The fragments were shifted by (0·1 0·0 0·2) and input to the various calculations. Table 3 gives the sequence numbers of the peaks that indicate the correct position of the fragments.

Comments on the calculations and discussion of the results

(1) VS. The programs were executed using a variety of selection parameters to find the best results (*a posteriori*).

(2) $Q(\mathbf{t})$. The function $\langle |E|^2 |E_p|^2 \rangle$ was calculated using various $|E|$ cut-off values; the best results were obtained using $|E| > 1{\cdot}0$.

(3) *TRADIR*. The function uses difference structure factors which are refined by the *DIRDIF* procedure in space group $P1$ (see Beurskens, van den Hark & Beurskens, 1976), with three or four refinement cycles.

The use of the VS programs requires some skill which, in the present test case, leads to slightly better results. On the other hand, computational aspects often speak in favor of reciprocal-space procedures.

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A Simple Computer Method for the Orientation of Single Crystals of Any Structure Using Laue Back-Reflection X-ray Photographs

BY C. A. CORNELIUS

Department of Physics, Monash University, Clayton, Victoria 3168, *Australia**

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Abstract

A simple computer program for the simulation and analysis of X-ray back-reflection Laue photographs of a single crystal with any structure and orientation has been developed in Fortran IV. Comparison of computer plots of the calculated patterns with the photographs enables rapid identification of approximate orientation. The program may ultimately be used to index an orientation from the identification of at least three spots from the photographs. The procedure incorporating use of the program requires only minimal knowledge of crystallography or computer methods.

1. Introduction

Orientation of single crystals or indexing of crystal faces *via* the Laue back-reflection X-ray technique can be a difficult and very time-consuming task. This is particularly the case when the crystal structure has symmetry lower than cubic, or orientations with low-symmetry directions are required.

Computer programs have been published by Krahl-

* Present address: Department of Physics, University of Southampton, Southampton SO9 5NH, England.

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Urban, Butz & Preuss (1973), Christiansen, Gerward & Alstrup (1975) and Preuss (1979) which simulate to various degrees the reflections expected for Laue back-reflection and transmission X-ray photographs.

The procedure due to Christiansen *et al.* (1975) is a precision technique and can only be used for cubic symmetry and monochromatic radiation. The Krahl-Urban *et al.* (1973) program is designed for 'white' radiation and any crystal structure. However, apart from 'on–off' reflection intensities, no graduation in intensity appears to be calculated. The Preuss (1979) program calculates and plots Laue-spot angular relationships and intensities and also produces a stereographic projection. The structure factors must be either taken from a ten-structure-factor library, which is part of the program, or read in *via* cards. In addition, the Krahl-Urban *et al.* (1973) and Preuss (1979) programs can, from the input of data for three indexed spots, calculate the crystal direction which is anti-parallel to the X-ray beam.

To assist those workers with no computing facilities, Preuss, Krahl-Urban & Butz (1974) have published a large number of plotted Laue back-reflection diagrams. Plots for only the most important crystal systems and orientations are present.

A Fortran IV computer program entitled *BACK-LAUE* has been constructed which allows simulation of both position and intensity of spots on the Laue back-reflection X-ray photograph of a single crystal with any structure (including alloys) and of any orientation with respect to the X-ray beam.

In addition, using the indices and (x,y) coordinates in centimetres of a spot relative to the centre of the pattern, the program may be used to calculate either the crystal direction which is antiparallel to the X-ray beam, or the Miller indices of the plane normal to the X-ray beam. In this calculation, account is taken of the possibility of an inaccurately known specimen–film separation.

Plotting facilities which were available on the Burrough's B6700, on which the program was developed, have enabled the computed pattern to be plotted to the same scale as the photograph. Orientation of low-symmetry directions to an accuracy better than 0·5° is therefore easily accomplished by moving the crystal so that the spots of the Laue photograph line up with those of the simulation. By use of a Greninger chart, the computed pattern can also be used to determine quickly the angular relationships between the directions.

2. The program

2.1. *Back-reflection simulation*

Apart from a set of variables controlling output and mode of operation, only the following information is required.

