

# Dynamic diffraction of neutrons by high-frequency acoustic molecules in perfect crystals

E. M. Iolin

*Physics Institute, Latvian Academy of Sciences*

I. R. Entin

*Institute of Solid State Physics, USSR Academy of Sciences*

(Submitted 6 April 1983)

Zh. Eksp. Teor. Fiz. **85**, 1692–1700 (November 1983)

It is shown that dynamic diffraction of neutrons is sensitive to very low energy transfer corresponding to ultrasound frequencies 10–100 MHz. The calculated position of the satellites on the reflection curves differs from that calculated from the kinematic formulas. It is shown that at sufficiently high frequency the increment to the integral reflection consists of a part that is proportional to the sound amplitude and a term that oscillates as a function of the amplitude.

PACS numbers: 61.12.Dw, 43.35.Gk

It is known that ultrasound oscillations of relatively low frequency (wavelength comparable with the sample size) influence noticeably the Bragg diffraction of x rays and of thermal neutrons in perfect crystals (see, e.g., Refs. 1–4). In this range, the spatial periodicity of the acoustic displacements does not manifest itself and the influence of the ultrasound does not depend on its wavelength  $\lambda_S$ . In the x-ray case a dependence on  $\lambda_S$  appears in the region  $\lambda_S \lesssim \tau$  ( $\tau$  is the extinction length). A transverse acoustic wave propagating in the scattering plane parallel to the reflecting planes causes resonant suppression of the anomalous passage at  $\lambda_S = \tau$  (Ref. 5). The resonance is due to interband scattering that mixes the Bloch states on two branches of the dispersion surface of the dynamic diffraction. The probability of interband scattering in neutron diffraction was calculated in Ref. 6 for the same geometry in a semikinematic approximation. In the Bragg geometry, the interband scattering that is possible at  $\lambda_S < \tau$  leads to an increment, linear in the sound amplitude, to the integral intensity of a reflected x-ray beam.<sup>7</sup> A theory of x-ray scattering by ultrasound oscillations was developed in Ref. 8 for  $\lambda_S \ll \tau$  and in Ref. 9 for the intermediate region  $\lambda_S \sim \tau$ . The related problem of scattering by thermal lattice vibrations was analyzed in Ref. 10.

Neutron diffraction by high-frequency oscillations in a crystal differ substantially from that of x rays. Since the thermal-neutron velocity is of the same order as of the sound, they pass through a sample  $\sim 1$  cm thick within a time  $\sim 10^2 T_S$ , where  $T_S$  is the period of the acoustic oscillations with wavelength equal to the extinction length. Thus, the neutron propagates in an oscillating crystal, whereas x rays, owing to the high speed of light, produce an instantaneous diffraction photograph of the crystal. As a result it is necessary to take into account in the diffraction of neutrons, in contrast to that of x rays, not only the quasimomentum conservation law but also the energy exchange between the neutron and the oscillating crystal. Thus, the satellite angular shift due to the change of the neutron energy is of the order of one second of angle at ultrasound frequencies  $\sim 100$  MHz and is fully commensurate both with the angle width of the diffraction maximum and with the shift due to momentum exchange between

the neutron and the acoustic wave. Consequently, the dynamic neutron diffraction turns out to be sensitive to very small energy transfers corresponding to frequencies 10–100 MHz. The subject of the present paper is a theoretical investigation of dynamic diffraction of neutrons by high-frequency oscillations at  $\lambda_S \sim \tau$ .

## BASIC EQUATIONS

The Schrödinger equation, which describes the propagation of a neutron in a crystal in which an acoustic wave is excited, is of the form

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi + V \Psi, \quad (1)$$

$$V(\mathbf{r}) = \frac{2\pi\hbar^2}{m} \sum_{l,j} a_j \delta(\mathbf{r} - \mathbf{r}_{lj}), \quad (2)$$

$$\mathbf{r}_{lj} = \mathbf{R}_{lj} + \mathbf{u}_{lj}, \quad (3)$$

where  $m$  and  $\mathbf{r}$  are the mass and radius-vector of the neutrons;  $a_j$  is the length of scattering by the  $j$ -th nucleus located in the  $l$ -th unit cell;  $\mathbf{R}_{lj}$  and  $\mathbf{u}_{lj}$  are the equilibrium position and displacement of the nucleus  $lj$  in a traveling acoustic wave:

$$\mathbf{u}_{lj} = \mathbf{W} \exp(i\mathbf{K}_S \mathbf{r}_{lj} - i\omega_S t) + \text{c.c.}, \quad (4)$$

