On the Geometrical Conditions for Recording X-ray Topographs of Large Crystal Slices

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Abstract

Geometrical aspects of large-scale transmission X-ray topography with Kα₁ radiation have been considered. It is shown that the height of a crystal slice which can be effectively recorded is given as 

\[ H_{\text{eff}} = 2L(\Delta\lambda/\lambda)^{1/2} \]

where \(L\) is the source-to-sample distance and \(\Delta\lambda\) is the wavelength difference for the Kα doublet. A geometrical scheme termed the moving-slit simulation has been developed to examine the influence of various experimental parameters such as the widths of source and slits, the involved distances and the adjustment of the sample. The usefulness of this scheme is demonstrated experimentally.

1. Introduction

Lindegaard-Andersen & Ribe (1976), in their paper on a camera for large-scale X-ray topography, derived the condition for recording topographs of large-diameter crystal slices that the minimum source-to-crystal distance is inversely proportional to the thickness of the slice [equation (1) of their paper]. As pointed out by one of the authors of the present paper (LZ), the assumption of the derivation is not correct. In view of the extended application of X-ray topography it, therefore, seems worthwhile to reconsider the problem.

This paper describes a theoretical and experimental investigation of the geometrical conditions for recording large-scale transmission topographs.

2. Theoretical conditions

Ideal point source

We consider first the hypothetical case of diffraction of monochromatic X-rays from an ideal point source as sketched in Fig. 1. The Bragg condition is satisfied along the surface of the cone with vertex \(O\), axis \(OO'\) and semivertex angle \(90 - \theta_{B}\), where \(O\) is the ideal monochromatic point source, \(O'\) is the projection of \(O\) onto a diffracting plane \((hkl)\) and \(\theta_{B}\) is the Bragg angle. The diffraction cone cuts the lattice plane in the circular arc \(CMC'\) and the entrance surface of the crystal slice in the arc \(CPC'\). The rays along the diffraction cone may be prevented from reaching the crystal by the slit \(S\).

Referring to Fig. 1, we choose a cartesian coordinate system with origin at \(O\), \(x\) axis along the central ray \(OM\), \(y\) axis in the vertical plane through the \(x\) axis so the \(z\) axis will then be in the horizontal plane through \(O\). In this reference system the analytical expression for the diffraction cone is

\[ z^2(1 - \cot^2 \theta_{B}) - 2xz \cot \theta_{B} + y^2 = 0. \] (1)

The slit \(S\) (Fig. 1) is placed perpendicular to the central ray at the distance \(L\) from the source and the edges of the slit are assumed to be parallel to the \(y\) axis. The equation of the slit plane is simply \(x = l\), and inserting this in (1) we get

\[ s^2 \cot^2 \theta_{B} - 2sl \cot \theta_{B} + l^2 = 0. \] (2)

Fig. 1. Experimental set-up for X-ray transmission topography (schematic). Ideal point source \(O\), extended source \(OADB\), slit \(S\), crystal sample \(CMC'P\), diffracting lattice plane \((hkl)\).

Fig. 2. Intersection curves between diffraction cones and slit plane, see text.
find the curve of intersection between the diffraction cone and the slit plane:

$$y^2 = (2l \cot \theta_B)z + (\cot^2 \theta_B - 1)z^2.$$  \hspace{1cm} (2)

The positive branch ($z \geq 0$) of this hyperbola is plotted in Fig. 2 ($O_1$ curve) for the case of the 220 reflexion with Mo $K\alpha_1$ radiation in Si ($\theta_B = \theta_1 = 10.65^\circ$, $l = 230$ mm). Notice the exaggerated $z$ scale. For a given slit width, $s$, inserting $z = s$ in (2) yields the height $h = 2y$ of the diffracting beam at the slit position:

$$h = 2[2ls \cot \theta_B + (\cot^2 \theta_B - 1)s^2]^{1/2}. \hspace{1cm} (3)$$

The last term in the bracket will usually be negligible. Even with such extreme values of the parameters as $l = 100$ mm, $s = 1$ mm and $\theta_B = 5^\circ$, the error will be less than 3%. So we put:

$$h = (8ls \cot \theta_B)^{1/2}. \hspace{1cm} (4)$$

The height $H$ of the crystal slice which can be imaged is then (Fig. 1):

$$H = hL/l = (8L^2s \cot \theta_B/l)^{1/2}. \hspace{1cm} (5)$$

We now assume that the ideal point source contains two wavelengths $\lambda_1$ and $\lambda_2$, as a $K\alpha$ doublet is usually applied in X-ray topography. The corresponding Bragg angles are $\theta_1$ and $\theta_2$. With the same reference system the equation of the $\lambda_2$ diffraction cone is given by:

$$z^2 \cos (\theta_2 + \theta_1) \cos (\theta_2 - \theta_1) + zx \sin 2\theta_1 - x^2 \sin (\theta_2 + \theta_1) \sin (\theta_2 - \theta_1) - y^2 \sin^2 \theta_2 = 0. \hspace{1cm} (6)$$

Intersecting this cone with the slit plane ($x = l$) yields the $O_2$ curve plotted in Fig. 2. It cuts the $z$ axis at $z = l \tan (\theta_2 - \theta_1)$ and its shape is practically identical to that of the $O_1$ curve.

