Crystal Subgrain Misorientations Observed by X-ray Topography in Reflection

BY R. W. ARMSTRONG
University of Maryland, College Park, MD 20742, USA
AND W. J. BOETTINGER AND M. KURIYAMA
National Bureau of Standards, Washington, DC 20234, USA

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Abstract
Based on the principles of conservation of momentum
and energy for X-ray diffraction, a vector description is
obtained for the displacement of adjacent subgrain
images in reflection topographs. The analysis includes,
in addition to those crystal parameters defining the
misorientation at a subgrain boundary, the combined
effects of (horizontal and vertical) divergence in the
incident X-ray beam and of the position where the X-
ray images are recorded. The vector description is
matched with a stereographic projection method of
analysis for describing the subgrain misorientations.
These total considerations are applied to the charac-
terization of subgrain boundaries grown into a nickel
single crystal solidified along [-010], including specifi-
cation of the dislocation structure within the
boundaries.

1. Introduction
Misoriented subgrains within imperfect single crystals
are directly observed in X-ray surface reflection
topographs for one or both of the following reasons: (a)
different reflected intensities occur for each subgrain
image; (b) the diffracted beams separate or overlap at
the borders of adjacent images (Armstrong & Wu,
1973). An example of this phenomenon is shown in Fig.
1 for a (110) nickel crystal surface cut through a
reasonably cylindrical specimen solidified along [010]
by the Czochralski method (Kuriyama, Boettinger &
Burdette, 1978). Fig. 1 is a (220) surface reflection
topograph obtained by the asymmetric crystal topogra-
phic (ACT) method with Cu Kα radiation (Boettinger,
Burdette, Kuriyama & Green, 1976). The plane of
diffraction, i.e. the plane containing the incident X-ray
beam, the diffracting plane normal for a single subgrain,
and hence the diffracted beam, is (110). Subgrains are
observed with different reflected intensities in Fig. 1,
which also includes a substantial number of absent
subgrain reflections, due to subtle differences in the
subgrain orientations and positions relative to the
incident X-ray beam.

The actual boundaries between subgrains of the
nickel crystal are represented in Fig. 1 by black or white
bands of varied widths. In Fig. 1, a white band is
indicative of an absence of X-ray intensity in the region
between separated X-ray images while black boun-
daries occur because of the addition of X-ray intensities
in regions where the reflections overlap. At the
endpoints of boundaries or at positions of changed
direction along any boundary, it is possible to
determine the relative displacement in the X-ray image
of identical points. For the prominent, mostly white
boundary AB on the right side of Fig. 1, this
displacement, s, whose direction is indicated at A, is
observed to be very nearly in the horizontal plane of
diffraction containing [220], perpendicular to the plane
of the figure. Measurement of this particular displace-
ment provides the basic information for determining
the misorientation of adjacent subgrains.

II. Vector description
Consider a sample containing a boundary between two
subgrains, 1 and 2, as indicated in Fig. 2. Let the

![Fig. 1. (220) ACT surface reflection topograph of nickel crystal
obtained with Cu Kα radiation in (110) plane of diffraction.]

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difference in orientation between the subgrains be defined by a rotation axis \( l \) imbedded in subgrain 2 and a rotation about this axis of \( \Delta \theta_0 \). In general, Bragg diffraction from each of the subgrains, \( i \), demands

\[
\mathbf{k}^{(i)}_{\text{out}} = \mathbf{k}^{(i)}_{\text{in}} + \mathbf{H}^{(i)}
\]

(1a)

and

\[
|\mathbf{k}^{(i)}_{\text{out}}| = |\mathbf{k}^{(i)}_{\text{in}}|,
\]

(1b)

where \( \mathbf{k}^{(i)}_{\text{in}}, \mathbf{k}^{(i)}_{\text{out}} \) and \( \mathbf{H}^{(i)} \) are, respectively, the incoming and outgoing wave vectors and the reciprocal-lattice vector for diffraction from the \( i \)th subgrain. We restrict our attention to the case where

\[
|\mathbf{k}^{(1)}_{\text{in}}| = |\mathbf{k}^{(2)}_{\text{in}}| = k,
\]

