PROCEEDINGS OF THE YEREVAN STATE UNIVERSITY

Physical and Mathematical Sciences 2012, № 3, p. 52–55

Physics

DIFFRACTION IMAGE OF PRIMARY NARROW X-RAY BEAM IN WEAKLY DEFORMED CRYSTAL

G. R. GRIGORYAN*

Gyumri State Pedagogic Institute after M. Nalbandyan, Armenia

Huygens–Fresnel principle for dynamical diffraction of X-rays in a crystal with weak deformation field of its space lattice is stated with a view to construction of the wave functions of diffracted beams in the crystal lattice at an arbitrary distance r of the point source of primary radiation from the crystal. In particular, the well-known approximations of an incident spherical ($r = 0$) and plane ($r \to \infty$) waves result as the limiting cases of the problem under consideration. Some features of the interference absorption (the Borrmann effect) of X-ray wave packages in a crystal with weak field of lattice displacements were discussed.

Keywords: X-ray diffraction in crystals, anomalous absorption, X-ray scattering.

The problem of dynamic diffraction of a narrow X-ray beam (in the spherical wave approximation) in a crystal with weak deformation field has been considered in [1]. Of special interest are the cases when the primary beam is formed in a source located at a finite distance from the crystal. In contrast to the case of spherical wave approximation, where the primary beam comprises all directions about the Bragg direction of this reflection for appropriate atomic planes of the lattice, an incident beam of the discussed type induces a wave field that considerably depends on the source-to-crystal direction. As a result of this beam diffraction in the crystal, two modes are excited in the crystal that correspond to the strongly and weakly absorbing modes [2] in the non-deformed crystal. In case of weakly deformed crystal the curvature of the trajectories of two mode beams of the wave field is negligible [3]. The curvature of trajectories of diffracted X-ray beams is due to the gradient of relative deformation of crystal lattice. The validity criterion of such an approach is the smallness of alterations of relative deformation within the extinction length that is the characteristic length of dynamic diffraction of X-rays on the space lattice of crystal. As a result of this assumption the beam trajectories prove to be the same as those in the non-deformed crystal, i.e. be rectilinear. In case of this approach an additional phase component due to the deformation field may be represented as an integral of displacement function describing the local deviation from the Bragg condition, taken along the beam trajectory.

* E-mail: gohar_grigoryan@bk.ru

So, consider now a symmetric Laue case with crystal oriented near the Bragg condition in regard to the source of primary X-rays when the reflecting planes are normal to the incidence surface of the crystal. According to the Kirchoff integral formulation of the Huygens–Fresnel principle [4], the quasiamplitudes ψ_0 and ψ_h of crystal wave field, representing the transmitted and reflecting waves, are related by influence functions $G_j(x,z)$ $(j=0,h)$ determining the influence of primary radiation $\psi_i(x',z')$ in (x',z') point of the plane of crystal incidence surface $(z=0)$ on the field in observation point $P(x,z)$ in the scattering plane:

$$\psi_j(x,z) = \int G_j(x-x', z-z')\psi_i(x',z')dx', \tag{1}$$

where the integration is over $z'=0$ section coinciding with the incidence surface of the crystal.

The x-axis of (x,z) reference system was taken to be parallel to the incidence surface of crystal, and z-axis be directed along the internal normal to that surface. Besides that, oblique coordinate axes (s_0, s_h) shall be also used below with axes parallel to wave vectors K_0 and K_h of diffracted waves in the lattice. The transition from one reference system to the other is made by means of transformations

$$z = (s_0 + s_h)\cos\theta_B, \qquad x = (s_0 - s_h)\sin\theta_B, \tag{2}$$

where θ_B is a Bragg angle.

Now consider the diffraction of hard X-rays on the space lattice of crystal, the displacement field of which is described by the square-law function of coordinates

$$\vec{h}\vec{u}(\vec{r}) = \alpha s_0 s_h, \tag{3}$$

where $\vec{h}$ is the vector of reciprocal lattice of the corresponding reflection.

