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Dynamic diffraction of thermal neutrons in weakly deformed crystals

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Abstract. Hamilton's equations for the dynamic diffraction of thermal neutrons in weakly deformed crystal are considered in the light of Riemann's integration of the hyperbolic differential equation in case of Laue geometry. Using the Green's function, an integral formulation is given for determining the quasi-amplitudes of the diffraction field of slow neutrons. Under conditions of extremely small linear absorption, the role of primary and secondary extinction in the formation of the wave field of thermal neutrons in the crystal lattice is considered.

Keywoards: thermal neutrons, Green's function, dynamic scattering, Huygens-Fresnel principle.

Dynamic scattering of slow neutrons in the crystal lattice is described a pair of differential equations of Hamilton [1] which in turn, are generalizations of the one- dimensional equations describing propagation of neutron waves quasi-amplitudes in crystal net:

$$\partial u_0 / \partial s_0 = -i\bar{\sigma} u_h$$

$$\partial u_h / \partial s_h = -i\sigma u_0 + i\alpha u_h \qquad (1)$$

Here , $\sigma = -i\pi k \chi_h$, $\bar{\sigma} = -i\pi k \chi_{-h}$, $\alpha = 2\pi k \partial(\boldsymbol{hu}) / \partial s_h$ determines the local displacement from the Bragg angle due to the lattice deformation, $k = 1/\lambda$ is the wave number of radiation in vacuum, λ is de Broglie wavelength of neutrons, χ_h and χ_{-h} structure factors for reflecting atomic planes for the reciprocal lattice vectors **h** and **-h** respectively.
Let us briefly stay on the features of neutron absorption and scattering in a medium compared with the absorption and scattering of x-ray waves. The absorption of waves of both X-ray and neutron waves is taken into account phenomenologically by attributing the imaginary part to the refractive indexes:

$$n = 1 - \delta + i\beta \qquad (2)$$

The real part for both radiations can be represented as

$$n_r = 1 - \delta \qquad (3)$$

and they are of the same order for both radiations. The situation is different for the imaginary parts. So for thermal neutrons the ratio δ / n_i is of the order of 10^5, for the X- rays δ / n_i is of the order 10^3 due to the Z^3 dependence of absorption coefficient. Thus, in neutron scattering in a crystal, absorption can be neglected $(n_i \approx 0)$ [2,3].On the other hand in the case of thermal neutrons the interaction range is too short compared to the de Broglie wavelength that it can be considered as Dirac's $\delta(\boldsymbol{r})$ function and described by Fermi's pseudo-potential:

$$V_F(\mathbf{r}) = (bh^2 / 2\pi m)\delta(\mathbf{r}) \qquad (4)$$

Now the structural factors χ_h and χ_{-h} defined as the Fourier coefficients of this pseudo-potential are complex conjugate numbers $\chi_h = \chi_{-h}{}^*$:

$$\chi_{\mathbf{h}} = \int V_f(\mathbf{r})e^{2\pi i\mathbf{hr}}d^3\mathbf{r} \ , \ \chi_{-\mathbf{h}} = \int V_F(\mathbf{r})e^{-2\pi\mathbf{hr}}d^3\mathbf{r} \qquad (5)$$

The propagation of neutron wave packets in a lattice is described by wave equations arising from the Hamilton equations (1). For the reflected beam with quasi-amplitude this equation is written in the form:

$$\partial^2 u_h / \partial s_0 \partial s_h - i\alpha\partial u_h / \partial s_0 + (\sigma\bar{\sigma} + i\partial^2\alpha / \partial s_0 \partial s_h) = 0 \qquad (6)$$

In case of small deformations, namely when

$$\left|\sigma\bar{\sigma} / i\alpha\right| \gg 1 \qquad (7)$$

The solution of (6) has an asymptotic representation [4]

$$u_h = e^{i\alpha s_0 s_h} J_0(2\sqrt{(\sigma\bar{\sigma} - i\alpha)s_0 s_h}) \ , \qquad (8)$$

where $J_0(Y)$ is the zero-order Bessel function of the complex argument.

This solution differs from the corresponding solution for a perfect (no deformed) crystal [5] by the first phase factor in (5), and also, in addition to the deformation parameter $i\alpha$, the term in the argument of the Bessel function. For the amplitude of the transmitted wave taking into account the second of the equations (1) we have

$$-i\sigma u_0 = e^{i\alpha s_0 s_h}\left(\sqrt{(\sigma\bar{\sigma} - i\alpha)s_0 / s_h}\right) J_1\left(2\sqrt{(\sigma\bar{\sigma} - i\alpha)s_0 s_h}\right) \ , \qquad (9)$$

where $J_1(Y)$ is the first-order Bessel function.

