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Formation of a Diffraction Field During Dynamic Scattering of Slow Neutrons in a Deformed Crystal

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Abstract. The problem of diffraction of slow neutrons with a de Broglie wavelength $\lambda \sim 10^{-10}$ m in a crystal with a deformed lattice is considered. Based on the Hamilton equations describing the dynamic diffraction of slow neutrons, the features of the formation of a dynamic diffraction field in a lattice in various regions of the deformation field characteristics, including weak fields, slowly changing fields and rapidly changing fields are discussed. Using a particular example of a deformation field with a displacement field quadratic in coordinates, analytical solutions are obtained for the wave functions of transmitted and reflected lattice waves.

Keywords: thermal neutrons, dynamic diffraction, coherent imaging

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1. Introduction

The Broglie wavelength of thermal neutrons is of the order of 10^{-10} m, whereas the radius of the interaction range between a nucleus and neutrons is of the order 10^{-15} m, so point-like for this interaction in reasonable approximation.

For the coherent interaction of neutron waves with condensed matter, it is thermal neutrons whose kinetic energy is about 10 meV that are needed, since it is the energy of this order that is necessary to excite many condensed matter, and besides, the de Broglie wavelength is on the order of interatomic distances which is necessary for the phenomena of elastic neutron scattering and the observation of diffraction phenomena during neutron diffraction on a crystal lattice.

2. Results and Discussions

The propagation of neutron waves and, in particular, thermal neutrons is described by the Schrödinger equation. The characteristic of the medium in this case is the scalar potential $\mathrm{V}(\boldsymbol{r})$, which describes the interaction of neutrons with the nuclei of atoms of the medium. The theory of neutron diffraction is based on the Fermi pseudo potential [1, 2]

$$\mathrm{V}(\boldsymbol{r}) = \frac{\mathrm{h}^2}{2\pi \mathrm{m_n}} \sum_{\mathrm{j}} \mathrm{b_j} \delta(\boldsymbol{r} - \boldsymbol{r}_j), \tag{1}$$

where $\mathrm{b_j}$ is the neutron scattering length, $\delta(\boldsymbol{r} - \boldsymbol{r}_j)$ is the Dirac function, $\boldsymbol{r}_j$ is the radius vector of j-th nucleus of the medium, and the summation is carried out over all $\boldsymbol{r}_j$. Naturally, in the Fermi pseudo potential, the scattering centers are considered point like. The propagation of neutron wave packets in the lattice is described by wave equations arising from the Schrödinger equation based on the assumption that the diffraction wave field of a crystal lattice can be represented as the sum of two modified Bloch waves for transmitted and reflected waves:

$$\mathrm{U}(\boldsymbol{r}) = U_0(\mathbf{r})\mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{K}_0\boldsymbol{r}} + U_h(\mathbf{r})\mathrm{e}^{-2\pi\mathrm{i}(\boldsymbol{K}_0+\boldsymbol{h})\boldsymbol{r}}. \tag{2}$$

The wave field of the crystal lattice is represented as a sum of these wave functions with quasi-amplitudes $U_0(\boldsymbol{r})$ and $U_h(\boldsymbol{r})$ taking into account the assumption that they are macroscopic functions of coordinates with spatial heterogeneity of the order of extinction length $\Lambda \sim 10^{-7}$ m, compared to exponential phase functions with spatial heterogeneity of the order $\lambda \sim 10^{-10}$ m.

Dynamic scattering of slow neutrons in the crystal lattice is described by a pair of differential equations of Hamilton [3, 4]:

$$\frac{\partial U_0}{\partial s_0} = -\mathrm{i}\bar{\sigma}U_h, \tag{3}$$

$$\frac{\partial U_h}{\partial s_h} = -\mathrm{i}\sigma U_0 + \mathrm{i}\alpha_h U_h, \tag{4}$$

$$\alpha_h = \frac{\partial \boldsymbol{hu}}{\partial s_h}, \qquad \boldsymbol{hu} = q s_0 s_h, \tag{5}$$

where q is parameter of deformation field.

Equations (3) and (4) lead to two equations of hyperbolic type for quasi-amplitudes U_0 and U_h for transmitted and reflected waves, respectively:

$$\frac{\partial^2 U_0}{\partial s_0 \partial s_h} - i\alpha_h \frac{\partial U_0}{\partial s_0} + \sigma\bar{\sigma}U_0 = 0, \tag{6}$$

$$\frac{\partial^2 U_h}{\partial s_0 \partial s_h} - i\alpha_h \frac{\partial U_h}{\partial s_0} + (\sigma\bar{\sigma} - iq)U_h = 0, \tag{7}$$

where σ and $\bar{\sigma}$ mean free path for Bragg scattering while α determines the local displacement from the Bragg angle θ_B due to the lattice deformation, $k = 1/\lambda$ is the wave number of radiation in vacuum, σ and $\bar{\sigma}$ are reciprocal mean free path for Bragg scattering for the reciprocal lattice vectors **h** and **-h** respectively.