(*a*) X-ray tube voltage.
(*b*) Specimen–film separation.
(*c*) Maximum spot-to-centre distance.
(*d*) Lattice parameters for the unit cell.
(*e*) The required scan range for each Miller index.
(*f*) The crystal orientation for which a simulation is required. This may be in terms of either a direction antiparallel to the X-ray beam or a plane normal to it.
(*g*) A list of data which includes the following for the atom sites which are occupied in the same way:
(i) atomic number of the atom;
(ii) the number of such sites;
(iii) the probability (in per cent) of finding the atom at these sites;
(iv) the coordinates of each site in this set.

The program includes copious comments concerning execution and the logic behind each step. In addition, possible incompatibilities between Burrough's Fortran IV and other versions of the language are also indicated.

2.2. *Calculation of orientation*

With the program, a catalogue of Laue patterns is generated for a few high-symmetry directions. The one for the orientation closest to that of the crystal is used to determine the indices of at least three spots on the photograph. The Miller indices and coordinates, (x,y), relative to the centre of the photograph for each of these spots, together with the unit-cell parameters are then used to calculate the most likely:

(*a*) specimen–film separation in centimetres;
(*b*) direction anti-parallel to the X-ray beam in terms of both real- and reciprocal-space vectors.

To enhance statistical accuracy, all possible combinations of three indexed spots are used. An estimate of the error in the determined orientation is also calculated.

3. Method

Calculation of spot position and intensity for a Laue back-reflection X-ray photograph can be reduced to the following:

(1) Definition of a coordinate representation for real and reciprocal space and the plane of the Laue photograph.
(2) Calculation of the X-ray beam scattering vector and spot position for a particular crystal plane.
(3) Calculation of the structure factor for a particular plane and other factors related to intensity.

3.1. *Coordinate representation*

For simplicity, the primitive crystal directions are referred to a set of rectangular Cartesian axes with equal scale units of length (Fig. 1)

$$\begin{aligned}\mathbf{a}_1 &= a_1\,\mathbf{i}\\ \mathbf{a}_2 &= a_2(\cos\gamma\mathbf{i} + \sin\gamma\mathbf{j})\\ \mathbf{a}_3 &= a_{3x}\,\mathbf{i} + a_{3y}\,\mathbf{j} + a_{3z}\,\mathbf{k},\end{aligned}$$

where

$$\begin{aligned}a_{3x} &= a_3\cos\beta\\ a_{3y} &= a_3(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma\\ a_{3z} &= (a_3^2 - a_{3x}^2 - a_{3y}^2)^{1/2}\end{aligned} \tag{3.1}$$

and a_1, a_2 and a_3 are the lattice parameters. **i**, **j** and **k** are the usual Cartesian unit vectors with respect to the x-, y- and z-axis respectively.

From (3.1), the reciprocal-lattice axes may be easily deduced from the conventional relationships

$$\mathbf{b}_i = (\mathbf{a}_j \times \mathbf{a}_k)/V, \tag{3.2}$$

where V is the volume of the real-space unit cell and the i, j, k obey the usual cyclic conventions.

The direction antiparallel to the incident X-ray beam may be expressed as a real- or reciprocal-space vector as follows:

$$\begin{aligned}\mathbf{S}_0 &= S_1\,\mathbf{a}_1 + S_2\,\mathbf{a}_2 + S_3\,\mathbf{a}_3 \quad \text{(real space)}\\ \mathbf{S}_0 &= S_1^*\,\mathbf{b}_1 + S_2^*\,\mathbf{b}_2 + \mathbf{S}_3^*\,\mathbf{b}_3 \quad \text{(reciprocal space)},\end{aligned} \tag{3.3}$$

where S_1, S_2 and S_3 are the real-space primitive-lattice vector components and S_1^*, S_2^* and S_3^* are the Miller indices of the plane normal to the X-ray beam direction.

To ensure independence of the procedure from the Cartesian representation, a coordinate system within the plane of the Laue photograph is used. It is defined so that the vertical or y axis of the pattern is coincident with a projection of either the $\mathbf{a}_2$ or $\mathbf{a}_3$ axis, whichever is closest to the plane of the photograph. This projection is designated $\mathbf{C}_p$. An x axis, designated **t**, may then be defined as

$$\mathbf{t} = \mathbf{C}_p \times \mathbf{S}_0. \tag{3.4}$$

Both **t** and $\mathbf{C}_p$ are converted to real-space vectors by the program so that the relationship between the photograph and real-space axes may be easily seen.