From these formulas it is obvious that the field amplitude of one mode grows with growth α, and the other decreases, and the direction of energy transfer between the transmitted and reflected modes depends on the sign of the deformation parameter.

Thus, an approximation (5, 6) allows us to formulate the Huygens-Fresnel principle for all the initial wave packets exciting the diffraction field in the crystal lattice. To do this, we pass from the oblique coordinate system (s_0, s_h) to the Cartesian (x, z) system using transformations:

$$x = (s_0 - s_h)\sin\theta_B \qquad z = (s_0 + s_h)\cos\theta_B \tag{10}$$

The coordinate system (x, z) is chosen as follows: the x axis is parallel to the entrance surface of the crystal, and the z axis is directed along the inner normal of this surface. The quasi-amplitudes of diffracted beams should be determined by influence function $G_h(x, z)$ and $G_0(x, z)$ (Green functions):

$$G_h(x,\ z) = i\sigma / \cos\theta_B e^{i\alpha/4((z/\cos\theta_B)^2 - (x/\sin\theta_B)^2)} J_0\left(\sqrt{(\sigma\bar{\sigma} - i\alpha)(z/\cos\theta_B)^2 - (x/\sin\theta_B)^2}\right)$$

$$G_0(x,\ z) = e^{i\alpha/4((z/\cos\theta_B)^2 - (x/\sin\theta_B)^2)} \sqrt{(1 - i\alpha/\sigma\bar{\sigma})(ztg\theta_B + x)/(ztg\theta_B - x)}\, J_1\left(\sqrt{(\sigma\bar{\sigma} - i\alpha)(z/\cos\theta_B)^2 - (x/\sin\theta_B)^2}\right) \tag{11}$$

The quasi-amplitudes u_0 and u_h of the crystal wave field constituting the transmitted and reflected wave in the crystal are related by the influence of $G_j(x,z)\ (j = 0, h)$, which determine the influence of the initial radiation $u^i(x)$ at the point (x', z') of the plane of the entrance surface of the crystal $(z = 0)$ on the field at the observation point (x, z) in the scattering plane:

$$u_j(x,z) = \int G_J(x - x', z - z') u^i(x', z') dx' \qquad (j = 0, h) \tag{12}$$

Where integration is carried out over the section $z = 0$ coinciding with the exit surface of the crystal.

In the case of a primary point source on the entrance surface of the crystal $u^i(x', 0) = \delta(x')$, where $\delta(x)$ is the Dirac function, the wave functions of the reflected and refracted waves will be directly determined by the functions $G_h(x,z)$ and $G_0(x,z)$.

$$u_h(x,z) = G_h(x,z),\ u_0(x,z) = G_0(x,z) \tag{13}$$

From these expressions it is seen that the practical absence of absorption of thermal neutrons in the crystal is revealed in the fact that at the edges of the Bormann delta, the beam amplitudes remain unchanged. With an increase in the strain parameter, the main field intensity is concentrating in the center of the beam. This is explained by the fact that in the absence of absorption, secondary extinction plays the main role in the formation of diffraction field. This means that the intensity is pumped from one mode of the wave field to another. This is directly seen from the asymptotic representation of the Bessel functions in (8, 9) far from the sides of the Bormann delta, i.e., for

$$\sigma\bar{\sigma}s_0 s_h \gg 1$$

$$J_0(\xi) \approx (2/\pi\xi)^{1/2}\cos(\xi-\pi/4) = (1/2\pi\xi)^{1/2}\exp(i\xi-i\pi/4)+\exp(-i\xi+i\pi/4)$$

$$J_1(\xi) \approx (2/\pi\xi)^{1/2}\sin(\xi-\pi/4) = (1/2\pi\xi)^{1/2}\exp(i\xi-i\pi/4)-\exp(-i\xi+i\pi/4)\ , \qquad (14)$$

where

$$\xi = \sqrt{(\sigma\bar{\sigma}\text{-}i\alpha)(z/\cos\theta_B)^2\text{-}(x/\sin\theta_B)^2} \qquad (15)$$

Such a representation corresponds to the fact that the wave field for each of the diffracted waves generated in the crystal is a superposition of two wave modes. From these formulas it is obvious that the field amplitudes of one mode grows, and the other decreases with growth of α, and the direction of changes on the amplitudes of modes depends on the sign of the strain parameter. With an increase in the strain parameter, the main field intensity is concentrated in the center of the beam. This is explained by the fact that in the absence of absorption, extinction plays the main role in the formation of diffraction wave field in crystal. Inside the Bormann delta, oscillations of the pendulum solution of spherical waves are observed. However, this interference effect quickly disappears with an increase in the deformation parameter, which is the result of the redistribution of the amplitudes of the two modes, which leads to an ever greater difference in the amplitudes of the interfering modes.

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