A quick and simple method for orienting cubic single crystals from Laue back-reflection photographs

Orienting single crystals by Laue back-reflection photographs is a universally applied method, because of the ease of sample preparation and speed of taking the photograph. The method of analyzing such photographs by use of the Greninger chart and the Wulff net is well described in standard texts, e.g. Cullity (1978), Azaroff (1968), Schwartz (1977). After some practice in analysis, an investigator can determine the orientation with fair accuracy by inspection, but must follow the procedure and trace conics of diffraction spots to ensure an accurate orientation. In our experience, neophytes find the standard method burdensome to learn initially and tedious to apply subsequently. Accordingly, we offer a simplified approach for orienting a cubic crystal, which also has the advantage of being rapid.

It is necessary to recall certain properties related to the Laue back-reflection method. Firstly, all of the planes of one zone reflect X-ray beams which lie on the surface of a zone, the axis of which is the zone axis. Therefore, the diffraction spots from these planes appearing on a back-reflection photograph lie on hyperbolas or straight lines, and the distance of any hyperbola from the center of the film is a measure of the inclination of the zone axis from the vertical. Fig. 1 shows schematically the relationship between the spot, the zone axis and planes in this zone. As shown in Fig. 1, \( \gamma \) is the angle between the zone axis and the incident beam and \( K \) is a reflected spot of the zone. The normal to this reflecting plane will intersect the film at \( M \). As is well known, the orientation of the plane normal in space can be described by its angular coordinates \( \gamma \) and \( \delta \) as shown in Fig. 1. From this figure it is clear that \( \gamma \) is equal to \( 90^\circ - \phi \). The Greninger chart provides directly the \( \gamma \) and \( \delta \) coordinates corresponding to any diffraction spot. The hyperbolas drawn on this chart, running from left to right, are curves of constant \( \gamma \), and one of these curves corresponds to the locus of diffraction spots from planes of a zone, the axis of which is tilted away from the plane of the film by an angle \( \gamma \). One row of such spots is shown in Fig. 1.

The quick method that we propose here for the determination of a crystal's orientation requires three simple steps:

1. Identify the conic corresponding to 001 and 011; find the \( \gamma \) value of that zone axis, and one other angle; and
2. Apply these results to a simple equation. The details are as follows.

Because of the high symmetry of the cubic system, the standard triangle is usually used to indicate a specimen's orientation. Let us arbitrarily consider \( hkl \) the orientation of a single crystal in the standard triangle 001-011-111. The center of the Laue photograph corresponds to this orientation, so if the Greninger chart is placed on the film, as shown in Fig. 2, then the angle, \( \delta \), between spot \( C \) (which is the 'reflection' of 001) and spot \( B \) (which is the reflection of 001) can be measured. The line of spots \( C, B, \ldots \) corresponds to the 001-011 zone, and spot \( C \) is easily identified by its fourfold symmetry. The angle between spot \( A \) (which is \( hkl \)) and spot \( B \) 001 is \( \gamma \). Clearly, spot \( B \) 001 might not exist because the corresponding structure factor might be zero. However, its location is securely identified by the vertical on the Greninger chart. The proof that the Miller indices of spot \( B \) should be \( 001 \) can be seen as follows. Since the 001-011 conic has zone axis 100, the angle \( \phi \), which is the angle between the zone axis and the crystal orientation, can be obtained from

\[
\cos \phi = \frac{h}{(h^2 + k^2 + l^2)^{1/2}} = \sin \gamma.
\]

If we assume spot \( B \) to have the Miller indices \( 001 \), the angle, \( \theta \), between \( B \) and \( A \) is given by

\[
\cos \theta = \frac{k^2 + l^2}{(h^2 + k^2 + l^2)^{1/2}} = \cos \delta \sin \gamma.
\]

By adding the squares of \( \sin \gamma \) and \( \cos \theta \), one sees that \( \gamma = \theta \). Therefore, since \( B \) lies at the intersection of the Greninger chart vertical, for which \( \delta = 0 \), and the 001-011 conic, then \( B \) has indices \( 001 \).

Rearrangement of (1) yields

\[
\frac{h}{k^2 + l^2} = \tan^2 \gamma. \tag{3}
\]

Since \( \delta \) corresponds to the angle between \( B \) and \( C \),

\[
\cos \delta = \frac{l}{(k^2 + l^2)^{1/2}}. \tag{4}
\]

The indices of the pole \( hkl \) can be simplified by normalization, written as \( \tilde{h} \tilde{k} \tilde{l} \); with this result and by solving (3) and (4) we find

\[
\tilde{l} = \cos \delta \cot \gamma
\]

and

\[
\tilde{k} = \sin \delta \cot \gamma.
\]

and \( \tilde{h} \) is equal to \( \tilde{1} \) by definition. Thus the Miller indices of the specimen orientation are identified.

As outlined above, the method for orientating a crystal proposed here is seen to consist of identifying the 001-011 conic, laying the Greninger chart on the photograph, reading off the values of \( \gamma \) and \( \delta \) and then employing (5). The method obviously can be generalized to other crystal systems, and it takes about 30 s to analyze a result. It is much quicker and more convenient than two previously published numerical approaches to solving Laue patterns (Huang, Christensen & Block, 1971; Lange & McKinstry, 1968).

This material is based upon work supported by the National Science Foundation, MRL program, Grant No. DMR 79-23647. We are grateful for this support, and also to J. B. Cohen for his critical comments.

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(Received 21 April 1981; accepted 28 May 1981)