3.2. *Spot position*

Defining the normal to the (hkl) plane in the usual reciprocal-space fashion, the position vector of a spot on the Laue photograph will be (Fig. 2)

$$\mathbf{S}_L = [2\cos\theta'\,\hat{\mathbf{p}} - \hat{\mathbf{S}}_0]/\cos 2\theta' - \hat{\mathbf{S}}_0, \tag{3.5}$$

where $\hat{}$ indicates a unit vector and θ' is the complement of the Bragg angle for the plane and is calculated from the dot product of the unit planar normal $\hat{\mathbf{p}}$ and $\hat{\mathbf{S}}_0$.

The x and y coordinates of the spot follow from the dot product of $\mathbf{S}_L$ with the vectors **t** and $\mathbf{C}_p$. The vector $\mathbf{S}_L$ is appropriately scaled according to the specimen–film separation (d). Also available from this data is the azimuthal angle of the spot on the photograph with respect to **t**. Thus, stereographic projections can also be produced if required.

3.3. *Spot intensity*

The intensity of a back-reflection spot may be written

$$I = \sum_{i=1}^{m} B(\lambda,\theta)|F(h_i k_i l_i)|^2, \tag{3.6}$$

where m is the number of planes contributing to a particular reflection and $F(h_i k_i l_i)$ is the structure factor for the $(h_i k_i l_i)$ plane. $B(\lambda,\theta)$ is an expression due to Preuss (1979) which incorporates corrections to

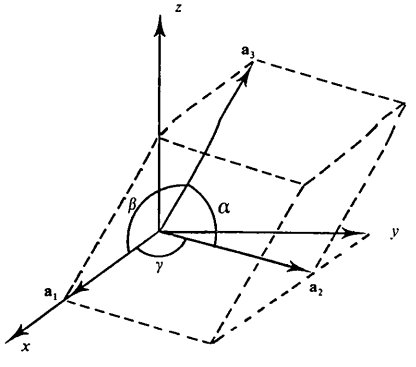


Fig. 1. Orientation of the crystallographic unit cell with respect to the Cartesian coordinate system.

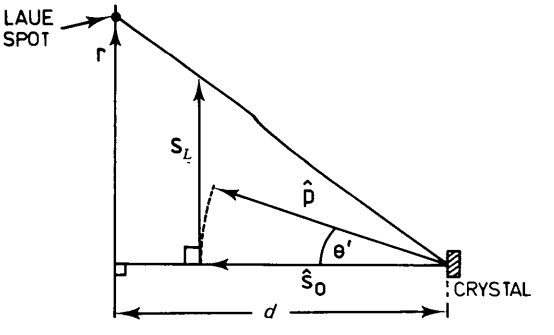


Fig. 2. Representation of the position of a Laue spot in terms of the unit planar normal $\hat{\mathbf{p}}$ and unit antiparallel X-ray direction $\hat{\mathbf{S}}_0$. The vector $\mathbf{S}_L$ is scaled by the specimen–film separation d to produce the spot position vector **r** in the photographic plane.

intensity which depend on the X-ray wavelength, λ, and Bragg angle, θ.

The m planes contributing to a particular reflection are deduced very simply by scanning the appropriate ranges of Miller indices. The individual reflection intensity is calculated for those planes which produce a spot within the physical dimensions of the photograph. A cumulative intensity is then calculated for those reflections which are too close to be resolved. For practical purposes, it was considered that spots within 0·2 mm of each other were not resolved. The printed output clearly indicates the actual positions of those spots considered by the program to be unresolved.

For reasons of multiplicity, it is important that the ranges of Miller indices input by the operator are sufficiently large. However, the program considerably reduces this guess-work by solving for the range of the Miller index corresponding to the reciprocal axis nearest to $\mathbf{S}_0$ (hereinafter called the third Miller index). The conditions for solution are that, given two Miller indices, the maximum and minimum values of the third are, respectively, such that a planar normal

(i) does not make an angle with $\mathbf{S}_0$ greater than half the maximum scattering angle recorded by the film (δ_{max}) and