(2a)

and

\[
|\mathbf{H}^{(1)}| = |\mathbf{H}^{(2)}| = H.
\]

(2b)

Consider, in particular, two diffracted rays emanating from adjacent points on the subgrain boundary, each ray undergoing diffraction from its respective (perfect) subgrain and striking a film plane with normal \( \mathbf{n} \) as shown in Fig. 2. The separation of the points where the two rays strike the film, \( s \), can be written as

\[
s = \sigma (\mathbf{k}^{(2)}_{\text{out}} - \mathbf{k}^{(1)}_{\text{out}}) + \alpha \mathbf{H}^{(2)} = \sigma \Delta \mathbf{k}_{\text{out}} + \alpha \mathbf{H}^{(2)},
\]

(3)

where \( \sigma \) and \( \alpha \) are scalars related to the film distance. Here we have introduced the following quantities:

\[
\Delta \mathbf{k}_{\text{out}} = \mathbf{k}^{(2)}_{\text{out}} - \mathbf{k}^{(1)}_{\text{out}},
\]

(4a)

\[
\Delta \mathbf{k}_{\text{in}} = \mathbf{k}^{(2)}_{\text{in}} - \mathbf{k}^{(1)}_{\text{in}},
\]

(4b)

and

\[
\Delta \mathbf{H} = \mathbf{H}^{(2)} - \mathbf{H}^{(1)}.
\]

(4c)

Since the projections of \( \sigma \Delta \mathbf{k}_{\text{out}} \) and \( \alpha \mathbf{H}^{(2)} \) on \( \mathbf{n} \) are equal but opposite in sign, as shown in Fig. 2, we obtain

\[
\sigma = - \frac{\Delta \mathbf{k}_{\text{out}} \cdot \mathbf{n}}{|\mathbf{k}^{(2)}_{\text{out}} \cdot \mathbf{n}|}.
\]

(5)

The length of the vector \( \sigma \mathbf{k}^{(1)}_{\text{out}} \) is the distance, \( d \), from the subgrain boundary to the film along beam 1. Equation (3) can now be written

\[
s = d \left\{ \Delta \mathbf{H} + \Delta \mathbf{k}_{\text{in}} - \frac{\Delta \mathbf{H} + \Delta \mathbf{k}_{\text{in}}}{\mathbf{k}^{(2)}_{\text{out}} \cdot \mathbf{n}} \mathbf{k}^{(2)}_{\text{out}} \cdot \mathbf{n} \right\},
\]

(6)

where

\[
\Delta \mathbf{k}_{\text{out}} = \Delta \mathbf{k}_{\text{in}} + \Delta \mathbf{H}
\]

(7)

from (1a) and (1b).

It is convenient to introduce the following unit vectors:

\[
\mathbf{g}^{(i)} = \frac{\mathbf{H}^{(i)}}{H},
\]

(8a)

\[
\mathbf{e}^{(i)}_{\text{in}} = \frac{\mathbf{k}^{(i)}_{\text{in}}}{k},
\]

(8b)

and

\[
\mathbf{e}^{(i)}_{\text{out}} = \frac{\mathbf{k}^{(i)}_{\text{out}}}{k}.
\]

(8c)

Associated with these quantities, we define

\[
\Delta \mathbf{g} = \frac{\Delta \mathbf{H}}{H},
\]

(9a)

and

\[
\Delta \mathbf{e}_{\text{in}} = \frac{\Delta \mathbf{k}_{\text{in}}}{k},
\]

(9b)

which are related to the angular misorientation of the two subgrains and the angular spread of the incoming X-ray beam, respectively. Then (6) is written

\[
s = d \left\{ (2 \sin \theta_B) \Delta \mathbf{g} + \frac{\Delta \mathbf{e}_{\text{in}}}{\mathbf{e}^{(2)}_{\text{out}} \cdot \mathbf{n}} \mathbf{e}^{(2)}_{\text{out}} \cdot \mathbf{n} \mathbf{e}^{(2)}_{\text{out}} \right\},
\]

