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Thermal Neutron Scattering of Un-Aligned Multi-walled Carbon Nanotubes

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Abstract: ***Neutron scattering is the scattering of free neutrons by matter. This process is used for the investigation of materials. Neutron scattering is an experimental technique which is applied in various areas of physics, physical chemistry, biophysics, crystallography and materials research. Neutron diffraction (elastic scattering) is used for determination of structures of materials. In this paper we attempted to study thermal neutron scattering in randomly un-aligned multi walled carbon nanotubes making use of an anisotropic dynamical model. This model includes the presence of both the surface modes and intertube coupling. Comparison of scattering cross section of un-aligned multiwalled carbon nanotubes has been done with fullerene and graphite. It was concluded that there is a significant difference between the values of scattering cross section for randomly un-aligned multiwalled carbon nanotubes and fullerene at higher values of energy.***

Keywords: Carbon nanotubes, Elastic scattering, Neutron Diffraction, Frequency distribution function, Specific heat

I. INTRODUCTION

The phonon frequency distribution function describes the experimentally measured temperature variation of specific heat in the temperature range 1-200K [1].Fast neutrons have a kinetic energy above 1 MeV. Their scattering by condensed substance can be compared to anelastic collision with a particle at rest. At each collision the fast neutron transfers a major portion of its kinetic energy to the scattering nucleus. In this way the neutron is slowed down until it reaches the stage of thermal equilibrium since neutrons are electrically neutral, they go through the sample moredeeper as compared to the electrically charged particles having comparable kinetic energy. They serve as rightprobes of bulk properties.

The kinetic energy of the free neutrons emitted by atomic nuclei in nuclear reactions is of the order of $10^6\ eV$ .Because of emitted major amount of energy, these neutrons cannot be used to study the dynamics of the crystals. They are passed through a moderator having large neutron scattering cross-section and small neutron absorption cross-section so that their energy gets minimised.

II. MATHEMATICAL FORMALISM

The expression of double differential scattering cross-section [2,3] of thermal neutrons, for a solid, in the present case randomly un-aligned multi walled carbon nanotubes, using the Fermi pseudo neutron-nuclear interaction potential, is expressed as follows:

$$\eta(E_1,E_2,\theta)=\frac{(c1+c2)}{4\pi}\left[\frac{E_2}{E_1}\right]^{1/2} e^{-2w}\left[\delta(\xi)+\hbar k^2\left\{\frac{e^{\xi\theta_D/T}-1}{2M\xi}\right\}^{-1} f(\xi)+multiexcitation\,terms\right] \quad (1)$$

where

E_1 and E_2 are the initial and final energy of the neutron respectively.

$\xi=(E_2-E_1)$ is the energy exchange. All energies are in units of $\xi_D=k_B\theta_D$, θ_D being the Debye temperature and k_B is the Boltzmann constant,

$c1=4\pi\ c_{coh}^2$ and $c2=4\pi\ c_{incoh}^2$ are the bound coherent and incoherent scattering cross-sections of the carbon atom respectively, where $c_{coh}=\langle c\rangle$ and $c_{incoh}=\sqrt{\langle c^2\rangle-\langle c\rangle^2}$ are the coherent and incoherent scattering amplitudes respectively,

$p=\hbar\vec{k}=\hbar(\vec{k}_1-\vec{k}_0)$ is the momentum transfer. $\vec{k}_0$ and $\vec{k}_1$ are initial and final wave vectors of the neutron respectively, $\hbar=\frac{h}{2\pi}$, h being the Planck's constant,

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e^{-2w} is the Debye-Waller factor where $2w = k^2\langle u^2\rangle_T$, $\hbar\vec{k} = \hbar|\vec{k}|$ is the magnitude of momentum transfer and $\langle u^2\rangle_T$ is the mean square displacement of the atom at temperature, *T*.

$\delta(\xi)$, represents the elastic or zero-phonon scattering contribution. The second term, in the bracket, containing $f(\xi)$, the phonon frequency distribution function, denotes the one-phonon scattering and the rest of the higher phonon scattering processes have been lumped into multi-excitation terms. Here only elastic scattering is taken into account.

The total phonon frequency distribution function, $f(\xi)$, is the sum of $f_l(\xi)$:

$$f(\xi) = \sum_l f_l(\xi)$$

In the present case, the anisotropic dynamical model for the frequency distribution function[4, 5] of phonons in randomly un-aligned multi walled carbon nanotubes is given by

$$\begin{aligned} f_l(\xi) &= Y_l\xi^2 \qquad 0 \le \xi \le \xi_{0l} \\ &= Z_l\xi \qquad \xi_{0l} \le \xi \le \xi_{ml} \\ &= 0 \qquad \xi > \xi_{ml} \end{aligned} \tag{2}$$

where $\xi_{0l} = k_B\theta_{0l}$, $\xi_{ml} = k_B\theta_{ml}$. θ_{0l} and θ_{ml} are the characteristic temperatures that define the extent of three-dimensionalmodes and two-dimensional mode region respectively, in a given direction l. Here ξ_{ml} is the maximum value of energy that two-dimensional modes can have. $l = x, y, z$ (x, y, z represents the directions in the Cartesian coordinates and also the polarization of the phonons). Y_l and Z_l are constants to be determined using the conditions:

1) Continuity of $f_l(\xi)$ at $\xi = \xi_{0l}$

2) Total number of modes is $3N$, N being the total number of atoms in the solid and

$$Y_l = \frac{6N}{\xi_{0l}(3\xi_{ml}^2 - \xi_{0l}^2)}$$

$$Z_l = \frac{6N}{(3\xi_{ml}^2 - \xi_{0l}^2)}$$

In the present case

$$f(\xi) = f_z(\xi) + 2\ f_{xy}(\xi) \tag{3}$$

where frequency distribution function in *xy* direction is given by $f_{xy}(\xi) = f_x(\xi) = f_y(\xi)$.

A. Elastic Scattering Cross-section

The elastic scattering cross-section of thermal neutrons, of energy E, using anisotropic frequency distribution functioncan be given as follows:

$$\eta_{el}(E) = \frac{(c1 + c2)}{4E\gamma}(1 - e^{-4E\gamma}) \tag{4}$$

where

$$\gamma = \frac{m_0}{M} \times \frac{1}{k_B T} \times \varepsilon_{ac} \tag{5}$$

with ε_{ac} as given below:

$$\varepsilon_{ac} = \frac{1}{3} \times \{W1 + W2 + W3 + W4\} \quad (6)$$

and

$$W1 = \frac{6}{z_{0z}\left(3z_{mz}^2 - z_{0z}^2\right)} \left[\frac{z_{0z}^2}{2} + 2\int_0^{z_{0z}} \frac{z}{\left(e^z - 1\right)}\, dz \right] \quad (7)$$

$$W2 = \frac{6}{\left(3z_{mz}^2 - z_{0z}^2\right)} \left[\left(z_{mz} - z_{0z}\right) + 2\int_{z_{0z}}^{z_{mz}} \frac{1}{\left(e^z - 1\right)}\, dz \right] \quad (8)$$

$$W3 = \frac{12}{z_{0xy}\left(3z_{mxy}^2 - z_{0xy}^2\right)} \left[\frac{z_{0xy}^2}{2} + 2\int_0^{z_{0xy}} \frac{z}{\left(e^z - 1\right)}\, dz \right] \quad (9)$$

$$W4 = \frac{12}{\left(3z_{mxy}^2 - z_{0xy}^2\right)} \left[\left(z_{mxy} - z_{0xy}\right) + 2\int_{z_{0xy}}^{z_{mxy}} \frac{1}{\left(e^z - 1\right)}\, dz \right] \quad (10)$$

where $z = \frac{\xi}{k_B T}$, ξ being the energy of the phonons, $z_{0z} = \frac{\theta_{0z}}{T}$, $z_{mz} = \frac{\theta_{mz}}{T}$, $z_{0xy} = \frac{\theta_{0xy}}{T}$ and $z_{mxy} = \frac{\theta_{mxy}}{T}$, m_0 is the mass of neutron and M is the mass of carbon atom.

III. RESULTS AND DISCUSSION

Using the above given equations and the appropriate values of the characteristic parameters $\theta_{0z} = 1.25K, \theta_{mz} = 905K, \theta_{0x} = \theta_{0y} = \theta_{0xy} = 1.25K$ and $\theta_{mxy} = 50K$ and $(c1 + c2) = 5.53\ barns$ $(1\ barn = 10^{-24}\ cm^2)$, elastic scattering cross section for randomly un-aligned multi walled carbon nanotubes have been evaluated for various values of incident neutron energies, *E*lying in the range $10^{-4}\ eV$ *to* $3 \times 10^{-1}\ eV$. These calculations are shown in figure1 by solid line(———). Also comparison of these values with fullerene (— — —) and graphite (- · - · -) has been plotted. Difference between the values of scattering cross section for randomly un-aligned multiwalled carbon nanotubes and fullerene is high at large values of energy.

