Structure of wave fields during diffraction of x-rays with total external reflection

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Diffraction of x-rays in conditions of total external reflection (DXTER) is a powerful new method of investigating the structures of the surfaces of crystal layers. The fundamental idea of this method was suggested by Marra et al.,[1] a theory for perfect crystals was developed by Afanas'ev and Melkonyan,[2] and an experimental scheme was realized by Imamov et al.[3]

In the DXTER method, the incident x-ray beam, on the one hand, satisfies the Laue diffraction condition for planes perpendicular to the surface of the crystal, and, on the other, makes a small angle Φ_0 with the surface and undergoes total external reflection. The diffracted wave is propagated in the crystal at a small angle to the surface and also undergoes total external reflection: A specularly reflected diffracted wave emerges from the crystal at a small angle Φ_h, making an angle $2\theta_B$ with the usual specularly reflected wave (Fig. 1).

In this article we give a theoretical analysis of the relations between the amplitudes of the wave fields in a crystal during DXTER, and also investigate the depth of penetration of the radiation into the crystal in relation to the angle of incidence Φ_0 when the exact Bragg condition is satisfied [$\alpha = 0$; $\alpha = -2\sin(2\theta_B)(\theta - \theta_B)$ is the standard parameter of deviation from the Bragg condition in the dynamic theory] and in relation to α for fixed Φ_0. For simplicity we considered only σ polarization. Afanas'ev and Melkonyan' showed that the angle Φ_h is determined not only by the angle of incidence but also by the deviation from the Bragg condition; in fact, the following relation holds:

$$\Phi_h^2 = \Phi_0^2 - \alpha. \tag{1}$$

Relation (1) enables us to represent the intensity of the reflected diffracted wave as a function of the angle of emergence – this is much simpler from the experimental point of view.[3] In this article, the dependence on α is therefore considered in the same way as the dependence on Φ_h.

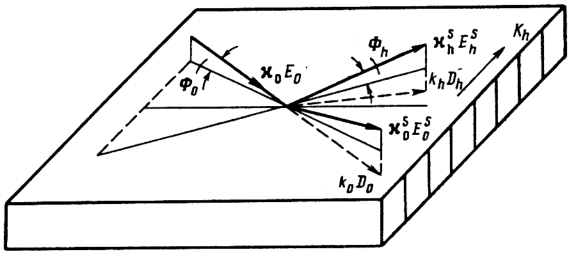

FIG. 1. Diffraction of x-rays in conditions of total external reflection. Vertical lines represent reflecting planes.

An analysis of the amplitudes of the wave fields and their depths of penetration makes it possible to determine at what values of Φ_0 and Φ_h the intensity of the reflected diffracted wave is most sensitive to disturbances in thin surface layers.

In DXTER, two wave fields are excited in the crystal,[2] each of which consists of transmitted D_0 and diffracted D_h waves. The depth of penetration of the fields is determined (for each of the fields the transmitted and diffracted waves have the same depth of penetration) by means of the expression

$$l_i = \frac{\lambda}{2\pi \,\mathrm{Im}\, u_i}, \tag{2}$$

where

$$u_i = \sqrt{\Phi_0^2 + \chi_0 - \frac{\alpha}{2} \pm \sqrt{\frac{\alpha^2}{4} + \chi_h \chi_{\bar{h}}}}, \qquad i = 1, 2. \tag{3}$$

Here χ_0, χ_h, and $\chi_{\bar{h}}$ are the corresponding Fourier components of the polarizability tensor, and λ is the wavelength of the incident radiation.

We see that when $\alpha = 0$ there are two characteristic angles of incidence associated with vanishing of u_i (in the absence of absorption), $\Phi_1 = (|\chi_0 - \chi_h|)^{1/2}$ and $\Phi_2 = (|\chi_0 + \chi_h|)^{1/2}$; Φ_1 corresponds to the critical angle of total external reflection for the first wave field, and Φ_2 for the second. In the case of scattering without diffraction ($\chi_h = 0$), there is one critical angle of total external reflection, $\Phi_{cr} = (|\chi_0|)^{1/2}$, where $\Phi_1 < \Phi_{cr} < \Phi_2$. The appearance of two critical angles is understandable from the physical point of view: The field for which the Bormann effect is realized corresponds to a small effective amplitude of interaction with the atoms of the substance, and thus a smaller critical angle; for the second field, on the other hand, there is strong interaction and thus a greater critical angle. The possibility of appearance of two critical angles for diffraction scattering was mentioned by Baryshevskii.[4] As an example, Fig. 2a plots the depths of penetration of both fields vs the angle of incidence for $\alpha = 0$, calculated for Si [(220) reflection, Cu Kα radiation]. For comparison we give the angular dependence of the depth of penetration of radiation into the crystal without diffraction,

$$l_0 = \frac{\lambda}{2\pi \,\mathrm{Im}\sqrt{\Phi_0^2 + \chi_0}}.$$

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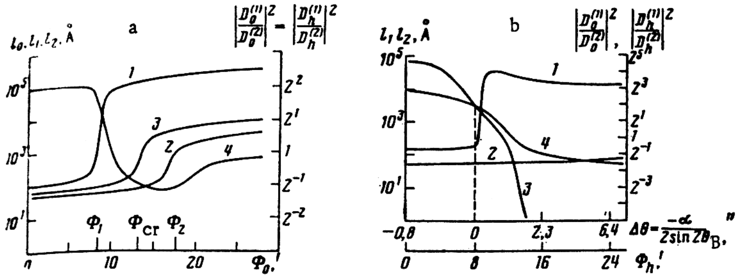