(10)

where the Bragg angle \( \theta_B \) is defined by

\[
\sin \theta_B = \frac{1}{2} \frac{H}{k}.
\]

(11)

The difference between the diffracting plane normals \( \Delta \mathbf{g} \) is given in terms of \( \mathbf{g}^{(2)} \) and the previously defined \( \mathbf{l} \) by

\[
\Delta \mathbf{g} \approx \Delta \theta_0 (\mathbf{g}^{(2)} \times \mathbf{l}),
\]

(12)

presuming that angles of order \( (\Delta \theta_0)^2 \) can be neglected. Obviously, the vector \( \Delta \mathbf{g} \) is perpendicular to both \( \mathbf{g}^{(2)} \) and \( \mathbf{l} \). Under the conditions represented by (2), it can be shown from (1a) and (1b), if the square of \( |\Delta \mathbf{e}_{\text{in}}| \) is neglected consistent with the approximation employed in (12), that

\[
\Delta \mathbf{e}_{\text{in}} \cdot \mathbf{g}^{(2)} = - \mathbf{e}^{(2)}_{\text{out}} \cdot \Delta \mathbf{g},
\]

(13)

and

\[
\Delta \mathbf{e}_{\text{in}} \cdot \mathbf{e}^{(2)}_{\text{out}} = 0.
\]

(14a)

Equations (10), (12), (13) and (14) contain the full information which Bragg diffraction conveys about misorientation contrast. Although (13) and (14a) restrict the value of \( \Delta \mathbf{e}_{\text{in}} \), they do not specify it fully to permit the calculation of \( s \) without any further assumption about \( \Delta \mathbf{e}_{\text{in}} \).

In order to consider the exact nature of the assumption required about \( \Delta \mathbf{e}_{\text{in}} \) and to develop easily usable formulas relating a subgrain rotation to \( s \), we decompose these vectors into component vectors lying in and perpendicular to the plane of diffraction of the reference grain 2. An arbitrary vector \( \mathbf{p} \) can be
composed of two vectors defined by
\[ p^\perp = (p \cdot v)v \]  
and
\[ p^\parallel = (p \cdot g)g + (p \cdot u)u, \]
where \( g, u \) and \( v \) form an orthonormal set
\[ v = (g \times e_{in})/|g \times e_{in}| \]
and
\[ u = v \times g. \]
The vectors \( u \) and \( v \) are parallel and perpendicular, respectively, to the plane of diffraction and \( u \) can be written explicitly as
\[ e_{in} - (e_{in} \cdot g)g / \left[ 1 - (e_{in} \cdot g)^2 \right]^{1/2}. \]
Because \( v \cdot g^{(2)} = 0 = e_{in}^{(2)} \cdot v \) and the orthogonal relation between \( A_c^{in} \) and \( e_{in}^{(2)} \) as well as between \( g^{(2)} \) and \( u \) gives the same angle, \( \theta_B \), in the scalar multiplication, it follows from (13) that
\[ |A_c^{in}| = |A g^{(2)}|. \] 
Equation (18) is essentially unchanged to give
\[ s^\parallel = d \left( (2 \sin \theta_B) A g^\parallel + A c^{in}_e \right). \] 

