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Neutron Scattering in Nanotubes

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Abstract: Neutron scattering has got numerous applications in various fields of research like material research, crystallography etc. Thermal neutron scattering in randomly un-aligned multi walled carbon nanotubes is based on its anisotropic frequency distribution function. This frequency distribution function is obtained using a dynamical model which includes the presence of both the surface modes and intertube coupling. Experimentally measured values of specific heat for randomly un-aligned multi walled carbon nanotubes has been studied to detect the phonon frequency distribution function. Elastic scattering is used for analyzing structures. Inelastic scattering is applied for the study of atomic vibrations. The dynamical model has been used to find the scattering values. Both scattering values are calculated and compared. It was concluded that the difference in their values is large. This difference would affect the transport processes in randomly un-aligned multi walled carbon nanotubes

Keywords: Specific heat, Elastic scattering, Inelastic scattering, Neutron Diffraction, Frequency Distribution Function

I. INTRODUCTION

Neutron scattering is a technique for examining the materials. The free neutrons which are emitted by atomic nuclei in nuclear reactions have high energy. So, these neutrons cannot be used to study the structure of the crystals. They are passed through a moderator of less atomic mass, high neutron scattering cross-section and thus their energy gets decreased.

Neutrons act together with atomic nuclei and magnetic fields from unpaired electrons. Energy transfer occurs in scattering experiments. Neutron scattering and absorption cross sections vary generally from isotope to isotope. The scattering consists of elastic and an inelastic component. The fraction of elastic scattering is described by the Debye-Waller factor or the Mossbauer-Lamb factor.

II. METHOD

A. Thermal Neutron Scattering Cross-Section

The dynamical model is applied to get frequency distribution function. [1,2]. Experimental values of specific heat for the case of un-aligned multi walled carbon nanotubes is given by Mizel etal [3]. These values have been studied to get frequency distribution function. The differential scattering cross-section [4, 5] of thermal neutrons, for the case of a solid, is expressed as follows:

$$\mu(E,E^{'},\theta)=\frac{(b1+b2)}{4\pi}\left[\frac{E2}{E1}\right]^{1/2}e^{-2w}\left[\delta(\xi)+\hbar k^{2}\left\{\frac{e^{\xi\theta_{D}/T}-1}{2M\xi}\right\}^{-1}d\left(\xi\right)+multiexcitationterms\right] \quad (1)$$

where $E1$ and $E2$ are the initial and final energy of the neutron respectively. Here Fermi-Pseudo neutron-nuclear interaction potential is used and the sample is un-aligned multi-walled carbon nanotubes.

$\delta(\xi)$, denotes the elastic or zero-phonon scattering contribution. The next containing $d(\xi)$, the phonon frequency distribution function represents the one-phonon scattering. The higher phonon scattering processes have been included in the last term i.e. multi-excitation terms.

$\xi=(E2-E1)$ is the difference between both final and initial energy. $\xi_D = k_B\theta_D$, k_B is the Boltzmann constant and θ_D is the Debye temperature.

Energy is taken in terms of Debye temperature. Here $b1 = 4\pi\ b_{coh}^2$ is the bound coherent scattering cross section and $b2 = 4\pi\ b_{incoh}^2$ is the bound incoherent scattering cross-sections of the carbon atom. Here $b_{coh} = \langle b\rangle$ is the coherent scattering amplitude and $b_{incoh}=\sqrt{\langle b^{2}\rangle-\langle b\rangle^{2}}$ represents the incoherent scattering amplitude.

$p = \hbar \vec{k} = \hbar(\vec{k}_1 - \vec{k}_0)$ indicates the transfer of momentum where $\vec{k}_0$ is the initial vector and $\vec{k}_1$ is the final wave vector of the neutron.

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

$$d(\xi) = \sum_p d_p(\xi)$$

The anisotropic dynamical model for the frequency distribution function of phonons in case of randomly un-aligned multi walled carbon nanotubes is given by:

$$\begin{aligned} d_p(\xi) &= Q_p \xi^2 && 0 \le \xi \le \xi_{0p} \\ &= R_p \xi && \xi_{0p} \le \xi \le \xi_{mp} \\ &= 0 && \xi > \xi_{mp} \end{aligned} \qquad (2)$$

where $\xi_{0p} = k_B \theta_{0p}$, $\xi_{mp} = k_B \theta_{mp}$. θ_{0p} and θ_{mp} are the characteristic temperatures. These temperatures represent the range of three-dimensional and two-dimensional mode region respectively, in a particular direction p. Here ξ_{mp} is the maximum value which two-dimensional modes can have. $p = x, y, z$ (x, y, z represents the directions in the Cartesian coordinates and also the polarization of the phonons). Q_p and R_p are constants which are calculated using two conditions:

1) Continuity of $d_p(\xi)$ at $\xi = \xi_{0p}$
2) Total number of modes is $3N$, N being the total number of atoms in the solid and

$$Q_p = \frac{6N}{\xi_{0p}(3\xi_{mp}^2 - \xi_{0p}^2)}$$

$$R_p = \frac{6N}{(3\xi_{mp}^2 - \xi_{0p}^2)}$$

In the present case

$$d(\xi) = d_z(\xi) + 2\, d_{xy}(\xi) \qquad (3)$$

where frequency distribution function in *xy* direction is given by $d_{xy}(\xi) = d_x(\xi) = d_y(\xi)$.

