serially along the line, with merely an indication of the changing indices.

In any case a large typescript table should be prepared (*e.g.*, as computer output) and considerably reduced to a photograph no larger than a full page in the journal. Such photographs (one or more) should be suitable for direct photographic reproduction. The editor of *Acta Crystallographica* reports that such a procedure greatly facilitates publication.

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Laue Ellipses and Reciprocal-Lattice Plane Packing Densities

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For each complete ellipse on a Laue photograph one can read off an inclination correction factor (ICF) from a chart and multiply it by the number (N) of reflexions counted on the ellipse. The product $D=N$. ICF is inversely proportional to the unit-cell area of the generating reciprocal-lattice plane and is often sufficient to identify the plane. Use is made of the facts that the reciprocal-lattice lines generating Laue reflexions are uniquely specified by their prime coordinate points in the reciprocal lattice (points with at least two coordinates prime to each other), and that these prime coordinate points are uniformly distributed over any n-dimensional lattice ($n \geq 2$).

Aim

Laue photographs seem to be used mainly to determine angles within the reciprocal lattice, or to find the orientation of a crystal. Another possible use is the identification of the generating reciprocal-lattice plane from its Laue ellipse, by means of counting the number of reflexions on the complete ellipse. It is shown below how this number, N, together with an inclination correction factor, ICF, obtained from a transparency superposed on the ellipse, can give a quick estimate of the relative inverse unit-cell area of the generating reciprocal-lattice plane; this is often sufficient to identify the reciprocal-lattice plane. It is also easy to calculate roughly the angular corrections required to swing that plane into, say, a horizontal orientation.

Terminology

Because complete Laue ellipses are required, a cylindrical camera with its wider angular range is better suited than a planar one; the term 'ellipse' will be retained, however. Reciprocal-lattice point, reciprocal-lattice line and reciprocal-lattice plane will be abbreviated to re point, relline and relplane, respectively.

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Reciprocal-lattice geometry and the number of reflexions on a Laue ellipse

The white radiation used for Laue photographs has a continuous spectrum which ranges from a well-defined minimum wavelength to a much less sharply defined tail in the long wavelength region. The corresponding Ewald spheres have radii from a maximum radius R down to a small, ill-defined minimum which we can assume to be zero. They are all nested inside each other and tangent in the relpoint O, as indicated in Fig. 1.

Any relpoint P' inside sphere C (the maximum Ewald sphere of radius R about C) has exactly one sphere C' of this set of spheres going through it and gives rise to a reflexion in the direction of $C'P'$. Let the projection of OP' meet sphere C in P. Then CP is parallel to $C'P'$ as well as to $C''P''$, *etc.*, where P', P'' *etc.* are successive relpoints on the same relline through O, and C', C'' *etc.* are the centres of the corresponding Ewald spheres through them. All the parallel reflexions superpose to form one spot on the film, and thus each relline $OP'P''\ldots$ gives rise to exactly one Laue reflexion, in the direction of CP, as long as at least the first point P' seen from O lies within sphere C.

Any relplane through O and intersecting sphere C will thus give rise to as many reflexions CP as there are 'first' points P' on the circular region of the plane inside sphere C. Fig. 2(*a*) shows such a circular region in a general relplane through O; the point C may lie either above or below the relplane. In any such relplane we can select two suitable rellines OH and OK as axes [Fig. 2(*b*)] and give the corresponding coordinates of any relpoint in the plane as a pair of integers (h,k). It is then obvious that for all 'first' points P' in this plane, and for no others, the coordinates h and k are prime to each other. We accordingly call the points P' 'prime coordinate points' (p.c.p.). The number of reflexions counted on a complete Laue ellipse is then

