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X-Ray Laue Diffraction with Allowance for Two-Dimensional Curvature of the Wavefront: the Concept a Locally Plane Wave

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Abstract—Symmetrical Laue diffraction in a perfect crystal with a plane entance surface is considered. The two dimensional curvature of the wave front of the incident beam is taken into account. Using the corresponding Green function, a general expression for the amplitude of diffracted wave in the crystal is presented. Based on this expression, the concept of a locally plane wave is analyzed taking into account two-dimensional curvature of the wave front. This concept is used for obtaining the rocking curves depending on the angles of deviation from the chosen exact Bragg direction in both the diffraction plane and in perpendicular direction. The obtained result is compared with the result of the standard dynamical diffraction theory.

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1. INTRODUCTION

Intensity of dynamically diffracted plane X-ray wave at the exit surface of a crystal depends on the parameter of deviation from the Bragg condition. This dependence is termed rocking curve [1, 2]. Work [3] has shown that the rocking curve can be obtained in diffraction from remote point source as the intensity distribution on the exit surface of crystal. In that work the incident wave is considered to be cylindrical (as in standard theory of dynamic diffraction). However, works [4, 5] (where also corresponding references are given) developed dynamic theory which takes into account two-dimensional curvature of the wavefront of the incident wave (in equations of dynamic diffraction the second derivatives of amplitudes are kept). This theory allows obtaining the rocking curves as a function of angles of deviation from a certain exact Bragg direction in both diffraction plane and the direction perpendicular to that. In this theory, as in [3], instead of consideration of different plane waves, diffraction from remote point source can be considered with using the notion of locally plane wave. In this case, crystal is in Fraunhofer zone of the source.

In the present work the rocking curve is obtained and discussed with use of diffraction of a wave from a remote point source with allowance for two-dimensional curvature of the wavefront of the incident radiation. The symmetric Laue case is examined.

2. LOCALLY PLANE WAVE WITH ALLOWANCE FOR TWO-DIMENSIONAL CURVATURE OF WAVEFRONT

According to work [5], the amplitude of the diffracted wave in the symmetric Laue case, with allowance for two-dimensional curvature of the wavefront of a wave incident at a crystal from a point source, may be written in the form

$$E'_h(\mathbf{r}) = Ae^{i\Phi_0(\mathbf{r})}\int_{-l}^{l} J_0\left(\sigma\sqrt{l^2 - x'^2}\right)e^{i\Phi(x')}dx', \quad (1)$$

where

$$\Phi_0 = kT\frac{\chi_0}{2\cos\theta} + \frac{k}{2L_s}\cos^2\theta x^2 + \frac{ky^2}{2L_s} - \frac{ky^2}{2L_s^2}\left(x\sin\theta + \frac{T}{\cos\theta}\right) - \frac{ky^4}{8L_s^3}, \quad (2)$$

$$\Phi = \beta x' + kx'^2\cos^2\theta/(2L_s), \quad (3)$$

$$\beta = \frac{k\cos\theta}{L_s}\left(x\cos\theta - \frac{\tan\theta y^2}{2L_s}\right). \quad (4)$$

Here $\sigma = k\sqrt{\chi_h\chi_{\bar{h}}}/(2\sin\theta)$, T is the crystal thickness, the source coordinates are taken $\xi_s = y_s = 0$, the deviation of central ray of the incident wave from the exact Bragg condition $\Delta\theta = 0$, L_s is the distance between the source and the crystal, and $l = T\tan\theta$. For other notations and chosen coordinate axes, see work [5]. The basic distinction of (1) from the standard theory [3] is dependence of the local parameter β of deviation from the Bragg condition on not only the coordinate x, but also y. Transition to locally plane wave is realized by neglecting in (3) the quadratic term with respect to x'. Corresponding estimation allowing such transition, can easily be obtained, according to (3), [3]:

$$T \ll (\lambda L_s)^{1/2}/\sin\theta. \quad (5)$$

Conditions of spatial and temporal coherence considered in [3, 5], are assumed to be met.