$\mathbf{W}$ ,  $\mathbf{K}_S$ , and  $\omega_S$  are the amplitude, wave vector, and frequency of the ultrasound. The phase of the wave (4) is chosen such that  $\mathbf{W}^* = \mathbf{W}$ . Transforming to Fourier components with respect to the frequency  $\Omega$  and to the wave vector  $\mathbf{q}$ , we obtain in the case of small displacements ( $|\mathbf{H} \cdot \mathbf{W}| \ll 1$ )

$$\Psi = \sum_{\mathbf{q}} \int \Psi(\mathbf{q}, \Omega) \exp(i\mathbf{q}\mathbf{r} - i\Omega t) d\Omega, \quad (5)$$

$$\left[ \hbar\Omega - \frac{\hbar^2 q^2}{2m} - \varepsilon F(0) \right] \Psi(\mathbf{q}, \Omega) - \varepsilon \sum_{\mathbf{H} \neq 0} F(\mathbf{H}) \Psi(\mathbf{q} + \mathbf{H}, \Omega) \quad (6)$$

$$-i\varepsilon \sum_{\alpha = \pm 1, \mathbf{H}} (\mathbf{H}\mathbf{W}) F(\mathbf{H}) \Psi(\mathbf{q} + \mathbf{H} + \alpha\mathbf{K}_S, \Omega + \alpha\omega_S) = 0,$$

$$F(\mathbf{H}) = \sum_j a_j \exp(i\mathbf{H}\mathbf{R}_{lj}), \quad (7)$$

where  $\varepsilon = 2\pi\hbar^2/m\kappa$ ,  $\mathbf{H}$  is the reciprocal-lattice vector,  $\kappa$  is the volume of the unit cell, and  $F(\mathbf{H})$  is a structure factor. For a centrosymmetric crystal without absorption  $F(-\mathbf{H}) = F(\mathbf{H})$ .

We shall assume that the two-wave case is realized in the crystal at  $W=0$ . Confining ourselves to the single-phonon approximation, we cut off the infinite system of coupled equations (6) and obtain the matrix equation for the determination of the six most significant components of the

wave function and of the corresponding wave vectors  $\mathbf{q}$  in the form

$$\hat{B}|\Psi\rangle=0, \quad (8)$$

where

$$\hat{B} \equiv \begin{vmatrix} C_0 & D & D \\ D & C_1 & 0 \\ D & 0 & C_{-1} \end{vmatrix}$$

contains the blocks

$$C_\alpha \equiv \begin{vmatrix} \hbar\Omega + \alpha\hbar\omega_s - \frac{\hbar^2(\mathbf{q} + \alpha\mathbf{K}_s)^2}{2m} - \varepsilon F(0) & -\varepsilon F(\mathbf{H}) \\ -\varepsilon F(\mathbf{H}) & \hbar\Omega + \alpha\hbar\omega_s - \frac{\hbar^2(\mathbf{q} + \mathbf{H} + \alpha\mathbf{K}_s)^2}{2m} - \varepsilon F(0) \end{vmatrix}, \quad (9)$$

$$D = (\mathbf{H}\mathbf{W})\varepsilon F(\mathbf{H}) \begin{vmatrix} 0 & -i \\ i & 0 \end{vmatrix},$$

and the wave function is

$$|\Psi\rangle \equiv \begin{vmatrix} \Psi_{00} \\ \Psi_{0\mathbf{H}} \\ \Psi_{10} \\ \Psi_{1\mathbf{H}} \\ \Psi_{-10} \\ \Psi_{-1\mathbf{H}} \end{vmatrix};$$

here

$$\Psi_{\alpha\mathbf{e}} \equiv \Psi(\mathbf{q} + \mathbf{G} + \alpha\mathbf{K}_s, \Omega + \alpha\omega_s)$$

are the amplitudes of the plane-wave components. To determine the wave fields we must use the condition that  $\Psi$  be continuous on the crystal surface. As usual, we neglect the continuity condition for the normal derivative of  $\Psi$ , since the refractive index of the neutron wave is close to unity.

