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THERMAL NEUTRON SCATTERING ON HYDROGEN ATOM NUCLEUS OF POLYETHYLENE

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ABSTRACT - Based on the assumptions, that the CH_2 unit is the basic unit of polyethylene affecting the thermal neutron scattering and that the phonon spectrum of polyethylene can be approximated by a discrete set of three Einstein frequencies, similar to a water molecule, a quantum mechanical expression for double differential cross section for the thermal neutron scattering on a hydrogen atom nucleus of polyethylene has been derived. For twenty-eight incident thermal neutron energies $E_0 \in [1\ meV, 1\ eV]$ the values of double and single differential cross sections, as well as the values of total scattering cross sections have been evaluated. The results obtained clearly show quantum inelastic effects of the creation and the destruction of polyethylene phonons, as well as highly pronounced quasielastic peaks, that occur at forward neutron scattering. The same property is also valid for inelastic scattering, but only when $E_0 \in [0.01\ eV, 1\ eV]$. However, when $E_0 \in [0.001\ eV, 0.01\ eV]$ then the destruction of phonons of the lowest energy shows a weak dependence on a scattering angle, which vanishes quickly with the increase of thermal neutron energy.

1. INTRODUCTION

It is known that the thermal neutron scattering on the atomic nuclei bound into molecules, can be successfully described by the Zemach-Glauber quantum-mechanical formalism [1]. It is also known that the thermal neutron scattering depends on the value of incident neutron energy, on the molecular space orientation, the collision time and molecular dynamical properties. Different methods have been developed in order to include the influence of the basic dynamical modes of a molecule motion on the thermal neutron scattering. The application of the incoherent approximation in the Zemach-Glauber formalism yields the following expression for double differential cross section of the thermal neutron scattering on the hydrogen atom nucleus of polyethylene (in the unit system where Planck's constant is $\hbar=1$ and the neutron mass $m_n=1$)

$$\frac{d^2\sigma}{dE\,d\nu} = \sigma(E_0 \to E, \nu) = \frac{\sigma_b}{4\pi}\sqrt{\frac{E}{E_0}} \int_{-\infty}^{+\infty} \exp(-i\varepsilon t) \langle \chi(\vec{\kappa}, t) \rangle_\Omega dt \,, \qquad (1)$$

where: E_0 and E are the energies of the incident and the scattered neutron, respectively; ν is the cosine of the scattering angle in the laboratory system; $\sigma_b = 81.66 \cdot 10^{-28} m^2$ is the bound effective microscopic cross section of the hydrogen atom nucleus for thermal neutron scattering; i is the imaginary unit, $\varepsilon = E - E_0$ is the neutron energy exchange; the symbol $\langle \ldots \rangle_\Omega$ denotes averaging over all space orientations of the CH_2 unit and $\chi(\vec{\kappa}, t)$ is an intermediary scattering

function including the influence of basic dynamic modes of a CH_2 unit motion on the thermal neutron scattering.

Polyethylene is a simple polymer and therefore has been the subject of various intensive physical studies. It can be crystallized to a very high degree, and is quite different from ordinary materials in the sense that its three-dimensional crystal is made essentially of long linear chains of CH_2 units. Due to that the dynamics of crystalline polyethylene is quite different from the usual three-dimensional materials. For crystalline polyethylene, a number of thermal neutron scattering kernels has been proposed. All these kernels utilize some dynamic model of polyethylene obtained from various experimental or theoretical studies. In most of these studies the focus was mainly on the energetic discrete modes; the proper account of the acoustic region has not been made.