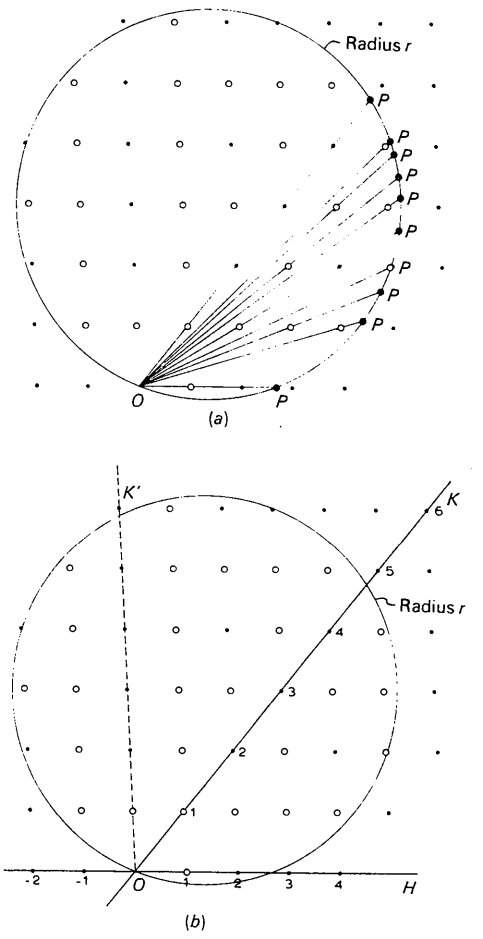

Fig. 2. Circular region of a relplane through O cut out by maximum Ewald sphere C. (*a*) Showing all the points P' enclosed (open circles) and some of the points P on the periphery (full circles). (*b*) Showing a pair of lattice lines, OH and OK, chosen as axes; OK' could have been used instead of OK, leaving the points P' unaltered but changing their coordinates.

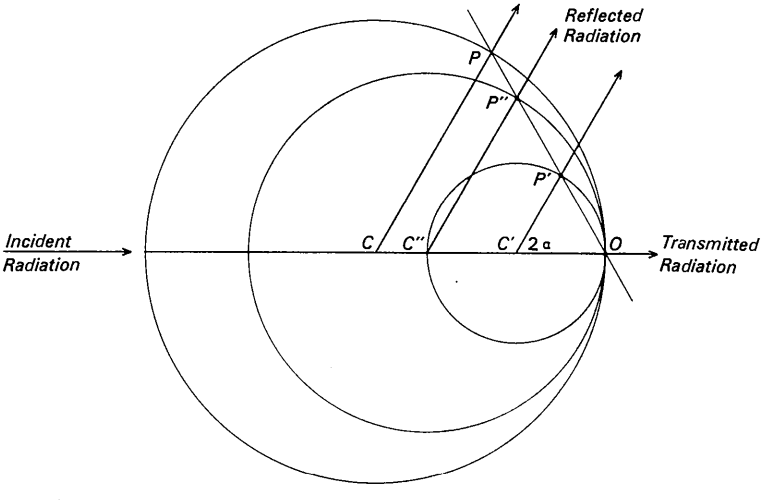

Fig. 1. The Ewald sphere construction for finding the direction of a Laue reflexion.

simply equal to the number of p.c.p. on that circular region of the generating relplane which is contained within the maximum Ewald sphere C.

The prime coordinate point theorem

We define a prime coordinate point in an n-dimensional space to be any point with integral coordinates, at least two of which are prime to each other. This ensures that we are always dealing with 'first' lattice points as seen from the origin.

The theorem then states that, given an n-dimensional space with general axes, the average prime coordinate point density is constant throughout that space and inversely proportional to the unit cell volume of the n-dimensional lattice formed by all the points with integral coordinates.

For the proof we begin with the two-dimensional case. First consider a unit square lattice as shown in Fig. 3(*a*). Along each line $k=$const. the p.c.p. form a repetition of some finite symmetrical pattern. The pattern length is equal to the product $\prod_{i=1}^{n_k} f_i$, where $f_1, f_2, \ldots, f_{n_k}$ are all the n_k different factors greater than 1 contained in k. For example, the lines $k=4$ and $k=8$ have the same pattern because in both cases k contains only the factor 2. If each factor f_i occurs only once in the decomposition of k, the pattern length is of course equal to k. The number of p.c.p. per pattern length is $\prod_{i=1}^{n_k}(f_i-1)$, except for $k=\pm 1$.