3. ROCKING CURVE WITH ALLOWANCE FOR TWO-DIMENSIONAL CURVATURE OF WAVEFRONT

After neglecting the quadratic term in (3), the amplitude (1) is proportional to the Fourier image of the point source function and its squared modulus is, on the one hand, intensity at the exit surface of crystal, on the other hand, rocking curve $R(\Delta\theta) = R(\Delta\theta_1 + \Delta\theta_2)$, which depends on the sum of the local angle of deviation from the Bragg condition in the diffraction plane, $\Delta\theta_1 = x\cos\theta/L_s$, and the local angle of deviation in the direction perpendicular to the diffraction plane, $\Delta\theta_2 = -\tan\theta y^2/(2L_s)$:

$$\Delta\theta = \Delta\theta_1 + \Delta\theta_2 = x\cos\theta/L_s - \tan\theta y^2/(2L_s^2). \quad (6)$$

Using table integral for amplitude, it is obtained from (1) in the approximation of locally plane wave:

$$E'_h(\mathbf{r}) = i\chi_h e^{i\Phi_0(\mathbf{r})}\sin[kT\Gamma/(2\cos\theta)]/\Gamma, \quad (7)$$

where

$$\Gamma = (\chi_h\chi_{\bar{h}} + \Delta\theta^2\sin^2 2\theta)^{1/2}, \quad (8)$$

with the incident wave amplitude normalized to unity.

4. EXAMPLE

Let us consider the reflection Si(220) with $\lambda = 0.71$ Å (17.46 keV), $T = 1.5\Lambda \approx 55$ μm, $L_s = 2$ m, and σ-polarization. Here $\Lambda = 36.6$ μm is the extinction length. Estimation (5) provides the upper limit of allowed thickness where the approximation of locally plane wave is still applicable, $T << 65$ μm. If the y-dependence in (6) is disregarded, the result of standard dynamical theory is obtained for an incident wave with cylindrical front. Calculation of squared modulus of amplitude from formula (7) leads in this case to a topogram of standard theory of diffraction shown in Fig. 1a [3] (brighter regions correspond to higher intensities). Figure 1b shows the intensity distribution, i.e., the rocking curve which corresponds to Fig. 1a (standard theory of diffraction, see also [3]). If the y-dependence in (6) is retained, i.e., the two-dimensional curvature of the wavefront of incident wave is taken into account, the topogram shown in Fig. 2a is obtained. The intensity distribution in Fig. 2a is rocking curve with allowance for two angles of deviation from the chosen exact Bragg direction. Figure 2b shows the rocking curve corresponding to Fig. 2a at x=0. Topogram of Fig. 2a can easily be understood by observing that the lines of constant intensity are parabolas $x\cos\theta - y^2\tan\theta/(2L_s)$ = const. The data of the crystal are taken from work [1].