One of the earliest kernels proposed for polyethylene is the Goldman kernel [2], which is an extension of the Nelkin kernel [3], used for water, to the case of polyethylene. Goldman suggested that the frequency distribution for the long chain molecules be represented by five Einstein frequencies analogous to those used by Nelkin for water. In the present paper Goldman's idea has been used in such a way, that the CH_2 unit, as well as a water molecule, has been considered as a basic structural unit. Owing to its dynamical properties it affects the thermal neutron scattering on the hydrogen atom nucleus of polyethylene. Kirouac's et al. assumption [4] has been accepted that the phonon spectrum without the acoustic branch can be successfully presented by a set of three discrete Einstein's frequencies ω_1=0.36 eV, ω_2=0.17 eV and ω_3=0.09 eV, with the corresponding effective vibrational masses m_{v1}=2.94 and m_{v2}=2.04 and effective rotational mass m_r=2.32. In addition it is considered that the CH_2 unit has the identical microdynamical structure of a water molecule as in [5]. The collision time of the thermal neutron and the hydrogen atom nucleus have been exactly described in [5]. The orientation averaging has been approximately performed by the Krieger-Nelkin procedure [6], which is applicable to the most general case of anisotropy of intramolecular vibrations [7].

Based on the above assumptions the following expression for double differential cross section of the thermal neutron scattering on the hydrogen atom nucleus of polyethylene is derived:

$$\sigma(E_o \to E,\nu) = \frac{d^2\sigma}{dE\,d\nu} = \frac{\sigma_b}{2}\frac{}{r+2}\left(\frac{EM}{\pi\alpha E_o kT}\right)^{1/2} \exp\left\{-\left[\frac{\alpha}{4MkT} + \frac{\varepsilon}{2kT} + \sum_{q=1}^{3} \bar{x}_q \operatorname{ch}\left(\frac{\omega_q}{2kT}\right)\right]\right\}$$
$$\cdot \sum_{j=1}^{8} \sum_{\ell=0}^{+\infty}{}' \sum_{m=0}^{+\infty}{}' \sum_{n=0}^{+\infty}{}' I_\ell(\bar{x}_1) I_m(\bar{x}_2) I_n(\bar{x}_3) \exp\left(-\frac{M}{4\alpha kT}(\varepsilon - D_j)^2\right). \qquad (2)$$

The definition of physical quantities used in expression (2), is given in reference [5].

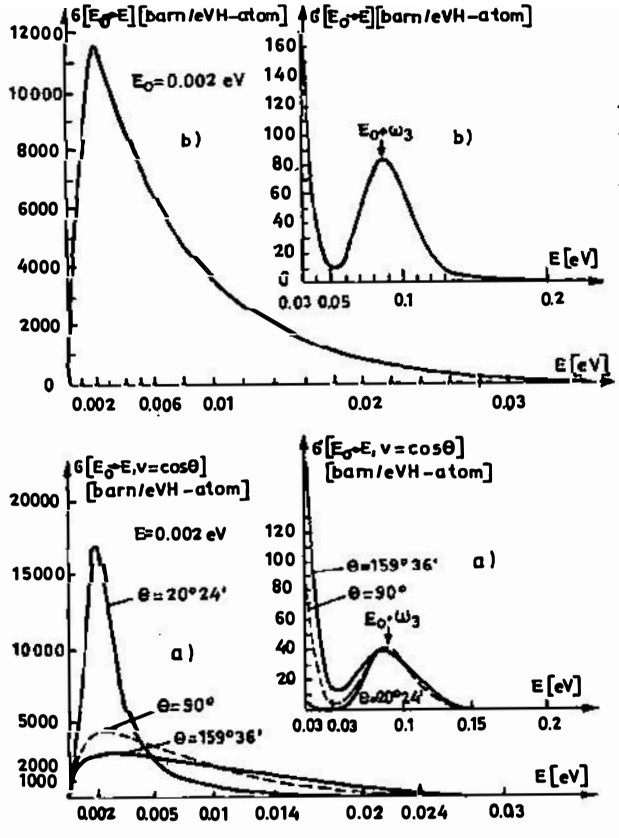

Fig. 1.