A few preliminary remarks are in order concerning the structure of Eq. (8). In the absence of sound, i.e., at  $D=0$ , the matrix  $\hat{B}$  is quasi-diagonal, and each of the matrices  $C_\alpha$  describes two-wave diffraction for the pair of waves  $|\mathbf{q} + \alpha\mathbf{K}_s\rangle, |\mathbf{q} + \mathbf{H} + \mathbf{K}_s\rangle$ . It is known<sup>11</sup> that the eigenvalues  $\mathbf{q}$  of the matrices  $C_\alpha$ , determined from the condition  $\det C_\alpha = 0$ , form in reciprocal space a two-sheeted dispersion surface. This surface is obtained at  $\alpha = \pm 1$  from the surface with  $\alpha = 0$  by shifting the latter by a certain vector  $\delta\mathbf{q}_\alpha$ . Neglecting small quantities of the order of  $(K_s/q)^2$  and  $(\delta q_\alpha/q)^2$ , we obtain

$$\delta\mathbf{q}_\alpha = \alpha(\mathbf{K}_s' - \Delta K_\omega \mathbf{e}), \quad \mathbf{K}_s' = \mathbf{K}_s - (\mathbf{K}_s \mathbf{f}) \mathbf{f}, \quad (10)$$

$$\Delta K_\omega = \omega_s/v \cos \theta_B, \quad \mathbf{e} = (\mathbf{e}_0 + \mathbf{e}_H)/2 \cos \theta_B,$$

where  $\mathbf{f}$  is a unit vector normal to the scattering plane,  $v$  is the neutron velocity,  $\mathbf{e}_0$  and  $\mathbf{e}_H$  are unit vectors in the directions of the incident and diffracted waves, and  $\theta_B$  is the Bragg angle.

The matrix  $D$  mixes the eigenfunctions with different  $\alpha$ . In the absence of degeneracy of the eigenvalue at different  $\alpha$ , small perturbation of  $D$  changes the eigenvalues by an amount  $\sim |\mathbf{H}\cdot\mathbf{W}|^2$  and the eigenfunctions by  $\sim |\mathbf{H}\cdot\mathbf{W}|$ . The

situation changes in the presence of degeneracy. Additional gaps appear on the dispersion surface in the branch intersection region, the eigenvalues change by an amount  $\sim |\mathbf{H}\cdot\mathbf{W}|$  and the eigenfunctions change by an amount  $\sim 1$ . Corresponding to the additional gaps are satellites on the reflection curves. In other words, one can speak of intraband scattering if branches of like type intersect, and of interband scattering if states of unlike type are mixed. It must be emphasized that the wave function of the considered nonstationary problem constitutes a superposition of waves of different frequency. The mixing waves with different  $\alpha$ , however, preserve their coherence because the acoustic perturbation is coherent.

The term  $\Delta K_\omega \mathbf{e}$  in (10) is the result of the Doppler effect on the traveling acoustic wave and of the change of the lengths of the wave vectors of the inelastically scattered neutrons. For thermal neutrons we have  $v \sim v_s$  ( $v_s$  is the speed of sound) and  $\Delta K_\omega \sim K_s$ , whereas for x-ray diffraction  $\Delta K_\omega$  is negligibly small. Depending on the mutual orientation of  $\mathbf{K}_s$  and  $\mathbf{e}$ , the momentum contribution  $\mathbf{K}_s'$  and the energy contribution  $\Delta K_\omega \mathbf{e}$  to  $\delta\mathbf{q}_\alpha$  can either cancel each other or add up. This leads to a change of  $|\delta\mathbf{q}_\alpha|$  and of the angle between the satellites when the direction of the traveling ultrasound wave is reversed. For a standing wave, the same circumstance gives rise to the appearance of four rather than two satellites in the x-ray case. Total mutual cancellation of the two contributions to  $|\delta\mathbf{q}_\alpha|$ , which is possible at  $\mathbf{K}_s' \parallel \mathbf{e}$ , takes place if the sound velocity is equal to the projection of the neutron velocity on the acoustic-wave propagation direction. In this case there is no interaction with the sound at all, since the phase of the oscillation and the magnitude of the displacement remain unchanged on the neutron path. On the other hand,  $\delta\mathbf{q}_\alpha \neq 0$  when the ultrasound propagates perpendicular to the scattering plane ( $\mathbf{K}_s' = 0$ ), so that in this geometry, in contrast to the x-ray case, the interaction with the acoustic wave does not vanish.