FIG. 2. Depths of penetration of wave fields and ratio of their intensities vs angle of incidence ($\alpha = 0$) (a), and deviation from Bragg condition for $\Phi_0 = 8' < \Phi_1$ (b). a) 1) Depth of penetration of first field; 2) of second field; 3) depth of penetration without diffraction; 4) ratio of squares of amplitudes of wave fields; $\left|\frac{D_h^{(1)}}{D_h^{(2)}}\right|^2 = \left|\frac{D_0^{(1)}}{D_0^{(2)}}\right|^2$, b) 1, 2) The same as in Fig. 2a; 3) deviation of squares of moduli of amplitudes of transmitted waves; 4) of diffracted waves.

For the case in question, the critical angles have the following values: $\Phi_1 = 8.4'$, $\Phi_{cr} = 13.3'$, $\Phi_2 = 16.8'$. When $\Phi_0 < \Phi_1$, both fields penetrate the crystal to a short depth ($l_1 \sim 100$ Å, $l_2 \sim 50$ Å), and the condition

$$l_1 > l_0 > l_2 \tag{4}$$

is satisfied ($l_0 \sim 70$ Å). Outside the region of total external reflection, the depths of penetration of the fields increase sharply, but condition (4) is preserved. For example, when $\Phi_0 = 20'$, $l_1 = 26\ \mu$, $l_0 = 6000$ Å, $l_2 = 2000$ Å. Thus we can reckon that DXTER has its greatest sensitivity to thin layers for angles of incidence $\Phi_0 < \Phi_1$.

To determine the contributions made by the first and second fields to the intensity of the reflected diffracted wave I_h^s, we analyze the ratio of their intensities at the surface of the crystal:

$$I_h{}^s = |D_h^{(1)} + D_h^{(2)}|^2,$$

$$\left|\frac{D_h^{(1)}}{D_h^{(2)}}\right|^2 = \left|\frac{u_2 + \Phi_0}{u_1 + \Phi_0}\right|^2. \tag{5}$$

The corresponding graph is shown in Fig. 2a. According to Eqs. (3) and (5), in the case $\alpha = 0$, as the angle of incidence decreases, the intensity ratio tends to the value $|(\chi_0 + \chi_h)/(\chi_0 - \chi_h)| \gtrsim 1$. When the angle of incidence changes from Φ_1 to Φ_2, ratio (3) decreases, and when $\Phi_0 = \Phi_2$ the intensity of the second field at the surface is greater than that of the first. The cause of the decrease in the relative contribution of the first field to the reflected diffracted wave is that when $\Phi_0 > \Phi_1$ the conditions of total external reflection cease to be satisfied for the first field, and it passes into the interior of the crystal. When $\Phi_0 > \Phi_2$, a similar phenomenon occurs for the second field, and the field intensity ratio tends to unity. On the whole we can state that the two fields make comparable contributions to the intensity of the reflected diffracted wave over the whole range of angles.

The dependence of the distribution of the wave fields in a crystal on the parameter α has different forms for different angles of incidence. Nevertheless we can formulate laws which are general to all angles Φ_0. In view of relation (1), when $\alpha > \Phi_0^2$ the angle Φ_h becomes imaginary, corresponding to the effect of total internal reflection for the diffracted wave (see Refs. 5 and 6). In this article we shall consider only the region $\alpha < \Phi_0^2$.

For deviations from the exact Bragg condition toward positive α ($\Phi_h \to 0$), the main role is played by the first field, but the contributions of both fields to the intensity of the reflected diffracted wave are comparable (Fig. 2b). The depths of penetration of the first and second fields are less than the corresponding values for $\alpha = 0$ (cf. Figs. 2a-b). In the region $\alpha \approx 0$ ($\Phi_h \approx \Phi_0$), the first field has maximum depth of penetration; this is an analogue of the Bormann effect.

For negative values of α ($\Phi_h > \Phi_0$), the depth of penetration of the first field is relatively great ($l_1 \gtrsim 1\ \mu$) for any angles of incidence, but its contribution to the intensity of the reflected diffracted wave decreases (Fig. 2b, curve 4). Nevertheless, if we do not consider very large deviations from the exact Bragg condition, the contributions made by the fields are comparable. Consequently, to investigate thin surface layers about 10-100 Å thick, we must choose angles of incidence in the range $\Phi_0 < \Phi_1$ and analyze the variation in the intensity of the reflected diffracted wave for angles of emergence of $\Phi_h < \Phi_0$; when $\Phi_h > \Phi_0$ the method is sensitive to disturbances in relatively thick layers (about 1000 Å to 1 μ).

For large deviations from the exact Bragg condition toward negative α ($\Phi_h \gg \Phi_0$), only the transmitted wave $D_0^{(2)}$ remains in the crystal, and its depth of penetration tends to the depth of penetration in the case of nondiffractive scattering, while the other waves ($D_0^{(1)}$, $D_h^{(1)}$, and $D_h^{(2)}$) vanish. Thus in the limit there is a transition to the case without diffraction.

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