In order to avoid simultaneous diffraction of the two $K\alpha$ components, the maximum useful slit width is $s_{\text{max}} = l \tan (\theta_2 - \theta_1)$ which, inserted in (5), yields the maximum height of the crystal which can be imaged:

$$H_{\text{max}} = L[8 \cot \theta_1 \tan (\theta_2 - \theta_1)]^{1/2}. \hspace{1cm} (7)$$
Putting \( \tan(\theta_2 - \theta_1) \approx \Delta \theta \), (7) can, by application of Bragg's law, be transformed to

\[
H_{\text{max}} = L \left[ 8 \Delta \lambda / \lambda \right]^{1/2},
\]

where \( \Delta \lambda = \lambda_2 - \lambda_1 \).

Extended source

Next we consider a horizontal, rectangular source of width \( w \) and depth \( p \) indicated as \( OADB \) in Fig. 1. The coordinates of the source corners are: \( O(0,0,0), A(0,0,w) \), \( B(-p \cos \gamma, p \sin \gamma, 0) \) and \( D(-p \cos \gamma, p \sin \gamma, w) \), where \( \gamma \) is the take-off angle for the central ray. By means of (1) and (6), the analytical expressions of diffraction cones from each corner of the source are derived. Curves of intersection with the slit plane \( (x=l) \) have been calculated and plotted in Fig. 2 for \( w=0.4 \text{ mm}, p=8 \text{ mm} \) and \( \gamma=6^\circ \). The \( A_1 \) curve is simply the \( O_1 \) curve translated a distance \( w \) along the \( z \) axis. The \( B_1 \) and \( D_1 \) curves deviate slightly from the \( O_1 \) and \( A_1 \) curves, respectively. In the following we will ignore this deviation because it does not appreciably affect the maximum recordable height of a crystal slice. It does, however, strongly influence the vertical resolution of X-ray topography (Tanner, 1976).

In the following we develop a geometrical scheme to account for the influences of the widths of source and slits, the distances involved and the angular setting \( \theta \) of the crystal (\( \theta \) is the angle between the diffracting lattice planes and the central incident ray). Fig. 3(a) represents a plane perpendicular to the slit through the central ray, whereas Fig. 3(b) represents the slit plane. In Fig. 3(b), curves of intersection of this plane with the diffraction cones for a certain wavelength (e.g. \( K\alpha_1 \) radiation) are sketched for five different angular settings of the crystal. For a given angular setting, only that part of the corresponding 'diffraction area' which is within the slit can contribute to the diffraction topograph. The effect of varying the \( \theta \) setting within the diffraction range of the experimental set-up is that the diffraction area moves from position 1 to position 5. An entrance slit usually causes the width of the diffraction area to vary slightly with the angular setting of the crystal as indicated in Fig. 3(b). However, around the optimal setting at position 2, the width of the diffraction area is close to its maximum width, which in the case represented in Fig. 3 is equal to the width of the source. An alternative way of simulating the variation of the \( \theta \) setting, in the following called the moving-slit simulation, is sketched in Fig. 3(c). Here the position of the diffraction area is fixed and the slit is travelling in the opposite direction to the one in Fig. 3(b). Equivalent slit positions 1 to 5 according to the scheme in Fig. 3(b) are indicated. Contractions of the diffraction area corresponding to slit positions 2 to 5 are also indicated, whereas contractions corresponding to slit positions...
like position 1 not cutting the diffraction area are of no importance.

The effective width of the source may be restricted by the entrance slit as sketched in Fig. 4. In this case the maximum width of the diffraction area is equal to the width of the entrance slit, but otherwise the case is identical to Fig. 3.