#### SYMMETRIC LAUE REFLECTION

Let a neutron with a wave vector  $\mathbf{Q}$  be incident on a plane-parallel plate of thickness  $T$  and let the angle  $\theta$  to the

reflecting planes be close to the Bragg angle  $\theta_B$ . The neutron has inside the crystal a wave vector  $\mathbf{q} = \mathbf{Q} - \mathbf{n}\xi$ , where  $\mathbf{n}$  is the inward normal to the surface and  $\xi$  is determined from the condition  $\det C_\alpha = 0$  at  $\Omega = \hbar^2 Q^2/2m$ . Neglecting the small quantities  $\sim (K_s/Q)^2$ , we obtain the eigenvalues  $\xi_{\alpha\pm}$  and the eigenfunctions  $\Psi_{\alpha\pm}$  corresponding to the two branches of the dispersion surface:

$$\begin{aligned} \xi_{\alpha\pm} &= -Q \sin \theta_B \Delta\theta + \frac{2\pi F(0)}{Q \cos \theta_B \kappa} \\ &- \alpha \left[ \frac{\omega_s}{v \cos \theta_B} - \frac{(\mathbf{e}_0 + \mathbf{e}_H) \mathbf{K}_s}{2 \cos \theta_B} \right] \mp \frac{\Delta K}{2}, \end{aligned} \quad (11)$$

$$\Psi_{\alpha+} = \begin{vmatrix} \sin(\gamma/2) \\ -\cos(\gamma/2) \end{vmatrix}$$

$$\Psi_{\alpha-} = \begin{vmatrix} \cos(\gamma/2) \\ \sin(\gamma/2) \end{vmatrix},$$

where

$$\Delta K = \Delta K_0 / \sin \gamma_\alpha$$

is the splitting of the two-wave dispersion surface for a definite angular deviation from the exact Bragg condition;

$$\Delta K_0 = 2\pi/\tau = 4\pi F(\mathbf{H})/Q \cos \theta_B \kappa$$

is the minimum value of the splitting  $\Delta K$ ;

$$\text{ctg } \gamma_\alpha = \frac{1}{\Delta K_0} \left( 2Q \sin \theta_B \Delta\theta - \alpha \frac{\mathbf{H} \mathbf{K}_s}{Q \cos \theta_B} \right); \quad \Delta\theta = \theta - \theta_B.$$

The boundary condition on the entrance surface of the plate is

$$\Psi_{\alpha 0} = \delta_{\alpha 0}, \quad \Psi_{\alpha H} = 0.$$

Let us consider a number of concrete cases.

1. We denote by  $I_{R0}$  the intensity of the reflected beam in the absence of an acoustic perturbation. Averaging of this quantity over the extinction beats yields<sup>11</sup>

$$\bar{I}_{R0} = \frac{1}{2} [1 + (\Delta\theta/\Delta\theta_0)^2]^{-1}, \quad (12)$$

where  $\Delta\theta_0 = d/\tau$  is the angle width of the diffraction maximum and  $d$  is the distance between the planes.

2. A transverse ultrasound wave is excited in the crystal and propagates perpendicular to the scattering plane,

$$\mathbf{H} \mathbf{K}_s = 0, \quad \mathbf{Q} \mathbf{K}_s = 0, \quad \mathbf{H} \mathbf{W} \neq 0$$

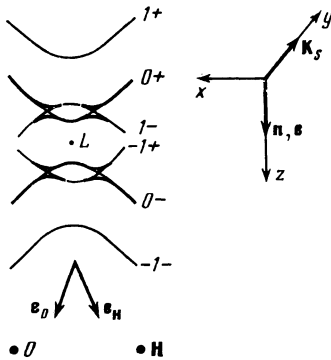


FIG. 1. Dispersion surface modified by interaction with an acoustic wave. The branch  $1+$  corresponds to  $\xi_{1+}$ , etc.

(each scattering plane oscillates as a unit, with a frequency  $\omega_s$ ). Intersection of the dispersion branches (see the figure) corresponds to the equations

$$\xi_{0+} = \xi_{1-}, \quad \xi_{0-} = \xi_{-1+}. \quad (13)$$

Using (22), we can rewrite the conditions (13) in the form

$$\Delta K = \Delta K_\omega. \quad (14)$$

It follows from (14) that the intersection of the dispersion surfaces takes place at  $\omega_s > \Delta K_0 v \cos \theta_B$ , the intersection points being symmetric about the Lorentz point  $L$ . For small  $|\mathbf{H} \cdot \mathbf{W}|$  near the degeneracy points (13) we obtain the perturbed eigenvalues of the matrix  $B$  in the form

$$\begin{aligned} \xi_{1,2} &= (\xi_{0+} + \xi_{1-})/2 \mp |\mathbf{H} \mathbf{W}| \Delta K_0/2 \sin \delta, \\ \xi_{3,4} &= (\xi_{0-} + \xi_{-1+})/2 \mp |\mathbf{H} \mathbf{W}| \Delta K_0/2 \sin \delta, \end{aligned} \quad (15)$$

where

$$\text{ctg } \delta = (\Delta K_\omega - \Delta K) / |\mathbf{H} \mathbf{W}| \Delta K_0.$$

