Analysis of X-ray Diffraction Conditions for Double-Crystal Topography

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Abstract

In recent years, with the advent of nearly perfect crystals, double-crystal topography has become very useful. For applications with such crystals the diffraction geometry in the double-crystal arrangement in three dimensions should be taken into account. Detailed studies of this problem are presented in this paper. Formulas for calculating the image height and displacement as the crystal is rotated are reported for various conditions. In the equispacing case, the image height is not limited provided the sample crystal is untilted with respect to the first crystal. However, if the crystal is tilted even a small amount then the image is limited and depends not only on the tilt angle $\phi$ but also on the distance between the X-ray source and the crystal $L$ and on the degree of crystal perfection $\beta$. In general, the tilt angle should not exceed 1' to obtain a large-area topograph and to measure the correct rocking curve in the asymmetric mode. In the unequispacing case, the image height is always limited. In this case, even when the crystal is not tilted, the image height is a function of $L$, $\phi$ and the difference in Bragg angle, $\Delta \theta$, between the diffraction planes of the two crystals. The image height is directly proportional to $\beta$ and inversely related to $\Delta \theta$. In this case, in order to obtain a large-area topograph of a nearly perfect crystal $L$ must be large or $\Delta \theta$ must be small. The different experimental conditions are explored for various types of first and second crystals to verify the analytical formulas that have been derived. The experimental data were found to be in good agreement qualitatively and quantitatively with the analysis.

I. Introduction

Double-crystal X-ray diffraction topography (DCT) is a useful technique for studying lattice defects in single crystals. This method was first reported by Bond & Andrus (1952) and Bonse & Kappler (1958) who employed two successive Bragg reflections in the (+,−) parallel setting to detect long-range variations of the lattice parameter. Using this technique, many investigations of defects in silicon and germanium semiconductor crystals as well as quartz single crystals were published by Bonse and co-workers (Bonse, 1962; Bonse & Hart, 1965a; b; Bonse & te Kaat, 1968), Renninger (1961, 1963, 1964, 1976), Kohra & co-workers (Kohra, Yoshimatsu & Shimizu, 1962; Kohra, 1976), Yoshimura & Kohra (1976), Yoshimura et al. (1979), Hart (1969, 1971, 1975), Chikawa, Asaeda & Fujimoto (1970), Stacy & Janssen (1974) and others. In order to study a variety of single crystals, other than nearly perfect semiconductors or quartz crystals, the non-parallel (+,−) or (+,+ ) settings were used by Bearden & Henins (1965), Deslattes (1968), Kohra, Hashizume & Yoshimura (1970), Yoshimura et al. (1976), Kuriyama, Boettinger & Burdette (1978) and Strocka & Willich (1982). In spite of the large volume of experimental work on DCT only Jäger (1965, 1966) has attempted to analyze in detail the problem of the influence of diffraction geometry on image formation. This type of analysis is usually conceived in terms of the DuMond diagram which analyzes the angles at which Bragg reflection occurs from a given set of lattice planes for various incident wavelengths. However, the DuMond diagram is only satisfied for diffraction occurring on the horizontal or zero plane. The diffraction geometry of the DCT arrangement is much more complex and to analyze it correctly calculations must be performed for the three-dimensional case. The present work will consider such a three-dimensional model and describe experiments which confirm the analysis.

II. Overview of experimental arrangements for double-crystal topography

There are two different types of settings for the DCT technique according to the arrangement of the incident and diffraction beams of the two crystals. This is illustrated schematically in Fig. 1. For each of the two settings (+,−) and (+,+), respectively, there are two different modes; equi- and unequispacing of diffraction planes. In Fig. 1(a) the crystals are in a parallel setting and for the other three cases (b), (c) and (d) they are non-parallel.

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Another factor which must be considered is the nature of the crystals used in DCT. One has the choice of using either symmetric or asymmetrically cut crystals. In the symmetrically cut case, the diffraction plane is parallel to the surface of the crystal and the diffracted-beam width is equal to the incident-beam width. While for the asymmetrically cut case the diffraction plane is inclined to the surface of the crystal by an angle $\delta$ and the diffracted beam is asymmetrical to the incident beam with respect to the surface of the crystal. In the latter case the width of the diffracted beam is increased or decreased by an asymmetric factor $m = \frac{\sin(\theta + \delta)}{\sin(\theta - \delta)}$ (Boettinger, Burdette, Kuriyama & Green, 1976).