For a given topograph, the quantities \( d, \theta_B \) and \( \gamma \) are known, and \( s^\parallel \) and \( s^\perp \) are measured. The sign of the measured distance is important: \( s^\perp > 0 \) if \( s \cdot v > 0 \) and \( s^\parallel > 0 \) if \( s \cdot u > 0 \). In many practical cases, the second term, \( A c^{in}_e \), in (20b) can be neglected compared to \( (2 \sin \theta_B) A g^\parallel \); otherwise \( A c^{in}_e \) must be experimentally determined either by possibly changing the ‘height’ of the X-ray source until one of the subgrain reflections vanishes or by using several film positions for a given diffraction condition. From these considerations, the desired quantities \( A g^\parallel \) and \( A g^\perp \) can be calculated by means of (20) and, in turn, \( A g \) is known. The rotation axis \( l \) can be found from two such \( A g \) values according to
\[ l = \frac{A g_1 \times A g_2}{|A g_1 \times A g_2|}, \]
where \( A g_1 \) and \( A g_2 \) are the \( A g \) vectors for two different topographs. After determining \( l \), \( \Delta \theta_0 \) can be calculated from (12) or, more simply, from \( A g^\perp = v \cdot A g \) by
\[ \Delta \theta_0 = A g^\perp / (u \cdot l). \]

III. Experimental results

The \((\bar{1}10)\) surface of the nickel crystal specimen shown in Fig. 1 was initially cut and then smoothed with an acid saw and polisher. The topograph of Fig. 1 and the subsequent ones to be described are printed to give mirror images of the crystal surface. The chosen axes and relevant directions on the actual nickel crystal have been identically transferred to the X-ray topographs. On the basis of Fig. 3, the observer is looking at each image along \(-n = [\bar{1}10]\) (with the darker regions of any figure having received more X-ray photons). Fig. 1 has \( H = [220] \) and \( v = [\bar{1}10] \) on the basis of Fig. 2 and (16a). Fig. 4(a), (b) and (c) shows topographs taken with \( H \) and \( v \) as follows: \([220]\) and \([001]\); \([400]\) and \([001]\); \([040]\) and \([001]\).
In Fig. 1, the shifted images of subgrains 1 and 2 were found to be formed by diffraction of $Kz_1$ and $Kz_2$ radiation individually. This result was made obvious during the initial crystal alignment procedure using the image intensifier (Boettinger, Burdette, Kuriyama & Green, 1976). With $s$ for the relative misorientation of subgrains 1 and 2 essentially in the horizontal plane of diffraction, i.e. the $(110)$, each subgrain could be seen to diffract first $Kz_1$ and then $Kz_2$ rays as the crystal was rotated about the vertical axis $\mathbf{v} = [\overline{1}10]$. The individual subgrains were of sufficient perfection that the $Kz_1$ and $Kz_2$ rays were diffracted at clearly different angular settings of the sample crystal. By direct measurement, a misorientation of 0.076° (274") was obtained for the $[\overline{2}20]$ diffracting plane normals of the subgrains through their sequential reflection of each wavelength. The ideal separation of the $Kz_1$ and $Kz_2$ peaks is computed to be 0.075° for double-crystal diffraction from silicon (111) and nickel (220) (Boettinger, Burdette, Kuriyama & Green, 1976). This separation is very much larger than the essentially negligible horizontal divergence of the incident radiation which is computed to be 0.00027° for asymmetric diffraction from the silicon crystal. The effect of the larger vertical divergence of 0.065° within the incident X-ray beam also contributes a negligible broadening in the horizontal plane of diffraction.

The quantitative confirmation that $s$ for these subgrains is in the $(1\overline{1}0)$ plane led to the consideration that reflection from both subgrains could be achieved more easily, even with $Kz_1$ rays alone, if the plane of diffraction were to be rotated 90° to become $(00\overline{1})$. The topographs of Fig. 4(a), (b) and (c) were taken in this way. The $Kz_1$ radiation was incident to the northern edge of Fig. 4(a), (b), and to the southern edge of Fig. 4(c). Besides subgrains 1 and 2 being found to be made simultaneously visible more easily in these topographs, they show that a substantially larger amount of the total crystal microstructure of subgrains is now in diffracting position at a single angular setting. Examination of the additional images which are numbered in Fig. 4(a), (b) and (c) confirms that large misorientations occur between the newly observed subgrains and the previous ones but, also, that the relative displacements of the new subgrains are very nearly in the same or opposite direction to that initially observed for subgrains 1 and 2.