Exact resonance corresponds to  $\delta = \pi/2$ . The acoustic perturbation lifts the degeneracy at the points of intersection and leads to formation of the gap  $|\mathbf{H} \cdot \mathbf{W}| \Delta K_0$ . Taking the boundary conditions into account we obtain the wave function of the neutron in the crystal:

$$\begin{aligned} \Psi &= \exp(i\mathbf{Q}\mathbf{r} - i\Omega t) \left\{ \sin \frac{\gamma}{2} \cos \frac{\delta}{2} \exp(-i\xi_1 z) \right. \\ &\times \left[ \cos \frac{\delta}{2} \begin{vmatrix} \sin(\gamma/2) \\ -\cos(\gamma/2) \exp(i\mathbf{H}\mathbf{r}) \end{vmatrix} + i \sin \frac{\delta}{2} \exp(i\mathbf{K}_s \mathbf{r} - i\omega_s t) \right. \\ &\times \left. \begin{vmatrix} \cos(\gamma/2) \\ \sin(\gamma/2) \exp(i\mathbf{H}\mathbf{r}) \end{vmatrix} \right] + \sin \frac{\gamma}{2} \sin \frac{\delta}{2} \exp(-i\xi_2 z) \\ &\times \left[ \sin \frac{\delta}{2} \begin{vmatrix} \sin(\gamma/2) \\ -\cos(\gamma/2) \exp(i\mathbf{H}\mathbf{r}) \end{vmatrix} - i \cos \frac{\delta}{2} \exp(i\mathbf{K}_s \mathbf{r} - i\omega_s t) \right. \\ &\times \left. \begin{vmatrix} \cos(\gamma/2) \\ \sin(\gamma/2) \exp(i\mathbf{H}\mathbf{r}) \end{vmatrix} \right] + \cos \frac{\gamma}{2} \sin \frac{\delta}{2} \exp(-i\xi_3 z) \\ &\times \left[ \sin \frac{\delta}{2} \begin{vmatrix} \cos(\gamma/2) \\ \sin(\gamma/2) \exp(i\mathbf{H}\mathbf{r}) \end{vmatrix} - i \cos \frac{\delta}{2} \exp(-i\mathbf{K}_s \mathbf{r} + i\omega_s t) \right. \\ &\times \left. \begin{vmatrix} \sin(\gamma/2) \\ -\cos(\gamma/2) \exp(i\mathbf{H}\mathbf{r}) \end{vmatrix} \right] + \cos \frac{\gamma}{2} \cos \frac{\delta}{2} \exp(-i\xi_4 z) \\ &\times \left[ \cos \frac{\delta}{2} \begin{vmatrix} \cos(\gamma/2) \\ \sin(\gamma/2) \exp(i\mathbf{H}\mathbf{r}) \end{vmatrix} + i \sin \frac{\delta}{2} \exp(-i\mathbf{K}_s \mathbf{r} + i\omega_s t) \right. \\ &\times \left. \begin{vmatrix} \sin(\gamma/2) \\ -\cos(\gamma/2) \exp(i\mathbf{H}\mathbf{r}) \end{vmatrix} \right] \left. \right\}; \end{aligned} \quad (16)$$

the  $z$  axis is directed along  $\mathbf{n}$ . The upper row of the two-dimensional vector  $\Psi$  corresponds to waves whose directions are close to the incident wave, and the lower row corresponds to the reflected beam. After averaging over the spatial dimensions of the neutron detector  $l \gg 2\pi/K_s$  and (or) over time intervals longer than  $2\pi/\omega_s$  we obtain the intensity  $I_{Re}$  of the elastically reflected wave and of the waves with increased ( $I_{R+}$ ) and decreased ( $I_{R-}$ ) frequencies:

$$\begin{aligned} I_{Re} &= \frac{\sin^2 \gamma}{4} \left| \sin^2 \frac{\delta}{2} [e^{-i\xi_1 \tau} - e^{-i\xi_2 \tau}] + \cos^2 \frac{\delta}{2} [e^{-i\xi_3 \tau} - e^{-i\xi_4 \tau}] \right|^2, \\ I_{R+} &= \frac{1}{4} \sin^4(\gamma/2) \sin^2 \delta |e^{-i\xi_1 \tau} - e^{-i\xi_2 \tau}|^2, \\ I_{R-} &= \frac{1}{4} \cos^4(\gamma/2) \sin^2 \delta |e^{-i\xi_3 \tau} - e^{-i\xi_4 \tau}|^2. \end{aligned} \quad (17)$$