(ii) does not make an angle of less than δ_{min} with the reciprocal axis corresponding to the third Miller index. Case (ii) is only important when the reciprocal axis corresponding to the third Miller index actually produces a reflection recorded by the film. The solution for the third index (m_3) is obtained by solving

$$\mathbf{p}(m_1,m_2,m_3).\mathbf{S}_0 = |\mathbf{p}(m_1,m_2,m_3)||\mathbf{S}_0| \cos \delta_{max}, \quad (3.7a)$$

for case (i), and for case (ii)

$$\mathbf{p}(m_1,m_2,m_3).\mathbf{b}_3 = |\mathbf{p}(m_1,m_2,m_3)||\mathbf{b}_3| \cos \delta_{min}, \quad (3.7b)$$

where $\mathbf{b}_3$ is the reciprocal axis corresponding to m_3 and is only the true $\mathbf{b}_3$ given by (3.2) when m_3 and l are equivalent. The solution to either of (3.7) is of the form

$$m_3 = (f_1 m_1 + f_2 m_2) \pm (f_{11} m_1^2 + f_{22} m_2^2 + f_{12} m_1 m_2)^{1/2}, \quad (3.8)$$

where the f_i and f_{ij} are complicated constants dependent only upon crystal symmetry and orientation.

The behaviour of the $B(\lambda,\theta)$ (Preuss, 1979) has been calculated as a function of λ and θ for a disk-like specimen. The behaviour of B as a function of θ indicates that no reflections of reasonable intensity are to be expected for a scattering angle greater than approximately 70°.

To retain complete generality, the structure factors are deduced from the usual relationship (here $K = \sin\theta/\lambda$)

$$F(h,k,l) = \sum_{p=1}^{n} A_p(K) \sum_{j=1}^{m_p} \exp i[hu_{pj} + kv_{pj} + lw_{pj}], \quad (3.9)$$

where n is the number of different atom types, $A_p(K)$ and m_p are respectively the atomic scattering factor and number of atoms of the pth type, and $[u_{pj},v_{pj},w_{pj}]$ is the unit-cell position of the jth atom of type p.

The atomic scattering factors are generated *via* the atomic number. The scattering factors for the majority of atoms in the Periodic Table have been calculated and fitted by Doyle & Turner (1968) to a sum of exponentials of the form

$$A(K) = \sum_{i=1}^{4} a_i \exp(b_i K^2) + c, \quad (3.10)$$

where c is a constant for each atom type. The a_i, b_i and c are stored within the program and called up *via* the atomic number. Only neutral atoms are included. If a set of coefficients is not available for a particular atom, the program terminates with the generation of a diagnostic.

For cases which fall into the latter category, the atomic scattering factors (from *International Tables for X-ray Crystallography*, 1965) may be fitted with a non-linear least-squares curve-fitting routine from Bevington (1969). For the majority of cases, the coefficients of Doyle & Turner (1968) are sufficient. However, some additional coefficients have been determined and are included. To reduce output of data for reflections of trivial intensity, a minimum intensity value is used to discriminate when printing or plotting. Since the program stores all reflection data in pack files rather than using large arrays or vast amounts of core, it may be run for the same orientation as many times as required without starting from the beginning and regenerating the same data. This facilitates alteration of the discriminator to increase or decrease the number of reflections in the output. In addition, the program imposes an upper limit on the number of reflections printed or plotted. This may also be altered as required without recompilation or rerunning the program from the beginning.

3.4. *Determination of orientation*

When three Laue spots have been indexed using computed patterns for orientations close to that of the specimen, another part of the program may be used to deduce the exact orientation. If more spots have been indexed, the orientation of the specimen is calculated using all possible combinations of three spots. The real- and reciprocal-space vectors antiparallel to the X-ray beam direction are then obtained by averaging the results for all combinations and deducing the standard deviation to indicate uncertainty. As indicated in § (2.2), the most likely specimen–film separation is calculated and used in all determinations.

With three spots, the procedure is as follows. The planar normal (which bisects the scattering angle), corresponding to each spot, may be written

$$\mathbf{n}_i = h_i \mathbf{b}_1 + k_i \mathbf{b}_2 + l_i \mathbf{b}_3 \ (i = 1, 2, 3). \quad (3.11)$$

If $\mathbf{S}_0$ is a vector in real space representing the desired orientation, then the dot product of $\mathbf{S}_0$ with each of the $\mathbf{n}_i$ will produce an estimate of half the scattering angle as measured from the Laue photograph using the (x_i,y_i) coordinates of each spot relative to the centre of the photograph (in centimetres). The calculation of this angle is explicitly dependent on the value of the specimen–film separation (d).