Detailed measurements of $s$ were made for the relatively large displacement between subgrains 2 and 4 using the enlarged topographs of Fig. 5(a), (b) and (c). Relevant data for the experimental conditions are given in Table 1(a). The topographic measurements for $s$ and the computed values of $Ag/|Ag|$ and $\Delta \theta_0$ are given in Table 1(b). Relative to the orientation of subgrain 2, the value of $I$ determined by the cross products of $Ag$ from the $[2\overline{2}0]$ and $[0\overline{4}0]$ topographs, according to (21), was $[+0.11, +0.992, -0.06]$; and, from the $[4\overline{0}0]$ and $[0\overline{4}0]$ topographs, was $[-0.05, +0.998, -0.03]$. Owing to the small difference in direction of $Ag$ for these subgrains in the $[4\overline{0}0]$ and $[2\overline{2}0]$ topographs, particu-
Fig. 5. Details of subgrain structures within ACT reflection topographs: (a) (220); (b) (400); (c) (040).

Table 1. Determination of subgrain misorientations

(a) Experimental conditions

<table>
<thead>
<tr>
<th>g</th>
<th>v</th>
<th>u</th>
<th>θ[°]</th>
<th>χ[°]</th>
<th>d(mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1/\sqrt{2})[1\overline{1}0]</td>
<td>[001]</td>
<td>(1/\sqrt{2})[1\overline{1}0]</td>
<td>38.2</td>
<td>0</td>
<td>21.0</td>
</tr>
<tr>
<td>[100]</td>
<td>[001]</td>
<td>[010]</td>
<td>60.7</td>
<td>45</td>
<td>14.5</td>
</tr>
</tbody>
</table>

(b) Measured variables and calculated parameters

| s[∥](mm) | s[⊥](mm) | Δg[∥] × 10³ | Δg[⊥] × 10³ | Δg/|Δg| | Δθ₀[°] |
|----------|----------|-------------|-------------|--------|--------|
| +0.044   | -0.367   | +1.29       | -14.1       | [0.064, 0.064, 0.996] | 1.1    |
| +0.0086  | -0.490   | +0.60       | -19.3       | [0, 0.03, 0.995] | 1.1    |
| -0.017   | +0.047   | -1.13       | +1.85       | [0.52, 0, 0.85] | 1.3    |
larly the small differences in $\Delta g^2$, this cross product is very inaccurate and, thus, was not used. The average of the two reliable determinations for $\mathbf{I}$ is $[+0.08, +0.996, -0.045]$, i.e. $\mathbf{I}$ is very close to the [010] crystal growth axis, as expected. An average value of $\Delta \theta_0 = 1.2^\circ$ is obtained using this value for $\mathbf{I}$ and the $\Delta g$ values for each of the three reflections in turn in (22).

IV. Discussion

The X-ray and crystal parameters which have been described for the simultaneous reflections of subgrains 1 and 2 in Fig. 1 are additionally illustrated in the stereographic projection presented as Fig. 6 (Wu & Armstrong, 1975). The effective 'X-ray source' position for the (220) surface topograph in Fig. 1 is shown on the left side of the horizontal equatorial plane. The separated short vertical lines at the 'X-ray source' position are the $-K_{\alpha_1}$ and $-K_{\alpha_2}$ beam directions established by reflection from the silicon first crystal while the Bragg angles $\theta_{B1}$ and $\theta_{B2}$ apply for diffraction from the adjacent subgrains. The diffracted X-ray beams are shown at positions 1’ and 2’ on the other side of the diffracting plane normals for subgrains 1 and 2, respectively.