We can separate in the total intensity  $I_R = I_{Re} + I_{R+} + I_{R-}$  of the reflected beam the terms with different dependences on the plate thickness:

$$I_R = I_1 + I_2 + I_3. \quad (18)$$

Here  $I_1$  does not depend on  $T$ , with

$$I_1 = \bar{I}_{R0} + \Delta I_1,$$

where

$$\Delta I_1 = \frac{1}{2} \cos^2 \gamma \frac{(\mathbf{H}\mathbf{W}\Delta K_0)^2}{(\mathbf{H}\mathbf{W}\Delta K_0)^2 + (\Delta K_\omega - \Delta K)^2}. \quad (19)$$

The quantity  $\Delta I_1$  reaches values  $\sim 1$  at angles satisfying the conditions (14), and decreases rapidly with the angle mismatch. Thus, expression (19) describes the onset, on the reflection curve, of satellites with angle width

$$\delta\theta = |\mathbf{H}\mathbf{W}| \Delta\theta_0 [1 - (\Delta K_\omega / \Delta K_0)^2]^{-1/2}.$$

At  $|\Delta K_\omega - \Delta k_0| \gg |\mathbf{H}\mathbf{W}|^2 \Delta K_0$  the satellites have a small angle width  $\delta\theta \ll \Delta\theta_0$ . We confine ourselves hereafter to this situation. The case of broad satellites, which corresponds to tangency of the branches of the dispersion surface, calls for a separate analysis and is not considered here. The second term in the right-hand side of (18) oscillates slowly with change of thickness:

$$I_2 = -1/2 \sin^2 \delta \cos^2 \gamma \cos [(\xi_1 - \xi_2) T], \quad (20)$$

and the third term oscillates with a small period on the order of the extinction length  $\tau$ :

$$I_3 = -1/4 \sin^2 \gamma \{ \sin^2 \delta \cos(\Delta K_\omega T) + 2 \sin^4(\delta/2) \cos[(\Delta K_\omega + \xi_1 - \xi_2) T] + 2 \cos^4(\delta/2) \cos[(\Delta K_\omega - \xi_1 + \xi_2) T] \}.$$

Assuming the crystal to be thick ( $T \gg \tau$ ), we average  $I_R$  over the rapid extinction beats and determine the ultrasound-induced increment  $\Delta R$  to the integral reflection:

$$\Delta R \equiv \int_{-\infty}^{\infty} (\Delta I_1 + I_2) d\theta, \quad (21)$$

$$\Delta R_1 \equiv \int_{-\infty}^{\infty} \Delta I_1 d\theta = 2 |\mathbf{H}\mathbf{W}| [1 - (\Delta K_\omega / \Delta K_0)^2]^{1/2} \bar{R},$$

where  $\bar{R}$  is the averaged integral reflection in the absence of oscillations:

$$\bar{R} \equiv \int_{-\infty}^{\infty} \bar{I}_{R0} d\theta = \frac{\pi}{2} \Delta\theta_0.$$

The quantity  $\Delta R_1$  is linear in the amplitude of the acoustic wave. At  $\omega_S < \Delta K_0 v \cos \theta_B$  there is no intersection of branches and  $\Delta R_1$  vanishes. It can be easily seen that in this case the increment to the integral reflection is quadratic in the sound amplitude.

Recognizing that  $\delta\theta \ll \Delta\theta_0$ , we obtain the oscillating increment to the integral reflection:

$$\Delta R_2 \equiv \int_{-\infty}^{\infty} I_2 d\theta \approx -\Delta R_1 \int_{|\mathbf{H}\mathbf{W}| \Delta K_0 T}^{\infty} J_0(x) dx, \quad (22)$$

where  $J_0(x)$  is a Bessel function of zero order. If

$|HW| \Delta K_0 T \ll 1$ , then  $\Delta R_2 \approx \Delta R_1$  and the amplitude dependence has a zero slope at  $W = 0$ . At  $|\mathbf{H}\mathbf{W}| \Delta K_0 T \gg 1$  we have

$$\Delta R_2 \approx - \frac{\Delta R_1}{(|\mathbf{H}\mathbf{W}| \Delta K_0 T)^{1/2}} \left[ 0.8 \cos \left( |\mathbf{H}\mathbf{W}| \Delta K_0 T + \frac{\pi}{4} \right) + \frac{0.5}{|\mathbf{H}\mathbf{W}| \Delta K_0 T} \sin \left( |\mathbf{H}\mathbf{W}| \Delta K_0 T + \frac{\pi}{4} \right) \right]. \quad (23)$$