The propagation of X-ray wave packages in the lattice is described by wave equations that ensue from the Takagi equations. For the reflected beam with quasiamplitude ψ_h this equation is described in the form:

$$\partial^2\psi_h / \partial s_0 \partial s_h - i\alpha\partial\psi_h / \partial s_0 + (\sigma\bar{\sigma} - i\alpha)\psi_h = 0, \tag{4}$$

here $\bar{\sigma} = \pi k c \chi_{\bar{h}}$, $\sigma = \pi k c \chi_h$, $\alpha_h = 2\pi k \dfrac{\partial \vec{h}\vec{u}(\vec{r})}{\partial s_n}$. Determines a local deviation from the Bragg angle that is due to the lattice deformation, c being the polarization factor equal to 1 or $\cos 2\theta_B$ for two independent polarization states of the radiation, χ_h and $\chi_{\bar{h}}$ are Fourier coefficients of crystal polarizability for the direct $(\vec{h})$ and reciprocal $(-\vec{h})$ vectors of diffraction respectively, $k = 1/\lambda$ being the wave number of radiation in vacuum.

In case of square-law function (3) of the displacement field, Eq. (4) is reduced by means of substitution $z = i\alpha s_0 s_h$ to the well-known equation for confluent hypergeometrical function [5]

$$z d^2\psi_h / dz^2 + (1-z)d\psi_h / dz - (1 - \sigma\bar{\sigma} / i\alpha)\psi_h = 0, \tag{5}$$

the solution of which is the Kummer function [6] ${}_1F_1(\alpha, 1, z)$:

$$\psi_h = {}_1F_1\left(1 - |\sigma\bar{\sigma} / i\alpha|, 1, i\alpha s_0 s_h\right). \tag{6}$$

In its turn in case of small deformations, namely for

$$\left|\frac{\sigma\bar{\sigma}}{i\alpha}\right| \gg 1, \tag{7}$$

the solution of (6) has an asymptotic representation [6]

$$\psi_h \cong e^{i\alpha s_0 s_h} J_0\left(2\sqrt{(\sigma\bar{\sigma} - i\alpha)s_0 s_h}\right), \tag{8}$$

where $J_0(Y)$ is zero order Bessel function of complex argument *Y*. This solution differs from an relevant solution for the perfect (non-deformed) crystal [7] by the first phase factor in (8) as well as the term $-i\alpha$ supplementary to parameter $\sigma\bar{\sigma}$ in the argument of the Bessel function. Taking into account the second of the Takagi equations [4]

$$-i\sigma\psi_0 = \frac{\partial\psi_h}{\partial s_h} - i\alpha_h\psi_h \ , \tag{9}$$

we have for the amplitude of transmitted wave ψ_0 from (8)

$$-i\sigma\psi_0 \cong e^{i\alpha s_0 s_h} \sqrt{(\sigma\bar{\sigma} - i\alpha)\frac{s_0}{s_h}} \cdot e^{i\alpha s_0 s_h} J_1\left(2\sqrt{(\sigma\bar{\sigma} - i\alpha)s_0 s_h}\right), \tag{10}$$

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

Using the solutions (8) and (10), one can find expressions for the point source influence functions $G_j(x,z)$, as the latter ones are solutions of the differential equation conjugate to Eq. (4) with δ-function in the right-hand member of the last equation and are known as Green functions of the corresponding problem.

Let the incident monochromatic X-rays be radiated by the point source distant from the origin of coordinates (x,y,z) at $-r\vec{k}_0/k$ vector, so that the wave field of primary beam be described by function

$$\frac{e^{-2\pi ikl}}{l}, \tag{11}$$

where *l* is distance between a source and the running point on $z=0$ surface. Due to the small effective domain about the point of origin $(x \ll l)$ in observation plane $y=0,l$, this function may be expanded into a series around $x=0$ point in the well-known parabolic approximation and assuming that $1 \cong r$ in the denominator of (11), we obtain by confining to square-law terms in x

$$\frac{e^{-2\pi ikl}}{l} \approx \frac{e^{-2\pi ikl(1+x^2/2r^2+x\sin\theta_B/r)}}{r}. \tag{12}$$