As shown in Fig. 2, in general, a point or horizontal line-focus X-ray source is used in the DCT method. The distance between the X-ray source and the first crystal $L_1$ and the distance between the first and second crystals $L_2$ has been varied by researchers from 150 to 1200 mm. The importance of changing these variables in terms of image formation will be discussed quantitatively later in the text. Definitions of other parameters used in the calculations below are described in Fig. 2.

### III. Analysis of diffracted image height

When the first crystal is properly adjusted the X-rays emitted from a point focus will diffract along a cone having a vertex angle $\pi - 2\theta$. In the symmetrically cut case the crystal surface and the diffraction cone will intersect along a circle or along an arc of a circle. Only those portions of the crystal in the intersection zone satisfy the Bragg condition. The diffraction cone of the first crystal becomes the incident-beam cone of the second crystal. When the second crystal is adjusted to the proper position, it will diffract some part of the X-rays from this cone. In the equispacing case the Bragg angle of the two crystals is the same. The X-rays from this whole cone can be diffracted and give a second crystal diffraction cone having the same vertex angle $\pi - 2\theta$ (see Fig. 3). In the unequispacing case the Bragg angle of the two crystals is not the same. Therefore, the vertex angle of the two cones is not identical and the whole diffraction cone from the first crystal cannot be completely diffracted.

In the discussions that follow the concept of 'ideal' and 'actual' crystal diffraction cones will be used. The ideal cone is defined in the following manner; consider the diffraction cone from the first crystal when it is adjusted to the exact Bragg condition (shown as cone $P$ in Figs. 3a, b); then the reflected image of that cone about the diffraction plane of the second crystal (shown as cone $Q$ in Figs. 3a, b) is the ideal diffraction cone. The actual diffraction cone is defined as the whole cone diffracted by the second crystal when the incident beam is divergent. With this concept the diffraction for various cases will next be considered.

#### (1) Equispacing case

In the equispacing case, if the second crystal is properly adjusted, the ideal X-ray diffraction cone and the actual cone coincide and complete diffraction occurs from the entire cone. These cones intersect with the second-crystal surface in a circle centered on $O$, Figs. 3a, b. However, when the second crystal (or first crystal) is tilted by an angle $\rho$ about the horizontal axis $y$, then these cones will not coincide and will only intersect with the crystal surface at the points $N$ and $M$ (see Fig. 4). Generally, the crystal is not very large and just intersects at one point $N$. The shapes of these two cones intersect the crystal surface in a circle and in an ellipse with centers $O$ and $E$ as shown in Fig. 4(b). Any incident or diffracted X-ray beam possesses some angular or wavelength spread. Therefore, the two
cones will have some finite thickness and intersect with the crystal surface not only at a geometric point $N$ but also with a certain area of intersection. From Fig. 4, one can show that $QB = QA = L$, $\angle BQD = \angle AQC = \rho$, $\angle QBD = \angle OAE = \theta$. $OB = ON = R = L \cos \theta$, where $L$ is the sum of the distances $L_1$ and $L_2$.

From triangles $ACQ$ and $BDQ$, one obtains $AC = p$ and $BD = q$:

$$p = L \sin \rho / \sin(\theta - \rho)$$  \hspace{1cm} (1)

$$q = L \sin \rho / \sin(\theta + \rho)$$  \hspace{1cm} (2)

so that the ellipse major axis is

$$2a = 2R - q + p = 2L \cos \theta (1 + K),$$  \hspace{1cm} (3)

where

$$K = \frac{\sin^2 \rho}{\sin(\theta + \rho) \sin(\theta - \rho)},$$  \hspace{1cm} (4)

and the ellipse minor axis is

$$2b = 2R = 2L \cos \theta$$  \hspace{1cm} (5)

The origin of the coordinate system is at point $I$, which is the projection point of the intersection of point $N$ on the $z$ axis. The distance between the origin $I$ and the ellipse center $E$ is $t$. Then, for the ellipse

$$[(z_1 - t)/a^2] + [y_1^2/b^2] = 1;$$  \hspace{1cm} (6)

and for the circle

$$(z_2 + s + t)^2 + y_2^2 = R^2;$$  \hspace{1cm} (7)

where $s$ is the distance between $O$ and $E$.