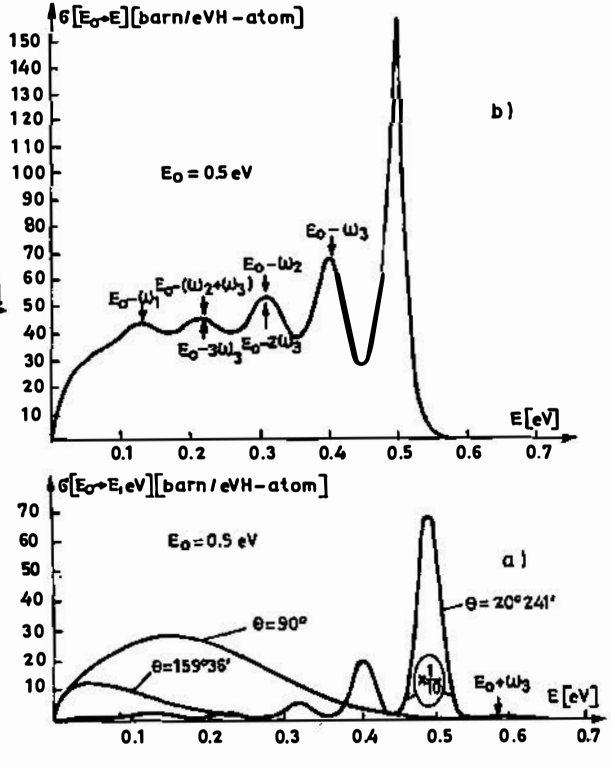

Fig. 2.

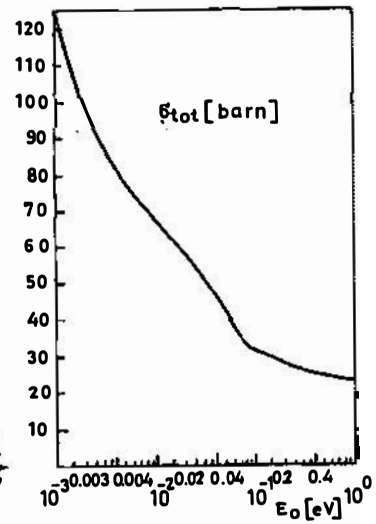

Fig. 3.

2. ANALYSIS OF THE RESULTS OBTAINED

Applying expression (2) for twenty-eight incident neutron energies $E_0 \in [1\ meV, 1\ eV]$, double and single differential scattering cross sections, as well as total cross sections, for the thermal neutrons, of the hydrogen atom nucleus of polyethylene, have been calculated. For the incident neutron energies $E_0=0.002$ eV and $E_0=0.5$ eV, in Figs.1a and 2a the dependence of double differential scattering cross sections $\sigma(E_0 \to E, \nu)$ versus E has been presented, for the following three values of the cosine of the scattering angle $\nu=-0.93727$, $\nu=0$ and $\nu=0.93727$. Both figures clearly show highly pronounced quasielastic peaks, when the thermal neutron is forward scattered. From Fig.1a it can be concluded that the phonon destruction of the lowest energy $\omega_3=0.09$ eV shows a weak dependence on a scattering angle. This property is valid for every $E_0 \in [0.001\ eV, 0.01\ eV]$, and with the increase of the incident thermal neutron energy it quickly vanishes. From Fig.2a it can be concluded that the quantum inelastic effects of the creation and the destruction of polyethylene phonons, as well as quasielastic peaks, occur at pronounced forward scattering. Quantum inelastic effects show this property only when $E_0 \in [0.01\ eV, 1\ eV]$.

For the same incident thermal neutron energies, the dependence of differential cross sections $\sigma(E_0 \to E)$ on the scattered energies has been shown in Figs.1b and 2b. These figures clearly show the effects of the creation and the destruction of polyethylene phonons, as well as highly pronounced quasielastic peaks. Fig.3 shows the dependence of total cross section of the incident thermal neutron energy. The evaluated values of total cross sections are in good agreement with the Armstrong experimental values [8].

3. CONCLUSION

The results obtained clearly show quantum inelastic effects of the creation and the destruction of polyethylene phonons, as well as highly pronounced quasielastic peaks. For all twenty-eight incident thermal neutron energies studied the quasielastic peaks occur at pronounced forward scattering, only when $E_0 \in [0.001\ eV, 0.01\ eV]$, then the phonon destruction of energy $\omega_3=0.09$ eV shows a weak dependence on a scattering angle. This property quickly vanishes with the increase of the incident thermal neutron energy.

4. REFERENCES

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