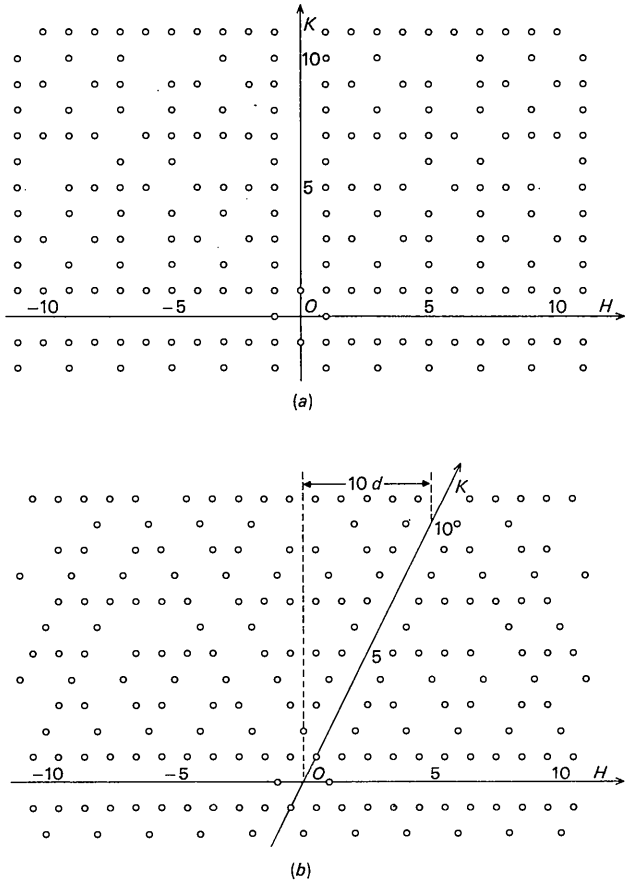

Fig. 3. Unit square lattice with only the p.c.p. shown; (*a*) before, (*b*) after a shear to the right, leaving the unit cell area constant.

The average density of p.c.p. along any line $k=$ const. is thus constant. We could now construct a reasonably large sampling frame of arbitrary shape, put it down anywhere on the plane and shift it through arbitrary distances parallel to OH, without changing the average number of p.c.p. enclosed. But the same applies equally well to the lines $h=$const. and shifts parallel to OK. Since any general displacement of the frame across the lattice can be resolved into two components along OH and OK, respectively, it follows that the average p.c.p. density over the whole lattice must be constant.

It will remain constant even if the axes are inclined at an arbitrary angle to each other (other than 0 or π), so long as the area of the unit cell does not change. Fig. 3(*b*) shows an example: The lattice of Fig. 3(*a*) has been sheared to the right so that each point on the lattice line $k=1$ has been moved to the right through a distance d, each point on $k=2$ through a distance $2d$, *etc.* The average p.c.p. density along each line $k=$const. remains the same as before the shear, and as long as the distance between them (and hence the unit-cell area) remains unchanged, too, the average p.c.p. density over the whole plane lattice will remain the same as before.

The proof for the three-dimensional case is an extension of the foregoing two-dimensional argument, and higher-dimensional cases follow similarly. It should be noted that for unit lattices the average p.c.p. density increases monotonically with the number of dimensions, and it might be interesting to find out whether it tends to 1 or not as $n \to \infty$.

To find the numerical value of the average p.c.p. density in a two-dimensional unit square lattice, two slightly different computer programs were written. Both use the same sampling method (varying the radius of a circle about the origin), but whereas the one actually determines the number of p.c.p. included by the sampling circle for successive lattice lines, the other one first finds the average line density and then multiplies by the length of line included in the sampling circle. Both methods give the same answer for the p.c.p. density, *viz.* 0·6079, and it seems that the method of sampling is more critical than the method of counting.

Application to Laue ellipses

We now know that the number of reflexions N counted on a complete Laue ellipse is proportional to the relpoint density on the generating relplane, *i.e.* inversely proportional to the unit-cell area on that relplane. Besides, N is still a function of the radius r of the

circular region of the relplane contained within sphere C. Thus we could find the p.c.p. density of that relplane by dividing N by πr^2. It is more convenient, however, to calculate only a relative p.c.p. density D for the ellipse concerned, by multiplying N by an inclination correction factor

$$\text{ICF}=\frac{\pi R^2}{\pi r^2}=\frac{\pi R^2}{\pi(R\sin\alpha)^2}=\text{cosec}^2\,\alpha\,,$$

where α is the semi-vertical angle of the generating cone of Laue reflexions. To get α, we use the 'extreme point' of the ellipse, corresponding to the maximum possible diffraction angle 2α for the ellipse. On a plane film, the loci of constant α and thus of constant ICF would be concentric circles; on a cylindrical film rolled flat, they are as shown in Fig. 4.

To obtain the various contours of constant $\text{cosec}^2\,\alpha$, it was noted that for a given α, the circles

$$x^2+y^2=(R\tan 2\alpha)^2$$

on a plane film transform into

$$(R\tan\Upsilon)^2+(z\sec\Upsilon)^2=(R\tan 2\alpha)^2$$

on a cylindrical film, where (x,y) are the rectangular coordinates on the plane film and (s,z) those on the tangent cylindrical film, of the points where an extreme reflexion would intersect the films, and where $\Upsilon=s/R$. This can be verified from Fig. 5:

$$x/R=\tan\Upsilon \quad\text{and}\quad y/(R\sec\Upsilon)=z/R$$

give

$$x=R\tan\Upsilon \quad\text{and}\quad y=z\sec\Upsilon\,.$$

Using the above relations, suitable values of $\text{cosec}^2\,\alpha$ were chosen and the corresponding contours calculated.