From Fig. 4(b),

$$s = a + q - R = (p + q)/2 = LK \sin \theta \cot \rho;$$  \hspace{1cm} (8)

noting that at point $N$, $z_1 = z_2 = 0$, $y_1 = y_2$, from (6) and (7),

$$t = [KL/(2 - K)] \sin \theta \cot \rho.$$  \hspace{1cm} (9)

At $z$ or points $F$ and $J$, $z_1 = z_2 = z$, from (6) and (7) one obtains

$$y_1^2 = R^2 - (z - t)^2(1 + K)^{-2}$$

$$= R^2 - (z - t)^2(1 - 2K)$$  \hspace{1cm} (10)

$$y_2^2 = R^2 - (z + s - t)^2.$$  \hspace{1cm} (11)

If the sum of the X-ray beam angular spreads, $\beta_1$ and $\beta_2$, for the two diffraction cones is $\beta$, then the linear spread at the second crystal surface is $L\beta$. When the linear spread $L\beta$ is larger than or equal to $y_1 - y_2$, the ellipse $E$ with thickness $L\beta_1$ and the circle $O$ with thickness $L\beta_2$ can intersect or touch each other and give a diffraction image. For the image border, $y_1 - y_2 = L\beta.$  \hspace{1cm} (12)

Substitution of (10) and (11) into (12) gives

Fig. 3. The diffraction cone in the equispacing case at (a) $(+, -)$ parallel setting and (b) $(+, +)$ non-parallel setting.

Fig. 4. The diffraction geometry analysis of the equispacing case with crystal tilted by an angle $\rho$ along the $y$ axis. $QB = L$, $NO = R$, $IE = t$, $OE = s$, $BD = q$, $AC = p$, $EC = a$ and $EH = b.$
\[(2K + \beta \sec \theta(z - t)^2 + 2s(1 + \beta \sec \theta)(z - t)
+ s^2(1 + \beta \sec \theta) - L^2\beta(\beta + 2 \cos \theta) = 0, \quad (13)\]
\[z = \frac{L^2\beta(\beta + 2 \cos \theta)}{2s(1 + \beta \sec \theta)} - \frac{s}{2} + t, \quad (14)\]
which is identical to
\[z = \frac{L\beta \cot \theta \tan \rho}{K} - \frac{LK^2 \sin \theta \cot \rho}{(2 - K)}. \quad (15)\]
The second term in the above formula is very small, approximately zero. Point N in Fig. 4(b) is approximately the central point of the diffraction image, therefore the image height is \(2z\), i.e.
\[H = \frac{L\beta \sin 2\theta \cot \rho}. \quad (16)\]

Thus the image height, in addition to the tilt angle \(\rho\), is also dependent on the three variables \(L\), \(\theta\) and \(\beta\), which has not generally been recognized. The height of the image is directly proportional to the angular spread \(\beta\) and distance \(L\).

According to the dynamical theory of X-ray diffraction, the X-ray beam angular spread or the width of a selective reflection for a symmetrically cut crystal is
\[\beta_s = \frac{2\lambda^2 N \mu^2 |F|^2}{m_0 c^2 \pi \sin 2\theta}, \quad (17)\]
where the symbols have the same meaning as those given by Warren (1969). The \(\beta_s\) of the first crystal for Si (111) and Si (400) is therefore 7.05 and 1.68°, respectively. The \(\beta_s\) of the second crystal for the same Si reflections is 7.17 and 2.69°, respectively.

In the asymmetrically cut case, the widths of the incident and diffracted beams \(\beta_0\) and \(\beta_o\) are given by \(\beta_0 = \beta_o m^{-1/2}\) and \(\beta_s = \beta_o m^{-1/2}\), respectively.