On account of the conventional Laue set-up, a precise measurement of d is not generally possible. An estimate is therefore deduced from a fit to the theoretical internormal angles for the indexed spots. A range of separations is assumed and the value which results in the least deviation of the measured internormal angles from those observed is assumed to be the most likely.

With the most probable value of d, the three indexed spots give the following three equations expressed in terms of the unknown vector $\mathbf{S}_0$.

$$\mathbf{n}_i.\mathbf{S}_0 = |\mathbf{n}_i||\mathbf{S}_0| \cos \delta_i \, (i = 1, 2, 3), \qquad (3.12)$$

where the δ_i are the angles between $\mathbf{S}_0$ and the $\mathbf{n}_i$ respectively.

Since the $\mathbf{n}_i$ and $\mathbf{S}_0$ are reciprocal- and real-space vectors respectively, by assuming $\mathbf{S}_0$ to be normalized

$$h_i S_{01} + k_i S_{02} + l_i S_{03} = |\mathbf{n}_i| \cos \delta_i \, (i = 1, 2, 3), \quad (3.13)$$

where the S_{0j} are the three real-space components of $\mathbf{S}_0$. Equations (3.13) may be solved for the S_{0j} by inversion of the 3×3 matrix of the h_i, k_i and l_i and post-multiplication of this inverse with the $|\mathbf{n}_i| \cos \delta_i$ vector. The uncertainty in the resultant real-space vector components as a result of the uncertainty in d may be calculated from the $\cos \delta_i$. The components of $\mathbf{S}_0$ are calculated for each set of three planes, and then the average values are calculated and printed. As an aid to interpretation, $\mathbf{S}_0$ is also converted to its reciprocal-space equivalent and printed along with the real-space form. The angles of the primitive real- and reciprocal-space vectors with respect to the film coordinate system are also calculated.

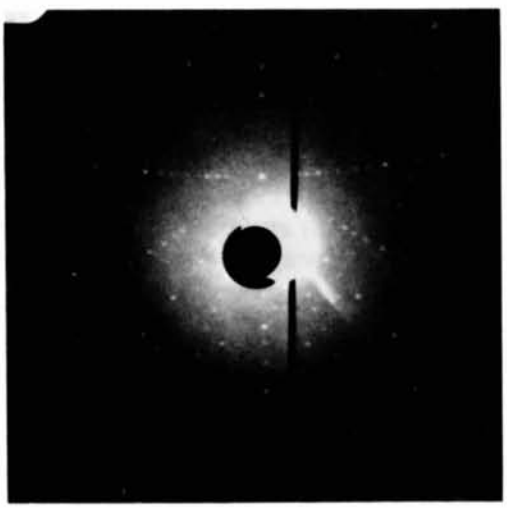
4. The procedure and the test case

Orientation determination for a crystal of monoclinic caesium dihydrogen phosphate (CDP) is used here as an example of the procedure. The Laue back-reflection photograph of the orientation which was determined is shown in Fig. 3(*a*). The X-ray tube voltage was 20 kV. The vertical line which is just to the right of centre is an artifact of the film holder designed to ensure correct viewing of the film.

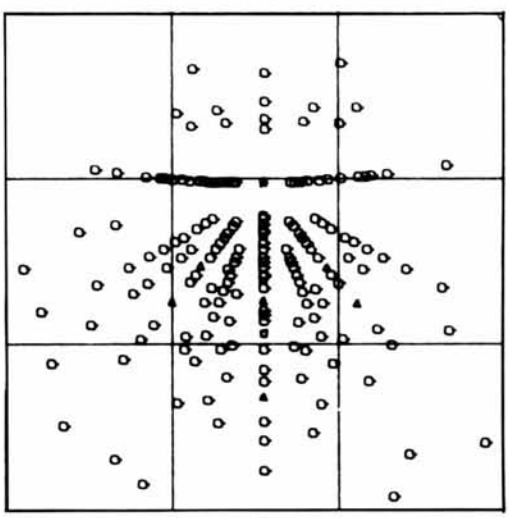
With the program and the information indicated in § 2.1 (lattice parameters and atom positions were obtained from Vesu & Kobayashi, 1976), a catalogue of Laue patterns was generated for the X-ray beam propagation vector antiparallel to the $\mathbf{b}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ axes. Visual comparison of these plots with Fig. 3(*a*) indicated that the orientation of the disk-shaped specimen was with the $\mathbf{b}_1$ axis making the least angle with the X-ray beam.

