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Phonon Mean Free Path in Graphite Nanotubes

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Thermal transport in solids is understood in terms of contributions from phonons and free electrons. Metals are good conductors of electricity and heat and a simple manifestation of this is seen in the constancy of Lorenz number in almost all metals at a given temperature. For semiconductors there is some variation in the Lorenz factor depending upon the level of doping. A theoretical understanding of this aspect is to be sought separately for various electron scattering mechanisms [1]. In the low carrier density regime the L values differ somewhat, and gradually approach the usual value with increase in carrier densities. In the degenerate limit all L values virtually converge to the usual metallic value of $\pi^2/3$.

The apparent proportionality between electrical and thermal transport is essentially true for simple metals and partially for semiconductors. However, this is totally redundant for insulators such as graphite and diamond. Even though electrical insulators these materials are the best known heat conductors with their thermal conductivities almost five times that of best known metallic values. Theoretical explanation can be provided on the basis of exceptionally large mean free path for phonons, which are the only carriers of heat. Large pure crystals being relatively free from impurity and boundary effects phonon mean free path is limited by only one mechanism: phonon-phonon scattering. Large thermal conductivity of graphite and diamond points to large phonon mean free paths, which mean an exceptionally small phonon-phonon scattering. Phonon-phonon scattering is due to the presence of anharmonic terms in the crystal potential which may have a low key presence in these materials as compared with others. However, interesting situations arise when one looks into thermal transport in nanotubes.

Nanotubes are well known for their interesting electronic properties, which are sensitive to method of preparation, helicity, tube diameter, and presence of molecular oxygen. There are considerable difficulties in such a venture due to lack of information on many parameters. However, some aspects such as heat capacity and phonon transport are relatively better understood. In this note we discuss some aspects of phonon heat transport in nanotubes which require more careful investigation.

Several researchers have investigated thermal conductivity in low dimensional systems both theoretically and experimentally [2-9]. Both in one and two-dimensional structures a marked reduction in thermal conductivity over the bulk values is reported depending upon the wire diameter or well depth. [6,7]. In a recent publication thermal conductivity of crystalline ropes of single walled carbon nano tubes has been reported .The thermal conductivity in single walled carbon nanotubes (SWNT) has shown a behavior quite different from that of the bulk materials. The usual peak in thermal conductivity temperature plot [5]around 10-20 ^{0}K is absent and thermal conductivity appears to reflect the temperature dependence of heat capacity in a rather wide temperature range 8-350 ^{0}K. The entire range is marked by a T^x dependence of thermal conductivity, where X=1-1.2. Since thermal conductivity appears to reflect the temperature-dependence of heat capacity. The usual simplified expression

$$k = cvl$$

suggests a T-independent mean-free-path l. For the sample under discussion reported values of the tube diameter is 1nm and length of the tube is 1000nm. The estimated value of the mean free path is 1000 nm, which is almost same as tube length. The point, which we wish to make out, is this: the tube diameter appears to play virtually no role in the entire range in limiting the mean-free-path of phonon. Usually expected confinement effects on phonon dispersion and also absence of the phonon-phonon process in a wide temperature range are points worth attention. Both phonon-phonon scattering and boundary scattering need to be looked in their right perspective and the data reanalyzed.

There could be yet another possibility. Phonon-phonon processes may play a role with probably T^Y dependence of heat capacity where Y may be around 1.5-2. There have been suggestions that heat capacity of nanotube may show 1D or 2D behavior depending upon tube diameter and temperature [9]. It is more likely to make a gradual transition and thus showing a mixed behavior in intermediate ranges. These aspects need to be investigated.

The heat capacity for two-dimensional system can be written as

$$C = \frac{Ah}{2\pi v^2}\left[\frac{k_B}{h}\right]^3 3T^2 \int \frac{x^2}{\exp(x)-1}dx$$

The simple expression of thermal conductivity is given by

$$k_L = Cv^2 \big/ \langle \tau^{-1} \rangle$$

Here τ refers to the phonon relaxation time and may include apart from boundary, impurity and phonon-phonon scattering. Averaging has to be done assuming a Debye spectrum. With phonon-phonon normal scattering included along with boundary and impurity and with the corresponding relaxation time given by

$\tau^{-1} = B\,\omega^2 T + A\,\omega^4 + L/v$

The three terms refer to scattering by phonon, impurities and boundary respectively.

Inclusion of all these into the thermal conductivity gives a rough estimate of its temperature variation. With increasing T the phonon-phonon term dominates and may result in a linear T dependence. At lower temperatures phonon phonon scattering will be insignificant but the system may behave as one-dimensional system and again show an approximate linear dependence.These are mere possibilities that could account for the observed data. More elaborate data on thermal conductivity in a wider range of temperature and for varying tube diameters would be required to provide a greater understanding of the phenomenon of heat transport.

Several authors have tried to obtain a theoretical estimate [2-6] of the changes in thermal conductivity of quantum wires and wells by considering the boundary scattering of phonons in which relative strengths of diffusive and specular reflections have been treated as a variable. The results indicated a steady decrease in thermal conductivity with wire diameter. For a wire diameter of 1 nm the thermal conductivity of the wire could be mere 0.02 per cent of the bulk value. Even for 2-D systems reduction in thermal conductivity is expected to be significant. In that case nanotubes may not be simple one are two-dimensional structures as regards phonon behavior. This result is not in contradiction with various reported measurements. However for nanotubes reported above the situation warrants a more detailed investigation. In absence of more data on these systems we feel that the simple analysis based on Eq, (1) may not suffice and a detailed study of dispersion relation and other features may have to be considered. This may include the electronic contribution to thermal transport along with the lattice contribution.

As perfect materials two extreme situations are of special interest. We may imagine a material, which are electrically good conductor and thermally insulator. Phonon glass, Electron crystal such materials theoretically are best choice for thermoelectric devices. The other extreme is that electron glass phonon crystal (EGPC) is Graphite and diamond and of course nanotube are good examples of such materials.The study of biological processes will require complete the structures and the dynamics of the mateirials. X- ray diffraction and nuclear magnetic resonance NMR spectroscopy are extremely powerful spectroscopic tools with the ability to determine structures of proteins or amino acids.

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