For the purpose of illustration in Fig. 6, a 5° misorientation is shown for the rotation of the two subgrains about an [010] axis. The separation of X-ray images along the length labelled $AB$ in Fig. 1 is produced by the crystal boundary whose trace is shown in Fig. 6, also, at a measured inclination running very nearly along $\pm [111]$. As indicated in Fig. 1, the boundary width in the X-ray image is established by shifting the trace of the real boundary in the crystal surface to the 1’ and 2’ diffracted-beam directions. The diffracted beams are relatively displaced in the same sense as was chosen for the separation of the diffracting plane normals. Thus, the subgrain misorientation produces a separation of the X-ray images. On the basis of Fig. 6, an overlapping of the subgrain images should occur for this same misorientation if the boundary direction is rotated forward past the equatorial [001] into the fourth quadrant of the figure. This condition is observed at two positions along the length of subgrain boundary $AB$ in Fig. 1.

Boundary $AB$ forms part of the 'lineage structure' for this nickel crystal and so the boundary interface should contain the [010] crystal growth axis. This direction should also normally be the rotation axis for the misorientation across the boundary. This observation is consistent with the displacement vector measured for the misorientation of subgrains 1 and 2. The [010] growth axis and the $\pm [111]$ trace for the boundary give the dashed (101) orientation in Fig. 6 for the plane of the boundary interface between the subgrains.

The line directions for the dislocations composing boundary $AB$ should be expected to run along [010], too. It may be seen in Fig. 6 that a choice of $(a/2)[101]$ Burgers vector for the dislocations aligned along the [010] growth axis gives a special case for explaining [010] being the rotation axis for the misorientation. In this instance, the dislocations are arranged in the form of a simple 'tilt' boundary because the Burgers vector is perpendicular to the boundary interface. This is the
only Burgers vector among the various \langle 110 \rangle which is able to satisfy this condition.

The total subgrain structure, as derived from all of the topographs in Figs. 1, 4 and 5, is sketched in Fig. 7. The subgrain boundaries CD, EF and LM appear at least as prominent as boundary AB in terms of their length and straightness in Fig. 4(a), (b) and (c). By reference to Fig. 6, it may be seen that these newly mentioned boundaries run very nearly along \( \pm [111] \). The dislocation character for them can be explained in a way analogous to that done for boundary AB. The boundary interface should be \( (010) \) and the Burgers vector of the dislocations in the boundaries should be \( (a/2) [010] \) so that they are essentially simple tilt boundaries also. The (essentially planar) orientations proposed for both kinds of boundaries are consistent with their appearance in Borrmann transmission topographs where the inclination of the boundaries through the crystal slice was able to be estimated from the width of the disruption images and the location of the entrance and exit surface edges of the boundaries (Boettinger, Burdette, Farabaugh & Kuriyama, 1977).

An interesting consideration relative to the dislocation character which is proposed for these boundaries is that, because of the interaction of their strain fields, the dislocations within, say, the \( (010) \) boundaries would be unstable were the orientation of the boundary surface to be changed to \( (101) \). This consideration may have contributed in an important way to determining the irregular shape of the total boundary length \( LC \) joining the otherwise straight lengths \( ML \) and \( CD \). Such an observation gives an indication of the potential significance of determining as completely as possible information about the boundary structures.

Isolated boundary segments such as those labelled \( GH \) and \( KB \) in Fig. 7 are seen to have a perfect \([010]\) rotation axis for their misorientations to the extent that no shift is observed for these boundary lengths in Fig. 5(c) as compared with 5(a) and 5(b). The directly comparable widths for the white appearance of boundary \( CD \) compared with the black appearance of \( LM \) in Fig. 4(c) indicate that misorientation contrast is responsible for these boundaries being observed. This consideration is shown most clearly for the total displacement of subgrain 4 in Fig. 4(c) for which the vector equations have been employed to show that the subgrain misorientation has a rotation axis close to but not quite at \([010]\).