The moving-slit simulation is an illustrative way to account for the effect of $\theta$ variation. The total power of the diffracted radiation is proportional to the diffraction area within the slit. The power contributing to the density of a traverse X-ray topograph varies in the 'vertical' direction ($y$ direction) in accordance with the variation of the width of the diffraction area within the slit. Fig. 5(a) and (b) illustrates cases of maximum diffracted power of $K\alpha_1$ radiation with and without overlap between $K\alpha_1$ and $K\alpha_2$ diffraction areas, respectively. The width of the diffraction area within the slit decreases to zero toward the upper and lower end of the slit resulting in zero density on a traverse topograph. We define the effective height, $H_{\text{eff}}$, of a crystal slice which can be recorded on the arbitrary basis that the width of the diffraction area within the slit should nowhere be less than half its maximum width. In the next section this will be shown experimentally to be a reasonable definition. In the case with overlap (Fig. 5a), $H_{\text{eff}}$ for maximum diffracted power is then obtained by inserting $s = \frac{1}{2}s_{\text{max}}$ in (5). Comparison with (7) and (8) yields:

$$H_{\text{eff}} = 2^{-1/2}H_{\text{max}} = 2(\Delta \lambda/\lambda)^{1/2}.$$  (9)

In the case without overlap (Fig. 5b), $H_{\text{eff}}$ is obtained by inserting a value $s > \frac{1}{2}s_{\text{max}}$ yielding $H_{\text{eff}} > 2(\Delta \lambda/\lambda)^{1/2}$. The maximum value of $H_{\text{eff}} \approx H_{\text{max}}$ can be obtained either with a wide source and a narrow exit slit or vice versa, provided the vertical divergence of the incident beam is sufficiently large.

In the following experimental section, the usefulness of the moving-slit simulation will be demonstrated.

![Fig. 7](attachment:fig7.png)

**Fig. 7.** Moving-slit simulation of the experimental conditions corresponding to Fig. 6(a) (a) and to Fig. 6(b) (b). Steps of 30' are indicated and a few slit positions are shown.

![Fig. 8](attachment:fig8.png)

**Fig. 8.** Variation of intensity with take-off angle (from Azaroff, 1968).

![Fig. 9](attachment:fig9.png)

**Fig. 9.** Section topographs, obtained by Mo $K\alpha$, of the 222 reflexion. Widths of entrance and exit slits were 0.2 mm and 0.1 mm, respectively. (a) Diffracting planes tilted in steps of 0.5° against the exit slit from -3° to +3°. (b) Series obtained at constant tilt angle of -3° by changing $\theta$ in steps of 30°.

![Fig. 10](attachment:fig10.png)

**Fig. 10.** Moving-slit simulation of the experimental results shown in Fig. 9. Two slit positions with different $\theta$ angle with the same tilt angle of -3° are shown.
3. Experiments

An experimental set-up like the one sketched in Fig. 1 was used with an additional entrance slit as indicated in Figs. 3(a) and 4(a). Fine-focus X-ray tubes with Mo and Cu anodes, respectively, were used. The horizontal source dimensions were \( p = 8 \text{ mm} \) and \( w = 0.4 \text{ mm} \). A dislocation-free Si slice of 63 mm diameter served as a sample crystal. The vertical divergence of the radiation passing the exit slit was about 11° as a result of take-off angles varying from 0° to 11.5°. The heights of the primary beam at the position of the slit (\( L = 230 \text{ mm} \)) and the sample (\( L = 300 \text{ mm} \)) were 44.2 and 57.6 mm, respectively.

Fig. 6 shows two series of section topographs and a traverse topograph, obtained by Mo \( K\alpha \), of the 220 reflexion of the Si sample. Different combinations of slits were used in the two series of section topographs and successive topographs were recorded by increasing the angle \( \theta \) in steps of 30°. The angular steps correspond to steps \( \Delta z = 1 \Delta \theta = 0.034 \text{ mm} \) in the moving-slit simulation (Fig. 7). The section topographs marked \( vv \) in Fig. 6(a) and (b) were obtained by the optimal slit positions marked \( vv \) in Fig. 7(a) and (b), respectively. The traverse topograph shown in Fig. 6(c) was recorded under the same conditions as the \( vv \) section topograph in Fig. 6(b). Two factors contribute to the vertical photographic density distribution on the traverse topograph, namely the width of the diffraction area within the slit (Fig. 7b) and the variation of intensity with take-off angle of the primary beam. The latter has been considered by Azaroff (1968) and the results of some measurements are shown in Fig. 8. The diffracted power giving rise to the photographic density on the traverse topograph is the product of the two factors. \( H_{\text{max}} \) and \( H_{\text{eff}} \) are both indicated on Figs. 6(c) and 7(b).

Although the vertical divergence of the primary beam is too small for recording \( H_{\text{max}} \), Fig. 6(c) illustrates that the proposed definition of \( H_{\text{eff}} \) is reasonable. In the present case the take-off angle of the upper end of \( H_{\text{eff}} \) was 2.5°, where, according to Fig. 8, the intensity of the primary beam is 70% of the maximum intensity. The definition of \( H_{\text{eff}} \) is probably satisfactory down to an upper take-off angle of 1°, where the intensity is about 40% of the maximum intensity.

