ON EXCLUSION OF COHERENT SCATTERING FROM THE CROSS SECTION FOR SCATTERING OF SLOW NEUTRONS BY SIMPLE CRYSTAL LATTICES

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A method is proposed for measuring the cross section for scattering of slow neutrons by simple lattices, with coherent single-phonon scattering excluded. The pure incoherent scattering cross section can be used to determine the phonon distribution function in the crystal. The velocity of the incident neutrons should exceed the maximal velocity of sound in the crystal and the scattering cross section should be measured near those directions along which Bragg elastic scattering is possible. If the inelastic forward scattering cross section is measured, polycrystals can be employed. Depending on the crystal under investigation, the incident neutrons should not have a wavelength larger than 1.5—0.5 Å.

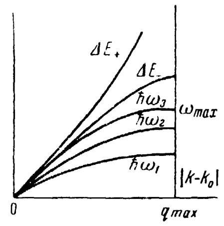
KNOWLEDGE of the distribution function of the frequencies of the phonon spectrum is very important in the study of the properties of a solid. Placzek and Van Hove [1] have shown that incoherent single-phonon scattering of neutrons makes it possible to determine the distribution function for cubic crystals with simple lattice. Tarasov [2] and Kagan [3,4] have considered the question of determining the distribution function in noncubic crystals. The determination of the phonon distribution function from incoherent neutron scattering may be complicated by simultaneous coherent scattering of the neutrons. Kagan [4] proposed a method for measuring the cross section of incoherent neutron scattering with constant variation of the wave vector of the neutron, equal to the reciprocal-lattice vector multiplied by 2π. In the case of a simple lattice, there is no coherent scattering in this case at all. In the present paper we propose a different method of eliminating the coherent neutron scattering in the case of simple lattices.

As is well known, coherent one-phonon scattering of neutrons proceeds in such a way that

$$\Delta E = \hbar^2 |k^2 - k_0^2| / 2m = \hbar\omega_j(\mathbf{q}), \qquad (1)$$

$$\mathbf{k} - \mathbf{k}_0 = \mathbf{q} + 2\pi\boldsymbol{\tau}, \qquad (2)$$

where ΔE is the change in neutron energy upon scattering, $\mathbf{k}_0$ and $\mathbf{k}_1$ the wave vectors of the neutron before and after scattering, m the neutron mass, $\omega_j(\mathbf{q})$ the phonon spectrum of the vibration branch j with wave vector $\mathbf{q}$, and $\boldsymbol{\tau}$ an arbitrary reciprocal-lattice vector. Let us consider the scattering of a neutron in a direction, such that



Bragg reflection is possible, that is, the neutron wave vector changes by 2π in elastic scattering. If the initial neutron wave vector $\mathbf{k}_0$ is assumed constant, then the change in its energy is a function of $\mathbf{k} - \mathbf{k}_0$. The figure shows the dependence of the variation of the neutron energy on the variation of its wave vector in scattering in this direction with an energy gain $\Delta E_+(\mathbf{k} - \mathbf{k}_0)$ and an energy loss $\Delta E_-(\mathbf{k} - \mathbf{k}_0)$, and the phonon energy $\hbar\omega_j(\mathbf{q})$ as a function of their wave vectors in the same direction. These curves should cross at the origin, for when $\mathbf{k} = \mathbf{k}_0$ we should have in this direction

$$\mathbf{k} - \mathbf{k}_0 = 2\pi\boldsymbol{\tau}, \quad \hbar\omega(2\pi\boldsymbol{\tau}) = \Delta E_{\pm}(k - k_0 = 0) = 0.$$

Coherent scattering is possible at the points of their intersection. If the slope of ΔE_+ at the origin is larger than or equal to the slope of the highest vibration branch ω_3, then the ΔE_+ and $\hbar\omega_j$ curves will not cross again anywhere and consequently, coherent scattering with a gain in energy is impossible. Thus, if

$$|\partial\Delta E/\partial \mathbf{k}|_{k=k_0} \geqslant \hbar\,|\partial\omega_j/\partial\mathbf{q}|_{\mathbf{q}=0}, \text{ i.e., } v_0 \geqslant v_{\mathrm{ac}}^{max}, \qquad (3)$$

we obtain pure incoherent scattering of the neutron with energy gain, from which we can determine the phonon distribution function[2,3]. (Here v_0 is the velocity of the incoming neutrons and v_{ac}^{max} is the maximum speed of sound in the crystal.)

If $\tau \neq 0$, the measurements must be carried out with a single crystal. If we investigate the inelastic forward scattering cross section, that is, for $\tau = 0$, then the specimen can be polycrystalline.

Let us estimate the incident-neutron wavelength λ necessary for such an experiment. The maximum (longitudinal) velocity of sound v_L in solids has a value $2 \times 10^5 - 6 \times 10^5$ cm/sec. The wavelength of the incoming neutron, as follows from (3), is

$$\lambda \leqslant \frac{2\pi\hbar}{mv_L} = 3.76 \cdot 10^{-3}\, v_L^{-1}, \tag{4}$$

that is, the upper limit of λ lies between 1.5 and 0.5 Å.

It is also possible to use the neutron energy loss. For this purpose the energy of the incident neutrons must be increased to such an extent, that when $k_0 - k = q_{max}$ the energy loss is

$$\Delta E_-(q_{max}) = \hbar^2 (k_0^2 - k^2)/2m > \hbar\omega_{max}. \tag{5}$$

Here q_{max} is the maximum wave vector of the phonons, equal to π/a_0, where a_0 is the lattice constant (for simplicity we consider a cubic crystal) and ω_{max} is the maximum phonon frequency. If we assume that the entire spectrum of the oscillations is elastic, then $\omega_{max} = v_L q_{max}$ and it follows from (5) that

$$v_0 > v_L + \pi\hbar/2ma_0. \tag{6}$$

The addition to the condition (4) is equal to approximately 0.5×10^5 cm/sec, that is, it is considerably less than v_L.

In measurements of the spectrum of the scattered neutrons in the direction of the Bragg peak, the following experimental difficulty arises: the number of elastically scattered neutrons is much larger than the number of inelastically scattered neutrons. This imposes stringent requirements on the energy resolution. This difficulty can be circumvented by setting up the experiment in such a way that in the elastic scattering the wave vector of the neutron changes by an amount somewhat smaller than $2\pi\tau$. Then there will be no Bragg peak in the measured direction. The $\hbar\omega$ and ΔE curves will intersect near the origin, giving coherent scattering at low phonon energies. This introduces an error in the determination of the initial part of the frequency distribution function of the phonon spectrum, which is immaterial, since this part can be readily determined from the elastic constants. This idea was advanced by S. V. Maleev.

The proposed method is simpler than that of constantly varying the wave vector of the neutron, since it is necessary to investigate here scattering in one direction at a constant crystal orientation. Its advantage is also the possibility of working with a polycrystal in the case of forward scattering. A shortcoming is the need for using hotter neutrons.

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