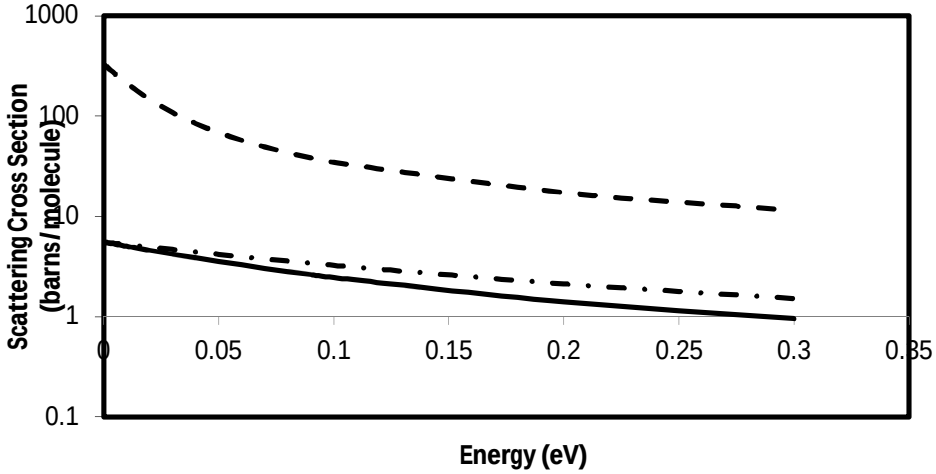

Fig 1: Comparison of variation of thermal neutron scattering cross-sectionswith the incident energy of neutrons at 300K for randomly un-aligned multi walled carbon nanotubes with fullerene and graphite.

Fullerene(— — —)

Graphite(-· - · -)

Randomly un-aligned multi walled carbon nanotube (——)

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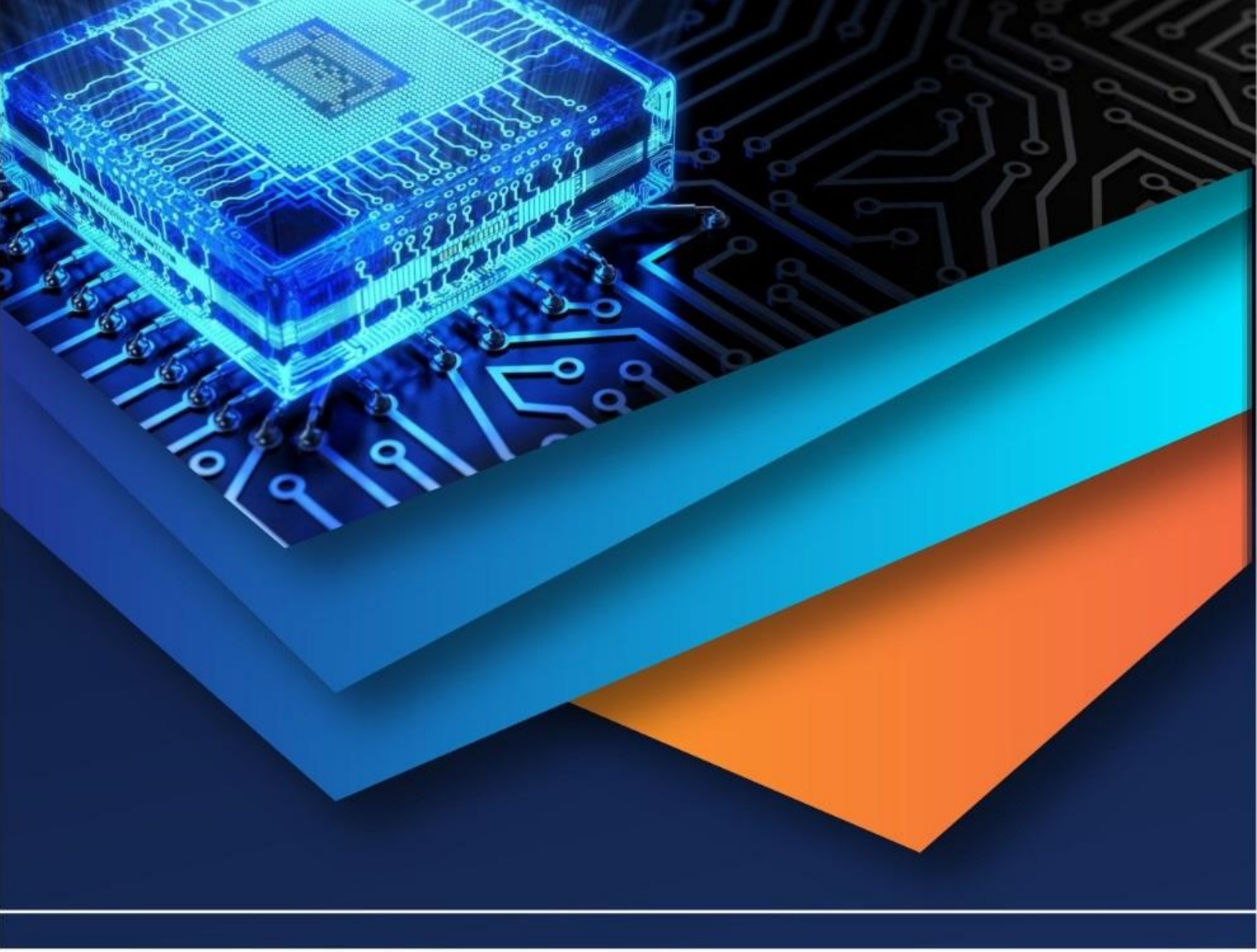

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