The effect of misalignment of the sample by tilting the diffracting lattice planes against the slit was also investigated. The results of an experiment in which a series of section topographs were recorded by successively tilting the sample crystal in steps of 0.5° from −3 to +3° are shown in Fig. 9(a). In the moving-slit simulation this misalignment can equally be represented by tilting the slit as indicated in Fig. 10. Because of the exaggerated \( z \) scale, the tilt angle is very

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**Fig. 11.** Section topographs, obtained by Cu \( K\alpha \), of the 422 reflexion. (a) and (b) show series obtained in steps of \( \Delta \theta = 50° \). Widths of entrance and exit slits, respectively: (a) 0.4 mm, 0.2 mm; (b) 1.0 mm, 0.6 mm. Take-off angle of central ray about 6°. (c) Diffracting planes tilted in steps of 1° against the exit slit from −6 to +6°. Slit widths 0.2 mm, 0.2 mm.
much enlarged. At tilt angles greater than about 1° the section topograph splits into two parts which, according to the moving-slit simulation, are due to simultaneous diffraction of the \( \alpha_1 \) and \( \alpha_2 \) components. With a fixed tilt angle of \(-3^\circ\), a series of section topographs were recorded by changing the \( \theta \) angle in steps of 30°. The results of this, which are shown in Fig. 9(b), give a vivid impression of the moving-slit simulation.

Two series of section topographs and a series of tilted topographs, obtained with Cu \( K\alpha \) 224 reflexions of the Si sample crystal are shown in Fig. 11. Each series of section topographs was recorded in angular steps \( \Delta \theta = 50^\circ \) and the series of tilted topographs in steps of 1° of the tilt angle from \(-6^\circ \) to \(+6^\circ \). Because the relative difference in wavelength between \( K\alpha_1 \) and \( K\alpha_2 \) is smaller for Cu than for Mo (see Table 1), the crystal height which can be depicted with Cu \( K\alpha_2 \) radiation is smaller than the height which can be depicted with Mo \( K\alpha_1 \) radiation. The slit positions corresponding to the section topographs marked \( vv \) recorded with a narrow exit slit (Fig. 11(a)) and a wide slit (Fig. 11(b)) are indicated in Fig. 12. Some of the tilt angles used in recording the tilted topographs (Fig. 11(c)) are also indicated in Fig. 12.

### 4. Discussion

Values of the important parameters in large-scale topography are listed in Table 1 for some usual radiations. The maximum take-off angle of most diffraction tubes is between 10° and 12°. Take-off angles smaller than about 1° are not very useful in large-scale topography because of the low intensity. According to Table 1 the vertical divergence will therefore be too small for recording \( H_{\text{max}} \) with Mo \( K\alpha_1 \) and Ag \( K\alpha_1 \) radiation. In other words, the whole vertical divergence of sufficiently intensive radiation from Mo and Ag diffraction tubes can be utilized in large-scale topography.

**Table 1. Parameters in large-scale transmission topography**

<table>
<thead>
<tr>
<th>Radiation</th>
<th>Cr ( K\alpha )</th>
<th>Fe ( K\alpha )</th>
<th>Cu ( K\alpha )</th>
<th>Mo ( K\alpha )</th>
<th>Ag ( K\alpha )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 10^3 \Delta \lambda )</td>
<td>1 70</td>
<td>2 04</td>
<td>2 48</td>
<td>6 04</td>
<td>7 89</td>
</tr>
<tr>
<td>( H_{\text{max}} ) (mm)</td>
<td>35</td>
<td>38</td>
<td>42</td>
<td>66</td>
<td>75</td>
</tr>
<tr>
<td>( \Delta \phi_{\text{max}} ) (°)</td>
<td>6 7</td>
<td>7 3</td>
<td>8 1</td>
<td>12 6</td>
<td>14 4</td>
</tr>
<tr>
<td>( H_{\text{int}} ) (mm)</td>
<td>25</td>
<td>27</td>
<td>30</td>
<td>47</td>
<td>53</td>
</tr>
<tr>
<td>( \Delta \phi_{\text{int}} ) (°)</td>
<td>4 7</td>
<td>5 2</td>
<td>5 7</td>
<td>8 9</td>
<td>10 2</td>
</tr>
</tbody>
</table>

### 5. Conclusion

Geometrical parameters involved in X-ray transmission topography have been investigated, emphasizing the maximum height of a crystal slice which can be imaged.

A moving-slit simulation of variations in the angular setting and tilt of the crystal sample has been developed. This simulation is shown to be of great use in evaluating the results which may be obtained by X-ray transmission topography.

**References**