A Greninger chart was used to obtain an approximate match of the observed interspot angles with those calculated. The correspondence of these angles was naturally subject to the specimen–film separation.

The indices and positions of nine of the brightest spots were fed back into the program and the true real-space direction antiparallel to the X-ray beam



(*a*)



(*b*)

Fig. 3.(*a*) X-ray back-reflection Laue photograph for caesium dihydrogen phosphate. (*b*) Simulated pattern for the [6·28, −0·16, 1·00] crystal direction antiparallel to the X-ray beam. Crystallographic vectors corresponding to the horizontal and vertical reference directions are indicated in the printout.

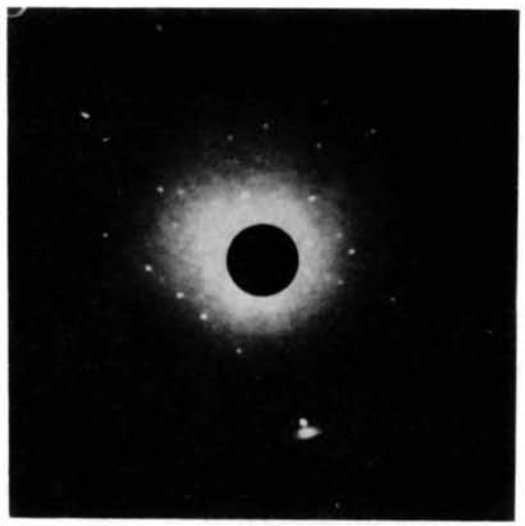
propagation vector was deduced to be [6·28(0·01), −0·16(0·03), 1·00(0·05)], where the standard deviation of the components is indicated in the round brackets. The experimental specimen–film separation was found to be (3·02 ± 0·02) cm.

As a final check, this vector and specimen–film separation were used by the program to calculate a Laue pattern which is displayed in Fig. 3(*b*). The different symbols represent a crude visual relative intensity gradation with the following meaning: * 80–100; ◊ 60–79; □ 40–59; △ 20–39; ○ I_{min}–19; where I_{min} is the value of the minimum intensity discriminator.

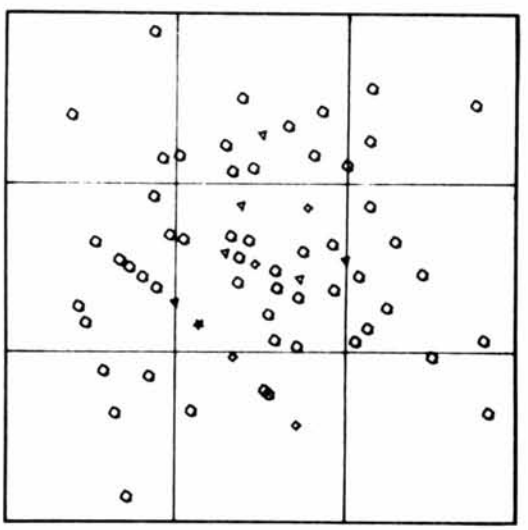
The agreement between Figs. 3(*a*) and 3(*b*) is extremely good as far as position is concerned for those spots which are present on both figures. Intensity, however, is a problem.

Fig. 3(*b*) was generated with a relative intensity discriminator of four. Whilst correctly indicating the most intense spots, the program indicates that considerably more contrast between spots should be visible. Unfortunately, this effect persists to the point of exclusion for some spots which should obviously be present when located in Fig. 3(*a*). This is particularly true for spots of relatively high scattering angle (*i.e.* greater than about 35°).

Subsequent runs of the program with a lower discriminator, while permitting more spots to be plotted than are present in Fig. 3(*b*) (discounting those plotted near the hole), allow indexing of every spot and,



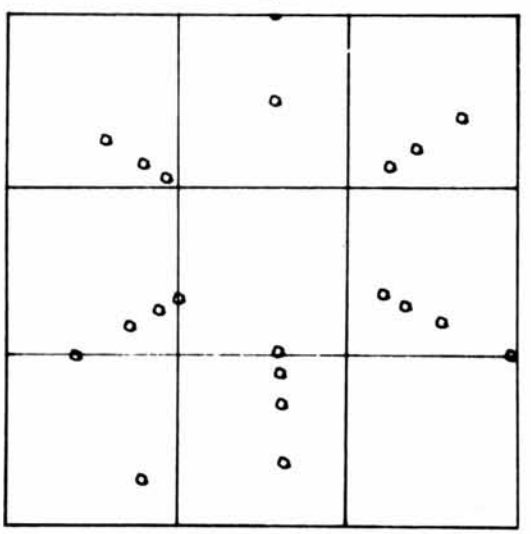
(*a*)