For this case of the equation for the diffraction field amplitudes, the Green-Riemann function [5, 6] which determines the influence functions of a point source is known [7-9], and has the form:

$$G_h = F_1\left(1 - \frac{\sigma\bar{\sigma}}{iq}, 1, iqs_0s_h\right). \tag{8}$$

System of equations (3) and (4) describes the propagation of quasi-amplitudes of diffracted waves in the crystal net and their relationship, since the existence of transmitted waves implies the existence of a reflected wave and vice versa. This relationship is determined by the parameters σ, $\bar{\sigma}$ and α_h. The first two parameters of the constant describe the lattice itself and characterize Bragg diffraction, the third parameter describes the local displacement from the Bragg condition due to deformation of the crystal lattice. If the deformations are small ($|\sigma| >> \alpha_h$) the role in the formation of the field in the crystal is played by the first two parameters, and the formed field is the field for a perfect crystal, with a characteristic relationship between the two fields in the lattice. If $\alpha_h >> |\sigma|$, then this relationship disappears and the crystal interacts only with the incident wave [10], which means a transition to kinematic scattering, and the effects of dynamic diffraction, i.e. multiple reflections of two fields in the crystal disappear. Note that if in equation (3) we neglect the first term in the first part of the equation, then the equation is immediately integrated, and by substituting this solution into equation (4) the amplitude U_0 of the passing wave is immediately determined.

We will consider in more detail what is possible using the example of diffraction of slow neutrons in a crystal lattice with a linear dependence on the coordinates of the displacement angle from the Bragg condition. Fig. 1 shows some examples of deformed crystals with such a deformation field [11].

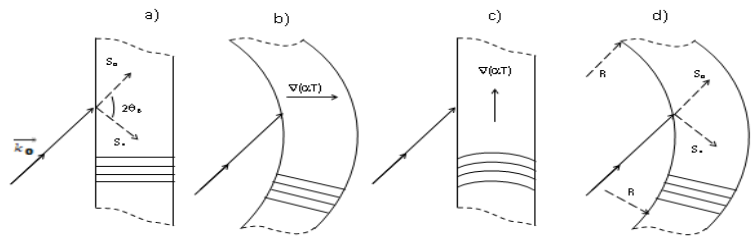

Fig.1. a) Undeformed crystal, b) crystal deformed by temperature gradient ∇(αT)⊥h, c) temperature gradient ∇(αT) ∥ h, d) crystal deformed by elastic bending (R is the bending radius of the entrance surface of the crystal).

Let us consider the case of lattice deformation induced by a temperature gradient. In this case, the planes perpendicular to $\boldsymbol{\nabla}(\alpha T)$ are curved, and the radius of curvature defined as:

$$\mathrm{R} = \pm|\boldsymbol{\nabla}(\alpha\mathrm{T})\,|^{-1}, \tag{10}$$

where the sign in front of the module is determined by the mutual orientation of the vectors **h** and $\boldsymbol{\nabla}(\alpha\mathrm{T})$, α- linear coefficient of thermal expansion.

The planes parallel to the temperature gradient remain flat, but are distributed in the form of a fan relative to each other. As a result, if the reciprocal lattice vectors **h** and the gradient $\boldsymbol{\nabla}(\alpha\mathrm{T})$are directed along the same line, i.e. parallel or antiparallel.

The next important parameter is the second derivative

$$\frac{\partial^2 \boldsymbol{hu}}{\partial s_0 \partial s_h} = q\ . \tag{11}$$

Which characterizes the phenomenon of the "speed" of pumping energy of beams in a deformed crystal from a passing to a reflected wave or vice versa from a reflected to a passing wave [3, 10], depending on the sign of q. This is explained by the fact that as the wave deepens into the crystal due to a change in the local displacement from the exact Bragg condition, the wave modes either approach or move away from this condition. The speed and direction of pumping is determined by the rate of change of the displacement angle from the Bragg condition defined in (11).

Now using the known asymptotic representations for the degenerate hypergeometric function [12], we obtain:

a) for perfect crystal ($q = 0$)

$$G(s_0, s_h) = J_0\big(2|\sigma|\sqrt{s_0 s_h}\big), \tag{12}$$

where J_0 is the zero-order Bessel function;

b) for slowly changing or light deformations ($\frac{q}{|\sigma|^2} \ll 1$) [12]

$$G(s_0, s_h) = e^{\frac{iqs_0s_h}{2}} J_0\Big(2\sqrt{\big(|\sigma|^2 - \tfrac{iq}{2}\big)s_0 s_h}\Big)\ , \tag{13}$$

c) for rapidly changing deformations ($\frac{q}{|\sigma|^2} \gg 1$)

$$G(s_0, s_h) = e^{\frac{iqs_0s_h}{2}} . \tag{14}$$

In full accordance with the above arguments.

3. Conclusions

Based on the system of Hamilton's equations describing the propagation of quasi-amplitudes of the diffraction field during dynamic diffraction of slow neutrons on a deformed crystal lattice. An analytical formula is obtained for the Green's function describing the dynamic deformation of slow neutrons in a deformed lattice, with a quadratic dependence of the deformed displacement field on the coordinates. The features of the formation of the diffraction field of slow neutrons in various regions of changes in deformation fields are considered and analyzed. Physical interpretations of the features of the formation of a crystalline diffraction field in different regions of lattice displacement fields are given.

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