The rotation axis for the misorientation of subgrains 2 and 4, as described by (21), can be determined on a stereographic projection basis, also, by a method employing measurements of the inclination of \( s \) relative to the plane of diffraction (Armstrong, 1977; Armstrong, Wu & Farabaugh, 1977). The stereographic projection method is based on determining planes which contain \( \mathbf{I} \) for each topograph and, subsequently, the intersection of these planes. Such planes are perpendicular to \( \Delta \mathbf{g} \) and contain \( \mathbf{g} \) from (12). To locate these planes, it is convenient to define an angle, \( \psi \), in terms of the magnitudes of the vector components \( s^t \) and \( s^i \) from (20a), (20b) as

\[
\psi = \cot^{-1}\left( \frac{|s^t|}{|s^i|} \right).
\]

This measured angle is related to \( \psi \) defined by

\[
\psi = \cot^{-1}\left( \frac{|\Delta \mathbf{g}^t|}{|\Delta \mathbf{g}^i|} \right),
\]

which is the angle between \( \Delta \mathbf{g} \) and \( \mathbf{v} \) given by

\[
\psi = \tan^{-1}\left( \frac{(2 \sin \theta_b) \sin (\theta_b + \chi) \tan \psi^i}{1 - 2 \sin \theta_b \sin (\theta_b + \chi)} \right),
\]

if \( \Delta e_{in} \) is negligible from (20a), (20b).

From \( \psi \) values determined on the basis of Table 1, the traces of planes containing \( \mathbf{A} \mathbf{g} \) and \( \mathbf{g}_2 \) are drawn in Fig. 8 as short segments of arc through the individual pairs of diffracting-plane normals. The rotation axis for the subgrain misorientation is determined in the figure as the intersection of the dashed great circles drawn perpendicular to these arcs. The rotation axis is shown to be \( \sim 6^\circ \) away from \([010]\) in agreement with the preceding vector determination of \( \mathbf{l} \) according to (21). To show the relative positions of the various diffracting plane normals for the two subgrains, a \( 5^\circ \) misorientation about the newly determined rotation axis was utilized in Fig. 8.

The measured misorientation of \( \Delta \theta = 1.2^\circ \) between subgrains 1 and 2, from (22) using \( \Delta \mathbf{g}^t = 0.076 \), gives dislocation separations within the boundaries of 120 and 1330 \text{Å}, respectively. The small value of even the larger computed spacing is consistent with the lack of any direct contrast effects being detected for the dislocation strain fields themselves (Armstrong & Wu, 1973).

At the greater magnification of Fig. 5(b), (c), an enhanced diffracted intensity is observed at numerous
clusters of points and short lines on the crystal surface. The enhanced intensity is probably due to the strain fields of small oxide particles which have formed on (110). Optical micrographs of such particles on the crystal surface were able to be matched with the X-ray structures. The absence of any direct contrast in Fig. 5(a) from these particles seems reasonable on this basis, too, because of the expectation that the nickel lattice displacements associated with the particles should be largely in the plane of the crystal surface. Also, at the greater magnification in Fig. 5 the boundaries of ferromagnetic domains may be observed to run vertically along ±[110] in Fig. 5(b), (c) and to run along ±[111] from boundary AF in Fig. 5(a), (c) (Kuriyama, Boettinger & Burdette, 1977). The reasonably clear observation of these boundaries gives another indication of the types of microstructural details which are resolvable with the ACT technique. In the present study, the domain boundaries provided a very useful crystallographic reference for measuring the positions and displacements of the various subgrain images.

V. Summary
A vector description is developed for determining the misorientation at boundaries between subgrains in otherwise perfect crystals as revealed by the technique of X-ray surface reflection topography. The effects of the X-ray parameters and the position of the recording film are taken into account. It is shown, for example, that subgrains having misorientations appreciably larger than the divergence within the incident (monochromatic) X-ray beam are able to reflect X-rays simultaneously if the rotation axis for the misorientation is positioned in the plane of diffraction. Topographical measurements are given for the rotation axes and angular misorientations of subgrains observed within a (110) nickel crystal surface cut from a specimen previously solidified along [010] by the Czochralski method. The crystallographic nature of the boundary interfaces is matched with the character and properties expected of dislocations being incorporated into the crystal during its growth process.

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References