The angular spread \(\beta\) in (14) is \(\beta_1 + \beta_2\). Here \(\beta_1\) is \(\beta_0\) of the first crystal and \(\beta_2\) is \(\beta_o\) of the second crystal. So for Si (111) and (400), with \(m=38\) for the first crystal, \(\beta\) is equal to 8.5° and 3.0°, respectively.

The results of these calculations for \(H\), for several cases, is given in Fig. 5. It can be seen in this figure that the diffraction image height becomes very small after tilting the crystal a small amount. In general, the height of the topographic image of the crystal will be small if the crystal is tilted more than 1 to 2° and full sample coverage will not be achieved.

(2) Unequispacing case

In the unequispacing case, the height of the diffraction image is limited because the apex angles of the ideal X-ray diffraction cone and the actual diffraction cone are not equal.

When the crystal is not tilted and has been adjusted to the proper orientation, these two cones can touch on a line \(QG\) (Fig. 6). The small cone intersects the bottom plane \(O_1GIJ\) of the large cone in an ellipse \(EFG\), which has major and minor axes \(EG\) and \(MH\). The diameters of the circles of the bottom plane of the two diffraction cones with apex angle \(\pi - 2\theta_1\) and \(\pi - 2\theta_2\) are
\[GJ = 2L \cos \theta_1 \text{ and } GC = 2L \cos \theta_2, \quad (18)\]
where \(\theta_1\) and \(\theta_2\) are the Bragg angles of the diffracting planes of the first and second crystals, respectively.

From the triangles \(EGC, AGO_2, QGA\) and \(ABQ\) and using the law of sines as before, one finds \(BG, AG, AO_2\) and \(AB\) as a function of \(L, \theta_1, \theta_2\) and \(\sigma\). By solving the algebra and simplifying one obtains
\[\cot \sigma = \frac{2 \sin \theta_1 \sin (\theta_2 - \theta_1)}{\cos^2 \theta_2 \sin 2(\theta_2 - \theta_1)} + \tan(\theta_2 - \theta_1), \quad (19)\]
where \(\sigma\) is the angle \(AQB\) in Fig. 6.

Next, from triangles \(QO_2G, QO_2D\) and \(QBG\) one finds \(QO_2, QD, DO_2\) and \(QB\) as functions of the same

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Fig. 5. The image height in equispacing case for different conditions as a function of the tilt angle \(\rho\). \(f_v\) is the vertical size of the focal spot.

Fig. 6. The diffraction geometry analysis of the image height in the unequispacing case. \(O_1C = L \cos \theta_2, O_1J = L \cos \theta_1, O_1W = L \cos \theta_1, UW = h, BN = r, NW = d = L\beta, BE = a\) and \(MB = b\).
variables, as above. From circle \( O_2 \), noting that \( DF \) is parallel to \( O_2 K \), one finds
\[
DF = L \cos \theta_2 [1 - \tan^2 \theta_2 \tan^2 \sigma]^{1/2}.
\] (20)

From similar triangles \( QBH \) and \( QDF \), one obtains \( b \), the minor axis of the ellipse:
\[
b = BH = \frac{L \sin \theta_1 \cos \theta_2 \cos \sigma}{\sqrt{1 - \tan^2 \theta_2 \tan^2 \sigma}}
\] (21)
\[
x \left[ \sin(2\theta_2 - \theta_1) \cos(\theta_2 + \sigma) + \sin^2 \theta_1 \cos^2 \phi \cos^2 \sigma \right]
\] (22)

The major axis of the ellipse is given by
\[
a = BG = L \sin \theta_2 \cos \sigma.
\] (23)

From Fig. 6, it is clear that the centers of the circle \( O_1 \) and the ellipse \( B \) are not at the same point. By substituting \( a \) and \( b \) from above for the ellipse equation in polar coordinates
\[
r = \frac{a^2 b^2}{a^2 \sin^2 \phi + b^2 \cos^2 \phi},
\] one obtains
\[
r = \frac{L \sin \theta_1 \sin \theta_2 \cos \theta_2 \cos \sigma}{\sqrt{1 - \tan^2 \theta_2 \tan^2 \sigma}}
\] (24)
\[
x \left[ \sin(2\theta_2 - \theta_1) \cos(\theta_2 + \sigma) + \sin^2 \theta_1 \cos^2 \phi \cos^2 \sigma \right]
\] (25)
\[
\frac{1}{\sqrt{1 - \tan^2 \theta_2 \tan^2 \sigma}}
\] (26)

Using (19), (25) and (28) and from the known values of \( L, \theta_1, \theta_2 \) and \( \beta \), one derives the image height \( h \). The results are displayed in Fig. 7.