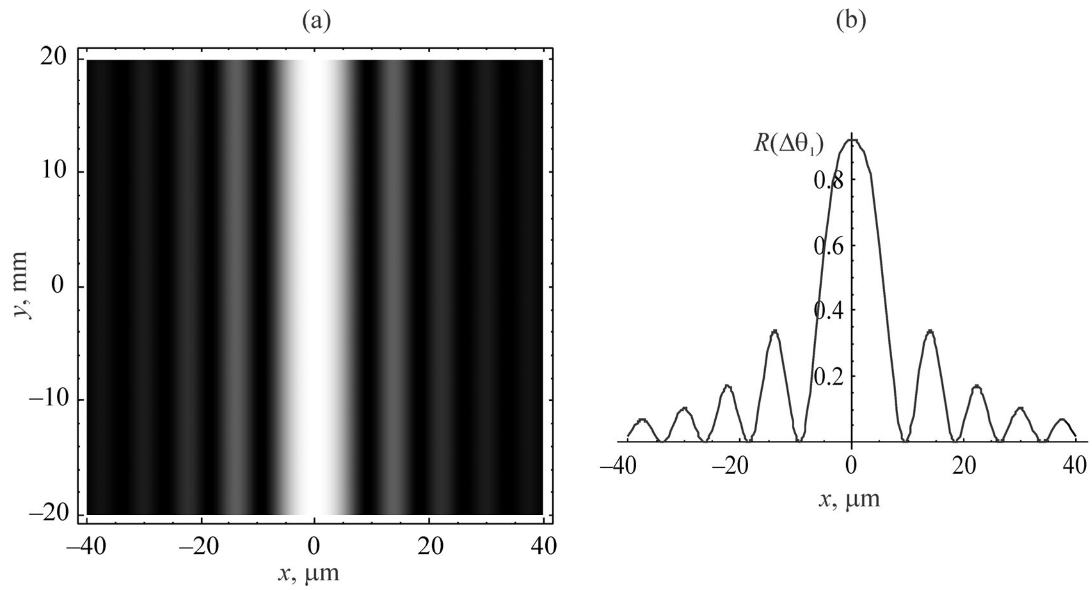

Fig. 1. (a) Calculated topogram in the locally plane wave approximation according to the standard theory of diffraction; (b) Rocking curve in case of locally plane wave, i.e., intensity distribution in topogram along x axis (standard theory).

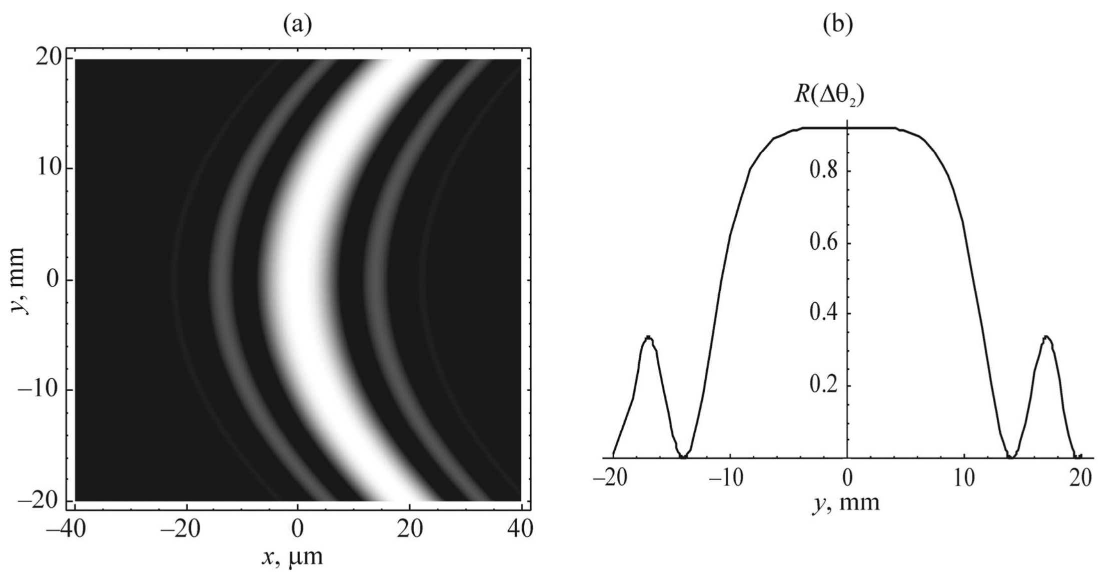

Fig. 2. (a) Calculated topogram in the locally plane wave approximation according to the theory of diffraction which takes into account two-dimensional curvature of wavefront; (b) Rocking curve on the line $x = 0$ depending on y (angular deviation in the direction perpendicular to the diffraction plane).

5. CONCLUSION

In general case the intensity of reflected wave depends on both deviation of the incident plane wave from a certain exact Bragg direction in the diffraction plane and deviation of the incident plane wave from this exact direction in the direction perpendicular to the diffraction plane. This means that the rocking curve depends on two angles of deviation. Work [3] exploits the concept of locally plane wave and obtains the rocking curve for diffraction of wave from remote point source. The incident wave is assumed to have a cylindrical front, as it is conventionally supposed in standard dynamical theory. The present work is based on the theory, which takes into account the two-dimensional curvature of the wavefront of incident radiation [4,5], uses the notion of locally plane wave, and obtains the rocking curve depending on two angles of deviation as a result of diffraction of a wave from remote point source.

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