It can be seen from (23) that the increment to the integral reflection contains a term that oscillates over the crystal thickness, with a period  $2\pi/|\mathbf{H}\mathbf{W}| \Delta K_0 \gg \tau$ . The long-wave oscillations are due to the onset of a gap in the region of the self-intersection of the dispersion surface, and are the analog of extinction beats for the case of a controllable scattering amplitude. Their observation can be used in principle for absolute measurement of the amplitude of high-frequency ultrasound. It must be emphasized that in the geometry considered the ultrasound does not influence the x-ray diffraction.<sup>12</sup>

3. A transverse ultrasound wave is excited in the crystal and propagates along the vector  $\mathbf{n}$ ,

$$\mathbf{H}\mathbf{K}_s = 0, \quad \mathbf{n}\mathbf{K}_s = K_s, \quad \mathbf{H}\mathbf{W} \neq 0.$$

Simple calculation shows that a pair of symmetrically located satellites is produced at the angles  $\Delta\theta$  given by the condition

$$[(\Delta\theta)^2 + (\Delta\theta_0)^2]^{1/2} = |(\omega_S - v K_s \cos \theta_B) / v Q \sin 2\theta_B|, \quad (24)$$

where the frequency must exceed a certain threshold value

$$\omega_S > \Delta K_0 v \cos \theta_B |1 - (v/v_S) \cos \theta_B|^{-1}.$$

When the propagation direction of the acoustic wave is reversed, we obtain in place of (24)

$$[(\Delta\theta)^2 + (\Delta\theta_0)^2]^{1/2} = (\omega_S + v K_s \cos \theta_B) / v Q \sin 2\theta_B \quad (25)$$

with a condition on the frequency

$$\omega_S > \Delta K_0 v \cos \theta_B [1 + (v/v_S) \cos \theta_B]^{-1}.$$

When a standing ultrasound wave is excited in the crystal, an increase of  $\Delta S$  leads first to satellites given by the condition (25), followed by an additional pair that satisfies (24). In the x-ray case, at analogous geometry, only two satellites appear at  $K_S > \Delta K_0$  (Ref. 7). It must be pointed out that (24) and (25) contain the quantity  $\Delta\theta_0$ . This leads to a deviation from the simple kinematic expression for the satellite angle at frequencies close to the threshold. The calculation of the increment to the integral reflection is similar to the one performed in example 2.

4. A longitudinal ultrasound wave propagates along a vector  $\mathbf{H}$ . Two cases are realized here.

a. At  $v \sin \theta_B > v_S$  and at an arbitrary frequency of the sound, branches with identical second index can intersect:

$$\xi_{0+} = \xi_{\pm 1+}, \quad \xi_{0-} = \xi_{\pm 1-}.$$

Four symmetrically placed satellites are produced at angles determined from the equation

$$[(\Delta\theta)^2 + (\Delta\theta_0)^2]^{1/2} - \left[ \left( \frac{v}{v_S} \frac{\Delta K_\omega}{Q} - \Delta\theta \right)^2 + (\Delta\theta_0)^2 \right]^{1/2} = \pm \frac{\Delta K_\omega}{Q \sin \theta_B}. \quad (26)$$

b. At  $v \sin \theta_B < v_S$  and at sufficiently high frequency

$$\omega_S > \Delta K_0 v \cos \theta_B [1 - (v \sin \theta_B / v_S)^2]^{-1/2}$$

four satellites appear and are connected with the branch intersections

$$\xi_{0+} = \xi_{1-}, \quad \xi_{0-} = \xi_{-1+}.$$

For the angles  $\Delta\theta$  we have in place of (26) the equation

$$\begin{aligned} & [(\Delta\theta)^2 + (\Delta\theta_0)^2]^{1/2} + \left[ \left( \frac{v}{v_S} \frac{\Delta K_0}{Q} \pm \Delta\theta \right)^2 + (\Delta\theta_0)^2 \right]^{1/2} \\ &= \frac{\Delta K_0}{Q \sin \theta_B}. \end{aligned} \quad (27)$$

Thus, in this case, in contrast to the cases considered above, excitation of a traveling acoustic wave in the crystal produces four satellites. Reversal of the sound-propagation direction or a transition to a standing wave does not alter the diffraction picture. We note that the condition  $v \sin \theta_B = v_S$  that distinguishes between cases a and b corresponds to displacement of the branches of the dispersion surface along their asymptotes and to the absence of satellites.

