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Bragg-surface dynamical diffraction

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In this work, the dispersion surface of Bragg-surface diffraction (BSD) is presented. A symmetric Bragg reflection plus a secondary diffracted wave nearly parallel to in-plane directions distinguish the BSD from an ordinary three-beam diffraction. The solutions of the fundamental equations of the dynamical theory of X-ray diffraction for the BSD demonstrate that measurable specular-reflected secondary waves are simultaneously excited with the diffracted waves.

1. Introduction

The multiple diffraction of X-rays in crystals, when treated by the plane-wave dynamical theory of diffraction, is basically a problem of solving the eigenvalues and eigenvectors of a square matrix, which is called the fundamental equations (Colella, 1974; Chang, 1984; Weckert & Hümmer, 1997). The eigenvalues (tie points) are related to the possible X-ray wave vectors in the crystal and the eigenvectors are the components of the wave fields assigned to each wave vector. For a general N-beam diffraction, there are $4N$ tie points: $2N$ for the specular-reflected and forward-transmitted waves (non-diffracting tie points) and $2N$ for the reflected and transmitted diffracted waves. In ordinary N-beam diffraction cases, when only strong Bragg reflected and Laue transmitted waves have to be considered, only the last $2N$ diffracting tie points are relevant, *i.e.* half of the waves can be neglected.

In this short communication, we call attention to a special case of three-beam diffraction, called Bragg-surface diffraction (BSD) (Hayashi *et al.*, 1997). In BSD, besides the Bragg reflected wave of the primary symmetrical reflection, the secondary diffracted wave is neither a Laue transmitted nor a Bragg reflected wave. It is instead nearly parallel to the in-plane direction. As illustrated in Fig. 1, near the geometrical BSD condition, **L**, the surface-normal direction, intercepts the dispersion surface of the secondary reflection twice, for instance at A and B in the figure. In terms of the eigenvalues of the fundamental equations, such a geometry provides four tie points for the secondary reflection. Therefore, it is expected for BSD that a total of eight significant tie points should be taken into account, instead of the six significant tie points for an ordinary three-beam diffraction. Here, these eight tie points are calculated for a particular BSD, $222/13\bar{1}$, which occurs in an Si (111) crystal.

We define $\mathbf{K}_2(j)$ as the secondary wavevector from the jth tie point ($j = 1, 2, \ldots, 8$) and $\hat{\mathbf{n}}$ as the outward surface-normal unit vector. The projection of $\mathbf{K}_2(j)$ in the surface-normal direction, $\delta = \mathbf{K}_2(j) \cdot \hat{\mathbf{n}}$, is plotted in Fig. 2 as a function of $\Delta\omega$, the deviation from the Bragg angle of the 222 primary reflection. The four tie points due to the secondary reflection appear as two pairs of conjugated values (gray lines in Fig. 2) when the tangent component of the incident beam falls in the outer region of the secondary Ewald sphere. For $\Delta\omega > 0.52''$, their imaginary parts become negligible. In terms of classifying them as non-diffracting or diffracting tie points, they are most likely to be

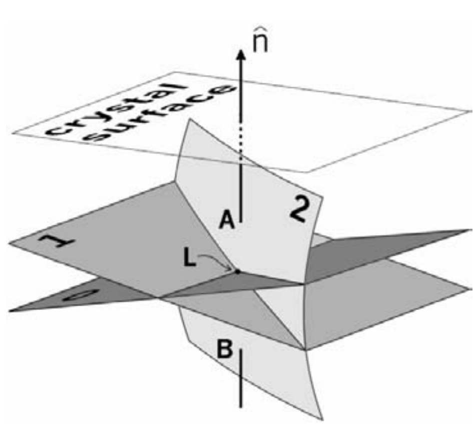

Figure 1
Geometrical condition of the BSD represented by the intersection, **L**, of three dispersion surfaces: 0, 1 and 2 centered, respectively, at the origin of the reciprocal space and at the primary and secondary reciprocal-lattice points.