(*b*)

Fig. 4.(*a*) X-ray back-reflection Laue photograph for V_3Si (cubic) with [421] approximately antiparallel to the X-ray beam direction. (*b*) Simulated pattern with [4·313, 2·215, 1] antiparallel to the X-ray beam direction.

(*a*)

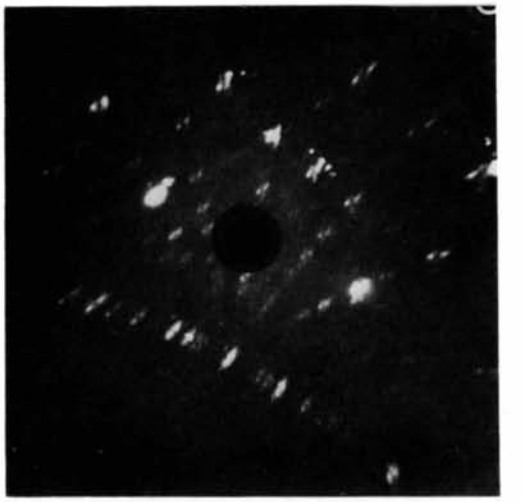


(*b*)

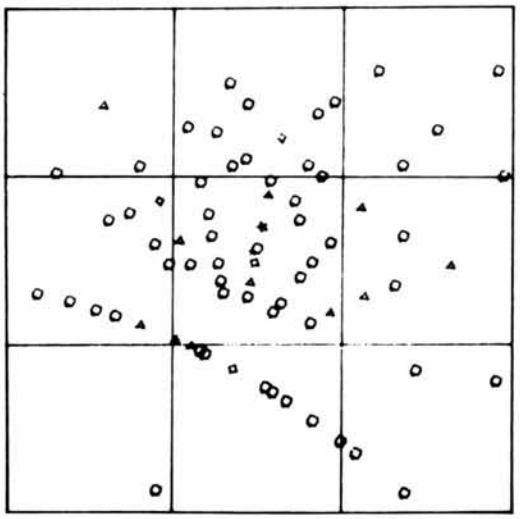
Fig. 5.(*a*) X-ray back-reflection Laue photograph for zinc (hexagonal) with [001] approximately antiparallel to the X-ray beam direction. (*b*) Simulated pattern with [0·202, −1, 7·127] antiparallel to the X-ray beam direction.

theoretically, an extremely accurate orientation determination.

At present this problem remains unsolved since there are many variables affecting the calculation and measurement of intensity, not the least of which is the physical condition and geometry of the specimen and the orientation of its cleavage faces with respect to the X-ray beam. In fact, a consideration of these latter two factors may render invalid the application of some of the factors contained in the $B(\lambda,\theta)$ in (3.6). Indeed the actual recording of intensity by the film may also be a problem.



(*a*)



(*b*)

Fig. 6.(*a*) X-ray back-reflection Laue photograph for strained uranium (orthorhombic) with [111] approximately antiparallel to the X-ray beam direction. (*b*) Simulated pattern with [1·188, 1·788, 1] antiparallel to the X-ray beam direction.

To some extent this intensity disagreement appears to be structure dependent. The program has been used widely for materials of cubic, hexagonal and orthorhombic symmetry and disagreement between calculated and recorded intensities was considerably less serious. Figs. 4, 5 and 6 show examples of orientations for each of these symmetries.

This difference in behaviour suggests inaccuracies in multiplicity or structure-factor calculation. However, careful examination of all outputs shows this not to be the case since the values calculated by the program for the m and $F(hkl)$ of (3.6) are as expected.

5. Summary

Despite some disagreement between the spot intensity calculated and that observed, the procedure outlined here both simplifies and speeds up the determination of orientation. Since the program requires only a limited amount of input information and is written with copious comments concerning both running and program procedure, it is simple to use. Owing to its wide use of pack files rather than run-time-dependent core space and array storage, the program may be run on a machine of only average capabilities.

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