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Acta Cryst. (1986). **A42**, 585–587

Extremely skew X-ray diffraction. By H. R. HÖCHE and O. BRÜMMER, *Martin-Luther-Universität Halle-Wittenberg, Sektion Physik, Friedemann-Bach-Platz 6, DDR-4020 Halle, German Democratic Republic*, and J. NIEBER, *Martin-Luther-Universität Halle-Wittenberg, Sektion Geographie, Domplatz 5, DDR-4020 Halle, German Democratic Republic*

(Received 10 February 1986; accepted 1 August 1986)

Abstract

Skew reflections are becoming more and more important in X-ray surface diffraction. A geometrical discussion of the whole dispersion surface in extremely skew cases gives the angular ranges of incidence and emergence in which the condition of X-ray diffraction is fulfilled. The main intensity comes from the incidence range given by $|\chi_0 - \chi_h|^{1/2} < \theta_i < |\chi_0 + \chi_h|^{1/2}$, where χ_0 and χ_h are the Fourier coefficients of dielectric susceptibility of the crystal. Furthermore, the exit angle of the diffracted beam is of the order of the critical angle of specular total reflection.

1. Introduction

In the dynamical theory of X-ray diffraction starting from P. P. Ewald's and M. von Laue's work (e.g. von Laue, 1960) the discussion of the dispersion surface is useful for the interpretation of X-ray beams. Usually the dispersion surface is discussed in its section with the diffraction plane consisting of the incident beam, the exit beam and the diffraction vector \mathbf{b}_h . For nearly all relevant experiments checking the dynamical theory, so-called zero-layer diffraction is realized (i.e. the normal to the entrance surface lies in the diffraction plane). Diffraction experiments using skew reflections can be treated on the basis of the conventional theory only for small angles between the surface normal and the diffraction plane. Especially in the case of grazing incidence the dynamical theory must be extended in such a manner that the curvature of the spheres of incidence and emergence must be taken into account, as given by Rustichelli (1975). Starting with the work of Marra, Eisenberger & Cho (1979) a new technique was developed, the so-called X-ray surface diffraction. The dynamical treatment of these diffraction experiments was given by Afanas'ev & Melkonyan (1983) by means of the extended dynamical theory of X-ray diffraction given by Bedynska (1973, 1974), Brümmer, Höche & Nieber (1976a, b, 1979)

and Härtwig (1976, 1977). The aim of this paper is the geometrical interpretation of the phenomena of X-ray surface diffraction on the basis of the three-dimensional dispersion surface.

2. The spatial dispersion surface

The beam geometry for skew X-ray reflections can be represented in a simple way. Generally all possible incident and exit beams are on cones with the diffraction vector \mathbf{b}_h as axis. In this paper we consider only the case where the diffraction vector lies in the crystal surface. This geometry corresponds to a symmetrically skew Laue case. The term 'symmetrically skew' means that the incident and exit beams make the same angles with the crystal surfaces of a plane parallel crystal and exact fulfilment of the Bragg condition is realized. Extremely skew reflections can be characterized by small angles between the diffraction vector and the crystal surface and a small angle between the incident X-ray beam and the crystal surface.

For the wave vectors outside and inside the crystal the component parallel to the crystal surface must be constant. Geometrically that means that both wave vectors have their starting points on the same normal to the crystal surface. By means of a complete representation of the dispersion surface it is possible to determine the angular ranges, which are of interest for measurements in extremely skew geometry. In Fig. 1 an attempt at a three-dimensional picture of the dispersion surface is presented; only the spheres with radius $r = nk$ (inside the crystal, n = refraction index, k = vacuum wave number) are sketched and the two branches of the hyperbolic planes are partially drawn. In the upper part the disc-like surface is shown. In the lower part the other hyperbolic surface is sketched. For clarity only one polarization state is considered. The equatorial plane of the two spheres represents the crystal surface. The section of the dispersion surface containing this plane is the well known picture (see Fig. 2a), but here the wave

vectors of the incident and exit beams are not in this plane. The following relations can be seen directly from Fig. 2(a):

$$\begin{aligned}\overline{MLa} &= k \cos \theta_B, \\ \overline{MLo} &= nk \cos \theta_B, \\ \overline{MA_1} &= (n - \chi_h/2)k \cos \theta_B, \\ \overline{MA_2} &= (n + \chi_h/2)k \cos \theta_B, \\ n &= 1 + \chi_0/2.\end{aligned}\quad (1)$$

χ_0 and χ_h are the Fourier coefficients of the dielectric susceptibility of the crystal. For non-centrosymmetric crystals χ_h must be replaced by $(\chi_h \chi_{\bar{h}})^{1/2}$.