B. Elastic Scattering Cross-Section

The elastic scattering cross-section of thermal neutrons [4,5] of energy E, using anisotropic frequency distribution function for the acoustic modes given by equations (2) and (3) can be expressed as follows:

$$\mu_{el}(E) = \frac{(b1 + b2)}{4E\rho}(1 - e^{-4E\rho}) \qquad (4)$$

C. Inelastic Scattering Cross-section

The expression of the inelastic scattering cross-section, $\mu_{in}^{(1)}(E)$, using the anisotropic frequency distribution function for acoustic modes when a neutron of initial energy $E1$ is scattered to final energy $E2$, due to one phonon exchange processes is as follows:

$$\mu_{in}^{(1)}(E) = \frac{(b1 + b2)}{12} \frac{M}{m_0} \frac{1}{z_0} \frac{d(|z|)}{z} \frac{1}{\varepsilon_{ac}^2} \left(e^z - 1\right)^{-1} \times \{\alpha 11 - \alpha 12\} \qquad (5)$$

where

$$\alpha 11 = e^{-m_0/M} \varepsilon_{ac} \left(\sqrt{z_0} - \sqrt{z_1}\right)^2 \left[\frac{m_0}{M} \varepsilon_{ac} \left(\sqrt{z_0} - \sqrt{z_1}\right)^2 + 1\right] \qquad (6)$$

$$\alpha 12 = e^{-m_0/M}\varepsilon_{ac}\left(\sqrt{z_0}+\sqrt{z_1}\right)^2\left[\frac{m_0}{M}\varepsilon_{ac}\left(\sqrt{z_0}+\sqrt{z_1}\right)^2 + 1\right] \quad (7)$$

z_0 and z_1 are the incident and the final energies of neutron respectively, which are expressed in units of $k_B T$ and $z = z_1 - z_0$. z is a dimensionless quantity which may have positive value or negative depending on whether neutron gains or loses energy. The contribution from two phonon processes is given by $\mu_{in}^{(2)}(E)$. Its contribution is quite small and therefore higher phonon processes have not been taken into account.

The total scattering cross-section is therefore:

$$\mu(E) = \mu_{el}(E) + \mu_{in}(E) \quad (8)$$

III. RESULTS AND DISCUSSION

Using the above described mathematical formalism and the relevant data of the characteristic temperatures or parameters for randomly un-aligned multi walled carbon nanotubes $\theta_{0z} = 1.245\ K$, $\theta_{mz} = 905\ K$, $\theta_{0x} = \theta_{0y} = \theta_{0xy} = 1.245\ K$ and $\theta_{mxy} = 2601\ K$ and $(b1 + b2) = 5.53\ barns$ $(1\ barn = 10^{-24}\ cm^2)$, elastic scattering cross section, inelastic scattering cross section and total have been computed for different values of incident neutron energies. The range of energy is *0.0001 < E < 0.3 eV*. The elastic scattering cross section is shown by long dash (— — —), inelastic by dash dot dash (- • - • -) and total by solid line **(——)** respectively. The contribution of two-phonon processes making use of effective Debye temperature is very less than the total scattering from one-phonon processes. This Debye temperature is obtained by the anisotropic model for the randomly un-aligned multi walled carbon nanotubes which is fixed by its characteristic temperatures The portion of higher phonon processes have not been included in the evaluation of scattering cross-section for the case of thermal neutrons. The elastic scattering part is determined by Debye Waller factor. Debye Waller factor is also called Mossbauer-Lamb factor. The value of two-phonon processes using effective Debye temperature equal to 1810K, obtained by the anisotropic model for the randomly un-aligned multi walled carbon nanotubes fixed by its characteristic temperatures which are given above, is almost two order less than the total scattering from one-phonon processes. Therefore, the effect of higher phonon processes have not been included in the evaluation of scattering cross-section of thermal neutrons. On comparing both scattering values, it was observed that the difference in the calculated values is large. Due to which, the transport processes in case of randomly un-aligned multi walled carbon nanotubes will be effected.

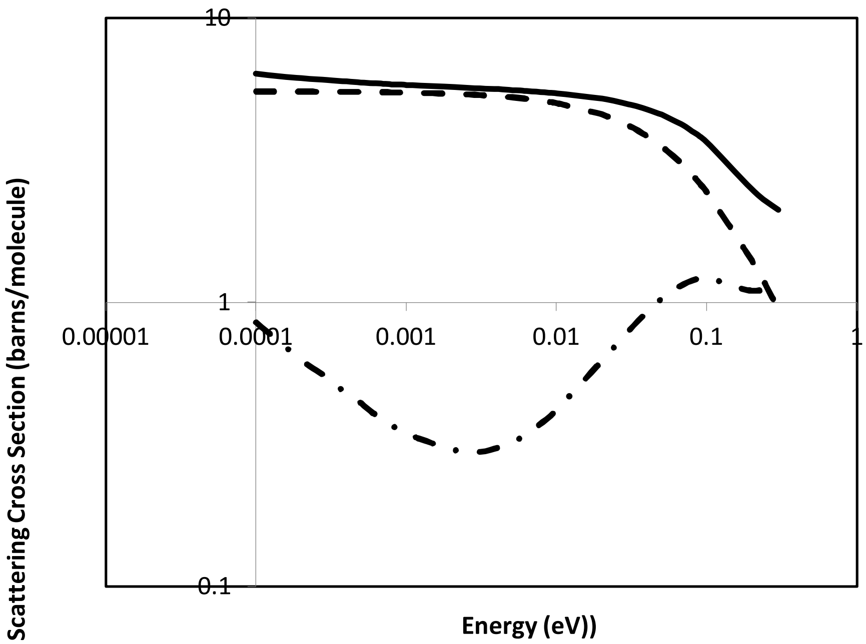

Fig 1: Thermal neutron scattering cross-sections, μ , with the incident energy of neutrons at 300K in randomly un-aligned multi walled carbon nanotubes.

Elastic: (— — —)
Inelastic: (- · - · -)
Total: (———).

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