## CONCLUSION

The investigation of dynamic diffraction of neutrons by high-frequency acoustic oscillations reduces in essence to an analysis of the cases of self-intersection of a modified dispersion surface. The result of the self-intersections is the onset of additional gaps of the dispersion surface and of satellites on the reflection curves. The presence of gaps leads to long-wave oscillations of the integral reflection as a function of the crystal thickness; the period of these oscillations is determined by the amplitude of the ultrasound.

An important role in our problem is played by not only momentum exchange but also energy exchange between the neutron and the acoustic wave. The energy transfer manifests itself in a change of the angle position and in an increase of the number of satellites compared with the x-ray case, and even to the appearance of satellites in a geometry in which there are no x-ray satellites at all.

Although the neutron energy change is by itself quite small ( $\sim 10^7$  eV), it turns out to be sufficient for a substantial change of the diffraction pattern in a narrow angle range ( $\sim 1^\circ$ ) of dynamic scattering.

The problem of diffraction by an acoustic wave is closely related to the problem of thermal diffuse scattering under conditions of dynamic diffraction. In particular, the divergence of the intensity of this scattering near a reciprocal-lattice site, which is well known in kinematic theory, is eli-

minated when account is taken of the frequency threshold for the formation of satellites on phonons with wave vector  $\mathbf{K}_S \perp \mathbf{H}$  or on account of vanishing of the matrix element of the interaction at small  $K_S$  in the case  $\mathbf{K}_S \parallel \mathbf{H}$ . This result was obtained earlier within the framework of a semi-kinematic theory<sup>10,13,14</sup> that takes into account the dynamic rescattering by atomic planes, and neglects scattering by the thermal phonon. Another obvious consequence of the dynamic analysis is the presence of diffuse scattering near a zero reciprocal-lattice site, if the crystal is close to the reflection position. This scattering is the result of reflection of the inelastically scattered radiation from the atomic planes of the crystal. Peculiar to neutron diffraction is a dependence of the effectiveness of thermal diffuse scattering on the neutron and sound velocity ratio.

We note finally that the results are directly applicable to the case of diffraction of modulated structures (static displacement wave,  $\omega_S = 0$ ).

The authors thank V. L. Indenbom for helpful hints.

<sup>1</sup>G. W. Fox and P. H. Carr, Phys. Rev. **37**, 1622 (1931).

<sup>2</sup>W. J. Spencer and G. T. Pearman, Adv. X-Ray Analysis, **13**, 507 (1970).

<sup>3</sup>B. Buras, T. Giebultowicz, W. Minor and A. Rajca, Phys. Stat. Sol. (a) **9**, 423 (1972).

<sup>4</sup>T. F. Parkinson, E. Gruman, S. K. Loyalka and L. D. Muhkestein, J. Appl. Phys. **45**, 2021 (1974).

<sup>5</sup>I. R. Entin, Pis'ma Zh. Eksp. Teor. Fiz. **26**, 392 (1977) [JETP Lett. **26**, 368 (1977)].

<sup>6</sup>V. G. Baryshevskii, Izv. AN BSSR, ser. fiz.-mat. nauk **3**, 117 (1980).

<sup>7</sup>K. P. Assur and I. R. Entin, Fiz. Tverd. Tela (Leningrad) **24**, 2122 (1982) [Sov. Phys. Solid State **24**, 1209 (1982)].

<sup>8</sup>R. Kohler, W. Mohling and H. Peibst, Phys. Stat. Sol. (b) **61**, 173 (1974).

<sup>9</sup>I. R. Entin, Zh. Eksp. Teor. Fiz. **77**, 214 (1979) [Sov. Phys. JETP **50**, 110 (1979)].

<sup>10</sup>A. M. Afanasev, Yu. Kagan and F. N. Chukhovskii, Phys. Stat. Sol. **28**, 287 (1968).

<sup>11</sup>Z. G. Pinsker, Rentgenovskaya kristallografika (Crystal X-ray Optics), Nauka, 1982.

<sup>12</sup>R. A. Young and C. E. Wagner, Brit. J. Appl. Phys. **17**, 723 (1966).

<sup>13</sup>S. Takagi, J. Phys. Soc. Japan **13**, 278 (1958).

<sup>14</sup>E. A. Tikhonova, Fiz. Tverd. Tela (Leningrad) **9**, 516 (1967) [Sov. Phys. Solid State **9**, 394 (1967)].

Translated by J. G. Adashko