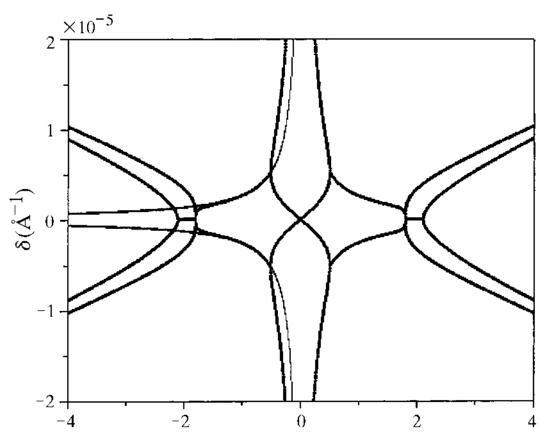

Figure 2
Components in the normal direction of the allowed X-ray secondary-wave vectors in the crystal, $\delta = \mathbf{K}_2(j) \cdot \hat{\mathbf{n}}$, as a function of $\Delta\omega$. Only the real part has been plotted, and the azimuthal rotation of the crystals is at the maximum of the $222/13\bar{1}$ BSD, wavelength 1.53793 Å. The eigenvalues were determined by Colella's formalism (Colella, 1974).

Table 1
Values of the projections (δ) and weights ($|q|$) for each allowed propagation mode, $j = 1, \ldots, 8$, in crystals with non-tilted and tilted surfaces.

The calculated values correspond to $\Delta\omega = 0.5''$ in Fig. 2 and a σ-polarized incident beam was assumed. The modes 1, 2, 7 and 8 are due to the secondary reflection.

	Non-tilted		Tilted (1.6″)	
j	δ ($\times 10^{-3}$ Å^{-1})	$\|q\|$	δ ($\times 10^{-3}$ Å^{-1})	$\|q\|$
1	0.829249	0.00276	0.829227	0.19599
2	0.819241	0.21316	0.819157	0.21524
3	0.004985 − 0.001105i	1.34862	0.009972 − 0.0011014i	1.34732
4	0.004985 + 0.001105i	0.15913	0.009972 + 0.0011014i	0.15992
5	−0.004985 − 0.001105i	2.16170	0.00000045 − 0.001103i	2.15053
6	−0.004985 + 0.001105i	0.25538	0.00000045 + 0.001103i	0.25419
7	−0.819241	1.45569	−0.819218	0.0000
8	−0.829249	0.06264	−0.829167	0.0000

non-diffracting ones since the components of their eigenvectors have significant values only for the wave fields of the secondary beam. However, the weights, $q(j)$, of these tie points for the total field in the crystal are of the same order of magnitude of the weight for the diffracting ones. For comparison, we show in Table 1 the eight $\delta(j)$ values, calculated at $\Delta\omega = 0.52''$, and the corresponding magnitude of $q(j)$. The weights were determined by solving a linear system of equations, which is constructed from applying the boundary conditions of the electromagnetic fields at the entrance and exit surfaces of the crystal slab (Weckert & Hümmer, 1997). Moreover, note that for an ordinary three-beam diffraction six linear equations are enough to determine the weights, while for the BSD eight equations would be necessary. The two extra equations are obtained here by splitting the secondary beam into one Bragg reflected beam, formed by the propagation modes with $\delta > 0$, and one Laue transmitted beam, formed by those modes with $\delta < 0$. The BSD becomes an ordinary three-beam diffraction when the crystal surface is tilted for a value large enough to make six propagation modes with δ of the same sign. This is also exemplified in Table 1.

The above examples demonstrate that the BSD geometry on a non-tilted surface gives relatively strong specular-reflected and forward-transmitted beams compared with any other three-beam diffraction geometry. Consequently, measurable specular-reflected waves are simultaneously excited with the diffracted waves, as observed by Campos *et al.* (1998). The forward-transmitted waves are also excited, although they should be experimentally more difficult to observe.

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