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Letters to the Editor

EXCITATION OF OPTICAL FREQUENCIES IN CRYSTALS BY SLOW NEUTRONS

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THE inelastic single-phonon scattering of slow neutrons with the excitation of an acoustical oscillation has been studied both from the theoretical and experimental points of view. In crystals with many atoms, neutron scattering can excite not only acoustical, but also optical modes of vibration in the lattice. Experimental difficulties make the identification of different modes of the dispersion function $\omega(\mathbf{q})$ either very difficult or impossible. However, it is possible to show that if the speed v of the incident neutrons is greater than the maximal speed of sound $c_{\max}$, and if they are incident at a Bragg angle, then the reflected beam will contain, in addition to elastically scattered neutrons, only neutrons scattered in the optical mode (not on the acoustical one). This circumstance can be used to determine optical frequencies experimentally.

The unavoidable presence of an angular spread Δ in the incident beam will lead to energies $E_0 - h\omega_{ac}$ in the spectrum of the scattered neutrons, which correspond to the excitation of acoustical frequencies (E_0 is the initial neutron energy). Let us see what limitations must be placed on Δ if we wish to separate the optical from the acoustical frequencies. It is clear that the maximal wave vector $q_{\max}$ of the emitted or absorbed phonon will be $\approx k_0 v$, where $k_0 = mv/h$ is the wave vector of the neutron. Taking v to be as small as it can, $c_{\max}$, we obtain

$$(h\omega_{\mathrm{ac}})_{\max} = mc_{\max}^2\Delta.$$

and hence obtain the desired relations:

$$\Delta \ll h\omega_{\mathrm{opt}}/mc_{\max}^2.$$

Now let us calculate the cross section for scattering with excitation of an optical mode. We denote the wave vector of the scattered neutron by $\mathbf{k}$, and that of the emitted phonon by $\mathbf{q}$. Generalizing formula (40.4) of Ref. 1 to a complex crystal, we obtain the following formula for the cross section of a given process, calculated per unit cell:

$$\frac{d\sigma}{d\mathbf{k}\,d\mathbf{q}} = \frac{1}{k_0}\left|\sum_\alpha m_\alpha^{-1/2} a_\alpha e^{-W_\alpha} \exp\{i(\boldsymbol{\varkappa}-\mathbf{q})\mathbf{r}_\alpha\}\,\boldsymbol{\varkappa}\mathbf{e}_{\mathbf{q}t}^{\alpha*}\right|^2$$

$$\frac{h(\bar{n}_{\mathbf{q}t}+1)}{\omega_{\mathbf{q}t}}\,\delta(\boldsymbol{\varkappa}-\mathbf{q}-2\pi\boldsymbol{\tau})\,\delta\left(k^2-k_0^2-\frac{2m}{h}\omega_{\mathbf{q}t}\right). \quad (1)$$

Here $\boldsymbol{\kappa} \equiv \mathbf{k}_0 - \mathbf{k}$; the index α labels the nuclei in unit cell; $\mathbf{r}_\alpha$, m_α, a_α, e^{-W_α} are the corresponding coordinates, masses, scattering amplitudes, and thermal factors; $\omega_{\mathbf{q}t}$ and $\bar{n}_{\mathbf{q}t}$ are the frequencies and mean occupation numbers of the oscillation $(\mathbf{q}, t)$; t labels the modes; $\mathbf{e}_{\mathbf{q}t}^{\alpha}$ are the displacement vectors of nucleus α in the oscillation $(\mathbf{q}, t)$, normalized as follows:

$$\sum_\alpha \mathbf{e}_{\mathbf{q}t}^{\alpha}\mathbf{e}_{\mathbf{q}t'}^{\alpha*} = \delta_{tt'}. \quad (2)$$

$\omega_{\mathbf{q}t}$ depends little on $\mathbf{q}$ for the optical modes. For example, according to the calculations of Tolpigo and Zaslavs'ka,[2] $\omega_{\mathbf{q}t}$ varies in NaCl by no more than 20% over the whole range of $\mathbf{q}$. Since, for our case, only small $\mathbf{q}$ appear.

$$\omega_{\mathbf{q}t} \approx \omega_{0t}, \qquad \bar{n}_{\mathbf{q}t} \approx \bar{n}_{0t} = (e^{h\omega_0 t/T}-1)^{-1}.$$

Then from (1) it follows that

$$\frac{d\sigma}{d\Omega} = \sqrt{1-\frac{2m\omega_{0t}}{hk_0^2}}\left|\sum_\alpha m_\alpha^{-1/2} a_\alpha e^{-W_\alpha} e^{i\varkappa\mathbf{r}_\alpha}\boldsymbol{\varkappa}\mathbf{e}_{\mathbf{q}t}^{\alpha*}\right|^2$$