**IV. Kz doublet line distance and displacement**

When only the case of the zero plane is considered the diffraction occurs only at one point on the crystal surface. If one considers the case of the whole crystal, one finds that diffraction occurs along an arc of a cone on the crystal surface. It is therefore necessary to analyze the diffraction geometry in the whole space. To do this consider the diffraction conditions from an arbitrary point \( P_1 \) on the first crystal surface (Fig. 8a). Let the first and second crystals both be symmetrically cut and designate the normals to the diffracting planes of these to be \( n_1 \) and \( n_2 \), respectively. The planes \( F_1J \) and \( P_1P_2W \) are parallel to the diffracting planes of the first crystal and the second crystal, respectively. The coordinate axes are shown in Fig. 8(a) with the \( y \) axis parallel to the main incident X-ray beam and the \( z \) axis normal to the horizontal plane. The coordinate of the point \( P_1 \) is \((x_1, y_1, z_1)\). The incident X-ray beam is shown by the line \( FP_1 \) and the diffracted ray by the line \( P_1P_2 \), which intersects the second crystal surface at the point \( P_2 \). \( P_1 \) is the projection point of \( P_1 \) on the horizontal plane. One can see that the angle \( \angle FP_1A = 90^\circ - \theta_1 \) is not equal to the angle \( \angle FP_1B = \alpha \). From triangle \( FP_1E \),
\[
\cos \omega = \frac{x_1 \cos \varepsilon_1 + (L_1 - y_1) \sin \varepsilon_1}{\sqrt{x_1^2 + (L_1 - y_1)^2}}
\] (29)

where \( \varepsilon_1 \) is the angle included between the incident beam \( FO_1 \) and the diffracting plane of the first crystal in the horizontal plane. Suppose the first crystal has been adjusted to the position that \( O_1 \) satisfies Bragg’s
law, then \( \epsilon_1 = \theta_1 \), therefore \( O_1 O_2 \) is the diffracted line of the point \( O_1 \) on the first crystal and angle \( DO_1 O_2 = 2\theta_1 = 2\epsilon_1 \). From right triangles \( FP_1 A \) and \( FP'_1 B \):

\[
\cos^2 \omega = \left[ \frac{x_1^2 + (L_1 - y_1)^2 + z_1^2}{x_1^2 + (L_1 - y_1)^2} \right] \sin^2 \theta_1.
\]

Solving (29) and (30) one obtains

\[
z_1^2 = \csc^2 \theta_1 \left[ x_1 \cos \epsilon_1 + (L_1 - y_1) \sin \epsilon_1 \right]^2 - x_1^2 - (L_1 - y_1)^2.
\]

Since \( x_1 \ll L_1 - y_1 \), from Fig. 8(a)

\[
y_1 = \frac{L_1 \cos \omega - \sin \epsilon_1}{\cos \epsilon_1 \tan(\epsilon_1 - \delta_1) + (\cos \omega - \sin \epsilon_1)}.
\]

From Fig. 8(b), \( l = P'_1 C + P'_2 C \), one gets

\[
l = [L_2 \sin(\theta_2 + \delta - \delta_2) - y_1 \sec(\epsilon_1 - \delta_1)]
\]

\[
\times \cos(\epsilon_1 - \omega) \sin(2\epsilon_1 - \theta_2 - \delta + \delta_2) \]

\[
\times \left[ \cos(\omega + \epsilon_1 + \delta - \theta_2 - \delta_2) \right]^{-1}
\]

\[
+ y_1 \tan(\epsilon_1 - \delta_1) \left[ \cos(\epsilon_1 - \omega) \right]^{-1}.
\]