In Fig. 2(b) the section of the dispersion surface containing the (x, z) plane is shown. From the continuity of the tangential component of the wave vectors it follows that two marked angles of incidence exist. For θ_1 it can be seen that

$$\cos \theta_1 = n - \chi_h/2 = 1 + \chi_0/2 - \chi_h/2.$$

For the small angles which are under discussion,

$$\theta_1 = |\chi_0 - \chi_h|^{1/2}. \quad (2)$$

The corresponding relations for θ_2 are

$$\cos \theta_2 = n + \chi_h/2 = 1 + \chi_0/2 + \chi_h/2,$$

and for small angles the series expansion gives

$$\theta_2 = |\chi_0 + \chi_h|^{1/2}. \quad (3)$$

Between these two angles the normal to the crystal surface has no real intersection point with the central part of the dispersion surface. This means that in this angular range a reflection can be expected. Fig. 2(c) shows the beam geometry in real space.

3. Concluding remarks

Only in the angular range between θ_1 and θ_2 can one expect significant diffracted reflected intensities. The direction of the reflected beams is represented by the bold portion of the sphere in Fig. 2(b). The angle of the diffracted reflected beam with the crystal surface is near the critical angle of specular total reflection. The main intensity will arise in the angular range of incidence $\theta_1 < \theta_i < \theta_c$, where θ_c is the critical angle of specular total reflection given by $\theta_c = |\chi_0|^{1/2}$. For incidence in the range $\theta_c < \theta_i < \theta_2$ the reflectivity drops drastically and for $\theta_i > \theta_2$ only negligible reflected intensity can be expected.

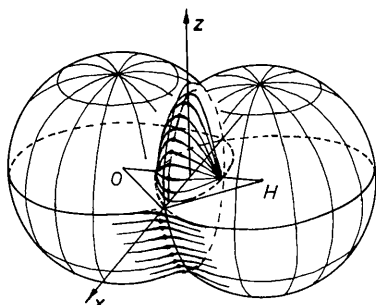


Fig. 1. Three-dimensional sketch of the dispersion surface.

These geometrical considerations agree with the results of a mathematical treatment on the basis of the extended dynamical theory as given by Afanas'ev & Melkonyan (1983) for the (001) surface of a Ge crystal and the 220 reflection of Cu $K\alpha$ radiation (see their Fig. 2). The relations become very complicated if the tie points of the internal wave fields are not in the (x, z) plane of Fig. 1. In particular, the discussion of the Poynting vectors and the coupling of the two polarization states will be rather complicated in the general case of extremely skew reflections.

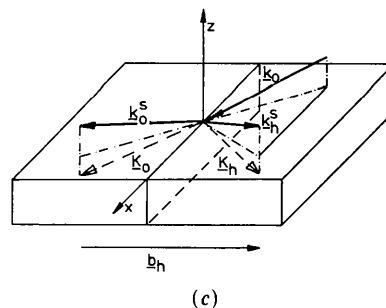
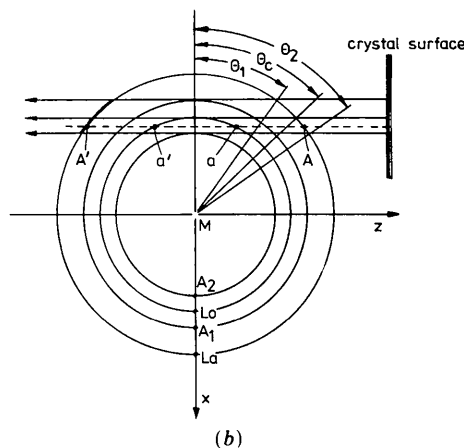
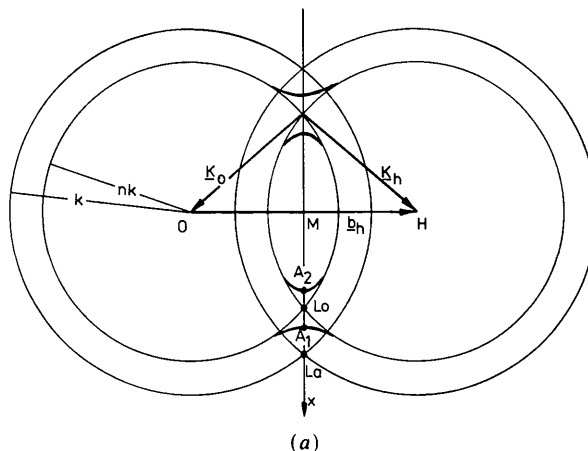


Fig. 2. (a) Section of the dispersion surface with the crystal surface. (b) Section of the dispersion surface with the (x, z) plane of Fig. 1. (c) Beam geometry in real space ($\mathbf{k}_0 \triangleq \mathbf{AO}$, $\mathbf{k}_0^s \triangleq \mathbf{A'O}$, $\mathbf{K}_0 \triangleq \mathbf{aO}$, $\mathbf{K}_h \triangleq \mathbf{aH}$ and $\mathbf{k}_h^s \triangleq \mathbf{a'H}$).

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Acta Cryst. (1986). **A42**, 587–588

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