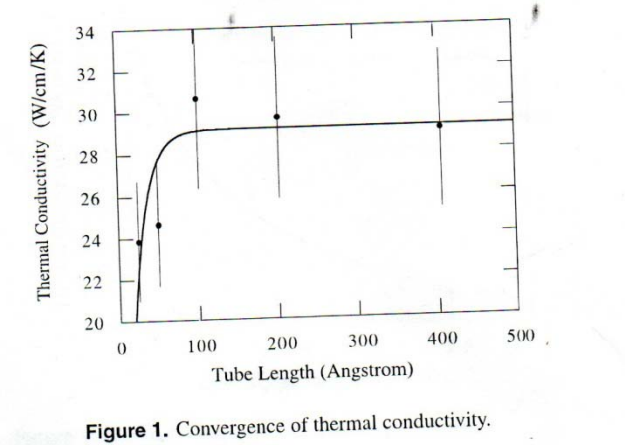

Figure 1. Convergence of thermal conductivity.

Theoretical predicted value approaches to, 29.8W/cm/K along the tube axis that is very high in comparison with conventional materials.

Later in this section we will show the thermal conductivity for nanotube bundles where the cross section is uniquely defined and the result can be used to compare with experiments and other materials.

In figure. 2, we show that the initial auto correlation function of the heat current along the tube axis for the system consisting of 4000 atoms.

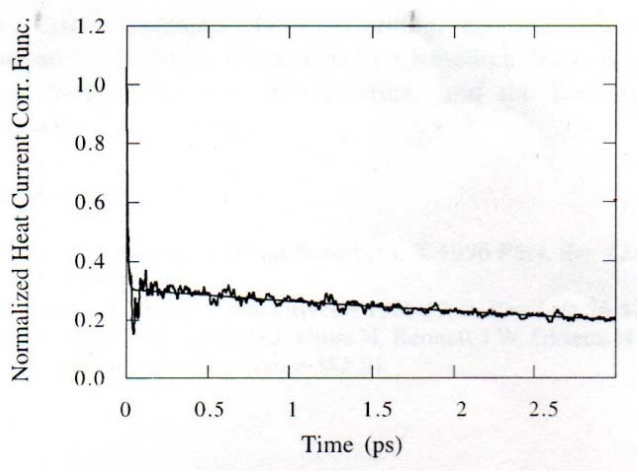

Fig. 2: Current autocorrelation function

The figure clearly shows very fast decay at the beginning followed by a very slow decay. The high vibrational mode do not contribute to the thermal conductivity in a significant way. The correlation function can well characterized by a double exponential function with two time constants[16].

Since nanotube having natural defects and vacancies. It is to important to know that how defects influence the thermal conduction properties of carbon nanotubes. As unlike macroscopic three dimensional materials, carbon nanotubes can be thought of as a quasi one dimensional wire.

The thermal conductivity can be calculated for various vacancies is demonstrated in fig.3.

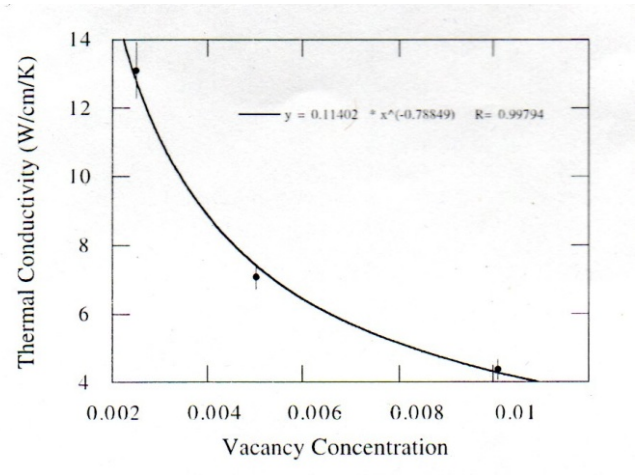

Fig. 3: Thermal conductivity as a function of vacancy concentration

The thermal conductivity decreases as vacancies concentration increases. Hence the rate of decrease in thermal conductivity is quite unexpected [17].

As we mentioned earlier the absolute value of an isolated single walled nanotubes are ambiguous the heat conduction cross-section is not uniquely defined. This problem is avoided in nanotube bundles, the cross-section can be well defined and it is surely unique. Therefore we can also carried out the thermal conductivity calculation of a(10,10)nanotube bundles in close packing condition. Nano tube bundles having very high thermal conductivity along the tube axis that is 9.5W/cm/K, that is comparable to simulated graphite in plane thermal conductivity that is 10 W/cm/K.

CONCLUSION

We have discuss that the thermal conductivity for single wall carbon nanotubes(SWCNT) based on the MD simulations. The thermal conductivity is used in nano tube based MEMS/NEMS devices. The thermal conductivity influenced by defects reveals an interesting phenomena that can not to known before. Origin of this behavior we have to collect the very deep information and discussion. Single walled carbon nanotubes having very high thermal conductivity than graphite sheet and diamond crystals.

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