where \( \epsilon_2 \) is the angle included between the beam \( O_1 O_2 \) and the diffracting plane of the second crystal in the horizontal plane. \( \epsilon_2 = \theta_2 + \Delta \), where \( \Delta \) is the deviation from the Bragg angle \( \theta_2 \). Next, from Fig. 8(a), noting that the right triangles \( FP_1 A = JP_1 A \), \( FP'_1 B = JP'_1 B \) and \( FP'_1 P_1 = P_1 JH \), we find that \( JH = HI = z_1 \); also \( P_1 K = P'_1 P_2 = l \), \( P_1 H = P'_1 I = FP'_1 \) and \( z_2 = JH(P_1 K / P_1 H) + HI \); therefore,

\[
z_2 = z_1 \left[ l \left[ x_1^2 + (L_1 - y_1) \right]^{1/2} \right] + z_1.
\]

Further, from triangles \( P'_2 QO_2 \) and \( P'_2 TO_2 \) one finds \( \psi = \epsilon_1 + \omega - \epsilon_2 \).

If the second crystal is set in the diffracting condition for ray \( FP_1 P'_2 \), then angle \( JP_2 V = 90^\circ - \theta_2 \). Then from right triangles \( P_2 VP_1 \) and \( P'_2 WP'_1 \) one has

\[
\left[ l^2 + (z_2 - z_1)^2 \right]^{1/2} \sin \theta_2 = l \cos(\epsilon_1 + \omega - \epsilon_2).
\]

Solving (35), (36), (31) and (29), one gets

\[
\cos(\epsilon_1 + \omega - \epsilon_2) = \frac{\sin \theta_2}{\sin \theta_1} \cos \omega,
\]

and simplifying and transposing terms one obtains

\[
\tan \omega = \frac{\sin \theta_2}{\sin \theta_1} \sin(\theta_2 + \Delta - \epsilon_1)] - \cot(\theta_2 + \Delta - \epsilon_1).
\]

Thus, one can use (31), (32), (34), (35) and (38) to evaluate \( z_2 \) at different values of \( \Delta \) or for other variables of interest. The computed results are shown in Fig. 9.

If we use \( \theta'_1 \) and \( \theta'_2 \) to represent the Bragg angles of the \( K\alpha_1 \) and \( K\alpha_2 \) doublet of the first crystal and \( \theta'_2 \) for the second crystal with \( \epsilon_1 = \theta'_1 \), then the plot for \( K\alpha_1 \) in Fig. 9 will pass through the origin and that for \( K\alpha_2 \) will not. The implications of this are physically explained in § V. Experimental results.

V. Experimental results

A double-crystal topography camera was developed by the Stony Brook group. The experimental arrangement is shown schematically in Fig. 2. The distance
between the X-ray focus and the first crystal, \( L_1 \), is 220 mm. The distance between the first and second crystals, \( L_2 \), can be varied from 100 to 500 mm. Both crystal stages can be rotated with an accuracy of 0.5°.

In addition to a film-plate holder this camera has provision for both an image intensifier tube and a photon detection counter.

In the present work the first crystal was an asymmetrically cut float zone silicon crystal. Two kinds of asymmetrically cut crystals were prepared for Cu K\( \alpha \) radiation. In the first instance an Si crystal was cut for optimum (400) diffraction with \( \delta = 33.2° \) and \( m = 39 \). Another crystal was cut for (111) diffraction with \( \delta = 13.5° \) and \( m = 38 \). The crystals were sliced with dimensions 50 x 50 x 12 mm and had a U-shaped groove cut parallel to the wide face of the crystal. This permitted strain-free mounting, which was verified by rocking-curve measurements to be nearly ideal.

The second crystals (i.e. samples) examined in the present experiments were Czochralski (CZ) silicon wafers, which had been either symmetrically or asymmetrically cut for (400), (220) and (111) diffraction.

(1) The image height for the equispacing case

In this case the first crystal was the Si (400) described above and the second crystal was a symmetrically cut Si (400) wafer with a thickness of 0.3 mm and a diameter of 75 mm. The measured rocking-curve width in this setting was 5.8° and the calculated rocking-curve width for Si (400) was \( \beta_1 = 2.7° \), therefore \( \beta = 3.0° \). The measured width was a little larger than the ideal and was attributable to the imperfections in the CZ wafer.