In the exponent of (12) the term linear in *x* describes an angular displacement from the exact Bragg condition in the respective component of the incident beam, where as the square-law term results from the wave front curvature of the primary beam. The latter vanishes when $r \to \infty$, that corresponds to transition to the plane wave approximation, and in case of $r \to 0$ the square-law term proves to be prevailing and corresponds to the approximation of spherical wave of Kato [8]. Thus, owing to the approximation of (12), it proved possible to formulate the Huygens–Fresnel principle over the full range $0 \le r < \infty$ of the source-to-crystal distances. Returning to the integral formulation (1) with due regard for (8), (10) and (12), the quasiamplitudes ψ_0 and ψ_h of the diffracted beams shall be replaced by influence functions $G_h(x-x',z)$:

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

$$G_0(x-x',z) = \tag{13}$$

$$= e^{\frac{i\alpha}{4}\left(\left(\frac{z}{\cos\theta_B}\right)^2 - \left(\frac{x-x'}{\sin\theta_B}\right)^2\right)} \sqrt{\frac{\frac{z}{\cos\theta_B} + \frac{x-x'}{\sin\theta_B}}{\frac{z}{\cos\theta_B} - \frac{x-x'}{\sin\theta_B}}} \left(1 - \frac{i\alpha}{\sigma\bar{\sigma}}\right) J_1 \sqrt{(\sigma\bar{\sigma} - i\alpha)\left(\left(\frac{z}{\cos\theta_B}\right)^2 - \left(\frac{x-x'}{\sin\theta_B}\right)^2\right)}.$$

With regard to (13) the approximation of incident spherical wave is obtained from (1) as a limiting case with $\psi_i(x',0) = \delta(x')$, where $\delta(x')$ is the Dirac delta function. The wave functions of reflected and transmitted waves will be given directly by $G_h(x,z)$ and $G_0(x,z)$ functions.

The plane wave approximation $(r \to \infty)$ results as the Fourier-image of $G_{0,h}(x,z)$ functions and the coefficients of reflection and transmission will be determined by analogous formulas with respective factors for perfect (non-deformed, $\alpha = 0$) crystals (see, e.g., [2]) by replacing $\sigma\bar{\sigma}$ by $\sigma\bar{\sigma} - i\alpha$. This fact specifies the features of interference absorption (the Borrmann effect). In particular, if for the perfect crystal the interference coefficient is determined by the imaginary part of $\sigma\bar{\sigma}$ $(\mathrm{Im}\{\sigma\bar{\sigma}\})$, for weakly deformed crystal the interference attenuation of waves will be determined by $\mathrm{Im}\{\sigma\bar{\sigma}\} - \alpha$ parameter. Here, if the first term determines non-coherent losses of wave energy, the second term represents the effects of energy transfer from the transmitting to the reflected wave and *vice versa*.

Received 29.06.2012

REFERENCES

1. **Truni K.G., Kocharyan V.R., Grigoryan G.R.** On Interference Absorption of X-rays in Weakly Deformed Crystals. // Izv. NAN Armenii. Fizika, 2012, v. 47, p. 131–138 (in Russian).
2. **Authier A.** Dynamical Theory of X-ray Diffraction. New York: Oxford University Press, 2001.
3. **Hourutunian L.A., Truni K.G.** Linear Trajectories Approximation in Geometrical Optics of dynamic X-ray Diffraction. // Izv. NAN Armenii. Fizika, 1999, v. 34, p. 272–281 (in Russian).
4. **Takagi S.** A Dynamical Theory of Diffraction for a Distorted Crystal. // Acta Crystallogr., 1963, v. 15, p. 1239–1253.
5. **Petrashen' P.V., Chukhovskii F.N.** Dynamical Scaterring of X-rays in a Crystal with Constant Deformation Gradient. // Sov. Phys. JETP, 1975, v. 2, p. 243–248.
6. **Indenbom V.L., Chukhovskii F.N.** Imaging Problem in X-ray Optics. // UFN, 1972, v. 107, p. 229–265 (in Russian).
7. **Janke E., Emde F., Lösch F.** Special Functions. M.: Nauka, 1968 (in Russian).
8. **Azaroff L.V., Kaplow R., Kato N., Weiss R.J., Wilson A.J.C., Young R.A.** X-ray Diffraction. New York: McGraw-Hill, 1974.