$$\times\frac{h}{2\omega_{0t}}(1-e^{-h\omega_{0t}/T})^{-1}. \quad (3)$$

As an example, let us consider the excitation of longitudinal optical vibrations in a crystal of NaCl. Since these are polarized along the main diagonal of the cubical NaCl lattice, we should take a Bragg angle such that $\boldsymbol{\kappa}$ is parallel to the main diagonal, i.e., $\boldsymbol{\kappa} = 2\pi p(\boldsymbol{\tau}_1 + \boldsymbol{\tau}_2 + \boldsymbol{\tau}_3)$, where the $\boldsymbol{\tau}_i$ are the basis vectors of the inverse lattice, and p is an integer. We find the vectors $\mathbf{e}_{\mathbf{q}\,\mathrm{long}}$ for the nuclei Na and Cl in the limit $q \to 0$. Since, for $q = 0$, the set of ions Na and Cl vibrate relative to each other bodily, these vectors can be found from the center-of-mass condition and the normalization (2). The thermal factors are calculated in the Einstein approximation. The optical frequencies are obtained from Ref. 2. The neutron velocity v appears only in the first factor in (3), which is always close to 1 for $v > c_{\max}$. We can neglect it. The result is the following differential scattering cross section for one molecule NaCl (in millibarns per steradian):

p	1	2	3	4	5	6
$d\sigma/d\Omega$	7.1	25	44.6	59	62.5	54.5

As a function of p, $d\sigma/d\Omega$ has a maximum due to competition between the factor κ^2 and the thermal factor.

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[1] A. I. Akhiezer and I. Ia. Pomeranchuk, Некоторые вопросы теории ядра (Certain Problems in Nuclear Theory), GITTL, 1950.

[2] K. B. Tolpigo and I. G. Zaslavs'ka, Укр. физ. журн. (Ukrainian Phys. J.) 1, 226 (1956).

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EQUATION OF STATE FOR THE MgO CRYSTAL

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THIS letter is a report on the calculation of the energy of the MgO crystal by a statistical method. The dependence of energy on volume at absolute zero has been found for pressures from zero to 10^7 atmospheres (at high pressures, the effect of temperature is small[1]).

In calculations for lattices of the alkali halide type it is customary to use a potential derived from the electron density of an isolated ion, i.e., to ignore the deformation of the ions in the lattice. But an isolated oxygen ion is not, in general, stable; in this work the electron density chosen for oxygen was found for a lattice at zero pressure by a variational method.[2] The magnesium ion deforms very litte, and the Hartree-Fock electron density is used in this case.[3] The energy calculations took into account the first quantum correction,[4] assuming an overlap of about 20%.

According to the statistical theory, the energy of any system of electrons with a density ρ is equal to:

$$\varepsilon(\rho) = \int \left\{ \varkappa_k \rho^{5/3} + \left(V_k + \frac{1}{2} V_p \right) \rho - \varkappa_a \rho^{4/3} - K(\rho) + \frac{1}{72} \frac{(\nabla \rho)^2}{\rho} \right\} dv,$$

$$\varkappa_k = 2.871, \quad \varkappa_a = 0.7386,$$

i.e., the sum of the kinetic (Fermi) and potential (Thomas-Fermi) energies of the electrons in the nuclear field, the Dirac exchange energy, the Wigner-Macke correlation energy, and the quantum correction of Kompaneev and Kirzhnits.[4-6] Atomic units are used throughout.

The correlation energy,

$$K(\rho) = 0.0306 \rho \left\{ \ln \left(1 + \frac{4}{\lambda} \right) - \frac{2}{1 + 2\lambda} \right\}, \quad 1/\lambda = 4.862 \rho^{1/3}$$

in the region of density $\rho = 0.2$ to 0.02 which we consider here, is approximately equal to

$$K(\rho) \approx 0.113 \varkappa_a \rho^{4/3}.$$

The ionic energy of the crystal is obtained by summing the interaction energy of one pair of ions over all the ion pairs in the lattice. The interaction energy of each pair of ions is equal to

$$U = \varepsilon(\rho_1 + \rho_2) - \varepsilon(\rho_1) - \varepsilon(\rho_2) = q_1 q_2 / r + U_s,$$

where q_1, q_2 are the charges on the ions, ρ_1, ρ_2 are the electron densities of the ions, and U_S is the energy required to remove the electron clouds from both ions.[5] The total energy of the crystal, referred to a single ion pair, has the form

$$E(\delta) = -\alpha q^2 / \delta + 6U_s^{+-}(\delta) + 6U_s^{--}(\sqrt{2}\delta) + 6U_s^{++}(\sqrt{2}\delta),$$

where $\alpha = 1.7476$ for a face-centered lattice, δ is the shortest distance between unlike ions, and U_S^{+-}, U_S^{--}, U_S^{++} are the overlap energies of the corresponding neighboring like and unlike ions.

In order to facilitate the numerical calculations, the electron densities of the ions taken from the literature[2,3] were approximated by the formulas

$$\rho_1(r) = 45 \exp(-4.9 r) \quad \text{magnesium.}$$

$$\rho_2(r) = \left\{ \begin{array}{lll} 280 \exp(-15 r) & \text{for} & r < 0.35 \\ 3.85 \exp(-2.3 r) & \text{"} & 0.35 < r < 1.6 \\ 1.54 \exp(-1.8 r) & \text{"} & r > 1.6 \end{array} \right\} \text{oxygen.}$$

Curves of crystal energy, referred to the energies of the free atoms, are shown in the figure (in atomic units). Curve 1 is the theoretical one. The lower part of Curve 2, where $p < 3 \times 10^4$ atmos, is based on Bridgman's experimental data[7] extrapolated to absolute zero; the portion of Curve 2 where $p > 3 \times 10^4$ atmos is an extrapolation of Bridgman's data to high pressures by Davydov's formula.[1]

In the range of pressures from zero to 10^6 atmospheres the theoretical Curve 1 can be approximated by the formula