This work used a small-focal-spot X-ray tube with focal spot size 0.8 mm vertical \((f_v) \times 12.5\) mm horizontal. The actual height of the diffraction image \( H' \) is the sum of \( f_v \) and the image height \( H \) calculated with (16).

The Bragg angle for Si (400) is 34.57° for Cu K\( \alpha \) radiation. In the experiments under discussion \( L = 500 \) mm and \( \beta = 6° \); the results for the measured image height \( H_m \) at different tilt angles \( \rho \) are compared to the calculated value \( H' = H + f_v \) in Table 1.

(2) Diffraction image for unequispacing case

In the unequispacing case, even if the crystal is not tilted, the diffraction image is limited. When the second crystal, or first crystal for that matter, is rotated, the K\( \alpha_1 \) horizontal diffraction line separates into two lines. The distance between these two lines expands continuously with increasing angle of rotation. The diffraction image in this process and the intersection pattern of the two diffraction cones are shown in Fig. 10. It can be seen that the K\( \alpha_2 \) line appears after the crystal is rotated to a certain angle. The K\( \alpha_2 \) line separates into two lines with increasing rotation angle.

The experimental results demonstrate the validity of the calculations given in § IV above. Some diffraction image pictures are shown in Fig. 11. In this unequispacing case the Si (111) diffraction was obtained from the first crystal. It was symmetrically cut with \( \delta = 13.5° \)

### Table 1. Comparison of observed image heights with theoretical values for equispacing case

<table>
<thead>
<tr>
<th>Tilt angle ( \rho ) (°)</th>
<th>Image height ( H_m ) (mm)</th>
<th>Calculated image ( H + f_v ) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( \infty )</td>
<td>( \infty )</td>
</tr>
<tr>
<td>2</td>
<td>25</td>
<td>24.2</td>
</tr>
<tr>
<td>3</td>
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<td>16.4</td>
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</tr>
<tr>
<td>300</td>
<td>0.8</td>
<td>1.0</td>
</tr>
</tbody>
</table>

![Fig. 10. A schematic diagram of image formation of the K\( \alpha \) doublet line in unequispacing case. (a) Section diagram of the two diffraction cones at the second crystal surface; (b) the corresponding topographic image.](image)

![Fig. 11. The X-ray double-crystal topograph of Si (111)-(400) in the unequispacing case for different rotation angles \( \phi \). The uneven split here into two images is entirely attributed to K\( \alpha_1 \) diffraction lines.](image)
Table 2. Comparison of measured data with theory for the unequispacing case

<table>
<thead>
<tr>
<th>Rotation $\Delta$ (°)</th>
<th>Measured $K_{2z_1}$ separation (mm)</th>
<th>Calculated $2z_2$ separation (mm)</th>
<th>Measured $h + f_v$ height (mm)</th>
<th>Calculated $h + f_v$ height (mm)</th>
</tr>
</thead>
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<tr>
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</tr>
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<td>-</td>
</tr>
<tr>
<td>35</td>
<td>23</td>
<td>22</td>
<td>-</td>
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</tr>
<tr>
<td>45</td>
<td>27</td>
<td>25</td>
<td>-</td>
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</tr>
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</table>

and $m = 38$. The second crystal was a symmetrically cut Si (400) wafer. The camera parameters were $L_1 = 220$ and $L_2 = 180$ mm, respectively. The measured values of the separation distance between the twin lines of $K_{2z_1}$ for various rotation angles $\Delta$ of the second crystal are given in Table 2. It can be seen that they are in agreement with the calculated values determined by (35). The distance between the first and second crystals and the film is approximately 20 mm, so one would expect the measured data to be slightly larger than the calculated values.

At very small rotation angles, $\Delta$, the twin line images overlap and the image height cannot be determined. Thus the image height is reported at the point where the twin lines are just separated, i.e. 25°. When the measurement is made at $\Delta = 2°$, the experimental value should be divided by two, giving a measured value of 6 mm which is very close to the calculated value ($h + f_v$) without rotation of 5.8 mm.

The smaller the difference between $\theta_2$ and $\theta_1$, or alternatively the larger the distance $L$ and the angular spread $\beta$, the greater the height of the diffraction image (see Fig. 7). This conclusion was checked by using different kinds of second crystal and different distances $L$. The different crystals used were CZ silicon (220), zinc (0002) and sodium nitrate (100). For Si (220), with $\theta_2 - \theta_1 = 9.42°$, the calculated image height was 10 mm when $\beta = 6°$ and $L = 560$ mm. The experimental observation was 13 mm. For Zn (0002) and sodium nitrate (100), the differences in the diffraction angles, $\theta_2 - \theta_1$, were 3.94 and 0.52°, respectively. These latter two crystals were, of course, not very perfect compared to Si, therefore the image height easily covered the entire crystal as expected.

If the crystal is tilted in the unequispacing case, two lines are found which are the $K_{2z_1}$ and $K_{2z_2}$ doublet. The height of the line and the distance between the $Kz$ doublet lines becomes much narrower as the tilt angle $\rho$ increases. Some topographs showing this effect are presented in Fig. 12.

VI. Discussion

(1) Comparison with crystal bending image formation

The horizontal image line (Fig. 13) caused by crystal tilt and/or diffraction geometry is different from the vertical or irregularly shaped line caused by crystal bending. If the second crystal is curved by a uniform bend stress, the diffraction image will be narrowed along this axis. For example, if the crystal is bent along a vertical axis, a vertical image line will be obtained in the topograph. When one rotates the second crystal about the normal to the diffraction plane then the diffraction line, owing to the curvature of the crystal, is correspondingly rotated. Therefore, in the present work, if the horizontal line is caused by crystal bending about the horizontal axis then after rotating the crystal 90° about the normal to the diffraction plane the diffraction image line should be rotated to a vertical line. However, this phenomenon was never observed; no matter how many degrees of rotation, the diffraction image line remains a horizontal line for the unequispacing case and for the equispacing case with crystal tilt. This type of experimental operation allows one to distinguish between bending and diffraction geometry effects.

(2) Large-area image coverage

In the unequispacing case, the diffraction image height depends on the distance $L$, the difference in
Bragg angle between the first and second crystal and on the degree of crystal perfection. If $L$ is very small or $\theta_2 - \theta_1$ is very large, then one never obtains large-area beam coverage for topography. There are two methods for obtaining large-area image coverage of very perfect samples: (a) increase the distance $L$ to as large a value as feasible; (b) select the first-crystal methods for obtaining large-area image coverage of beam coverage for topography. There are two cases for the rocking curve: if $L$ is very small, then one never obtains large-area coverage, as shown above, one has a choice for equivalent experimental accuracy; designing for large collimator distance from the source, $L_1$, with a short compact camera base, $L_2$, or alternatively being close to the source with a long camera base.

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(3) Consideration for rocking-curve measurements

When the image height is not very large as in the unequispacing case or in the equispacing case with tilt, then the horizontal diffraction line image will move up or down as the crystal is rotated about a vertical axis. In general, using the common method for observing a rocking curve, the width of the diffraction intensity curve incident on the second crystal is usually 10 to 20 times larger than the rocking curve being measured. The above discussion indicates that under certain conditions this usual assumption will not be followed. One can only measure the correct rocking curve for the case of the equispacing crystal that is unilted. Since the image height is very sensitive to the tilt of the crystal for the equispacing case one must take care to adjust the second crystal so that tilt is less than $10^\circ$.

(4) Implications for camera design

The image height is very sensitive to the tilt of the crystals and is not sensitive to rotations about the axis parallel to the normal to the diffraction plane. Hence one must have an accurate method for adjusting crystal tilt. This is particularly important when dealing with reflections that are not necessarily from an accurate reference surface on the sample. Finally, since $L_1$ and $L_2$ are interrelated in producing image coverage, as shown above, one has a choice for equivalent experimental accuracy; designing for large collimator distance from the source, $L_1$, with a short compact camera base, $L_2$, or alternatively being close to the source with a long camera base.

References