Table 1 indicates the accuracy involved. Two photographs (A and B) were taken of a crystal in two known positions, and another two (A' and B') after rotation of the crystal through 180° from those positions. A and A', as well as B and B', are then mirror images of each other in the horizontal centre line on the film. For each complete ellipse, a tracing was made, the transparent ICF chart of Fig. 4 superposed on it, and the ICF at the farthest point from the film centre reached by the ellipse was read off by interpolation between the contours. The relative density $D=N$. ICF then indicates the packing density of relpoints on the generating relplane. Ellipses I and VI stand out clearly from the next important ones, in spite of the scatter found for values of D. And indeed these two ellipses correspond to two major relplanes in the crystal concerned, both of practically equal unit cell area. The value $D=370$ for ellipse VI, photograph B', appears to be too high. In such cases of obvious discrepancy among a pair of values, it may be better to repeat the whole photograph after a slight rotation of the crystal, so as to increase the size of the ellipse(s) concerned.

If it is desired to swing the ellipse whose 'extreme point' has coordinates (s,z) as in Fig. 5, into a horizontal orientation, this can be done roughly as follows: Find Υ and α from s, z, camera radius R and the above relations. Then rotate the crystal (positioned at C) through an angle

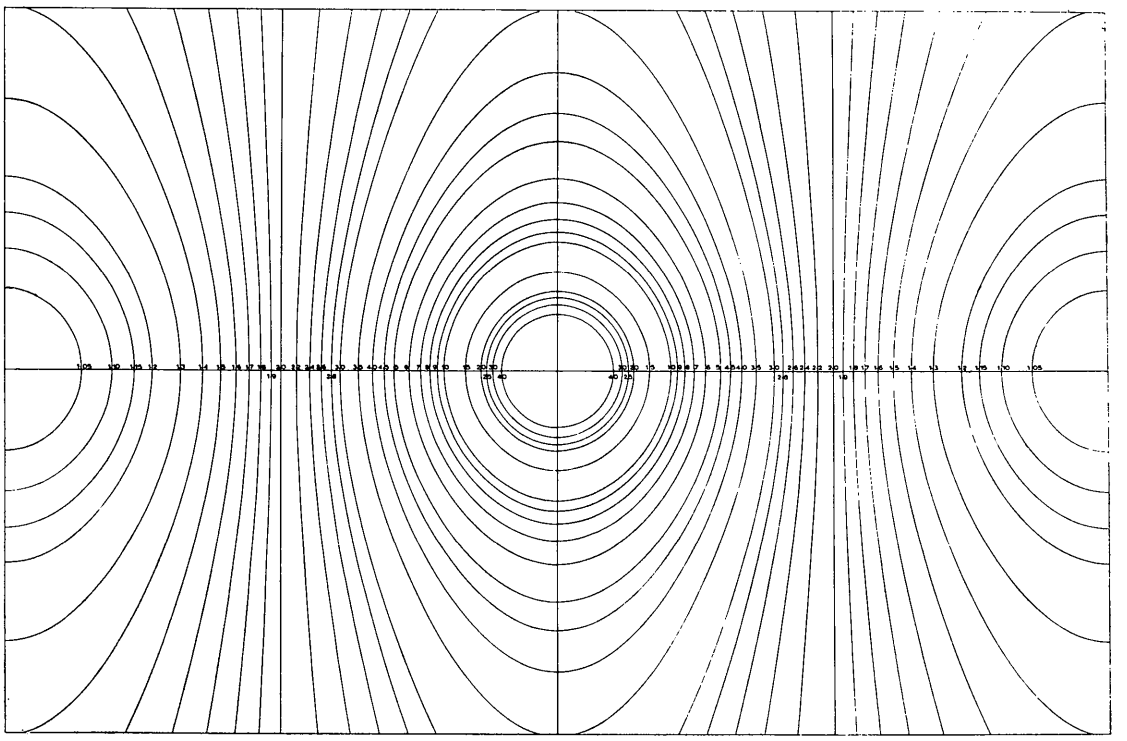

Fig. 4. ICF chart. Length proportional to camera radius and equal to 180 mm for a camera radius of 28·65 mm.

Table 1. *Comparison of relative p.c.p. densities D of various Laue ellipses, as measured on different photographs*

Ellipse no.	Photograph	N	ICF	D
I	A	19	15·5	294
	A'	19	16·5	314
II	A	19	12·0	228
	A'	20	11·5	230
III	A	40	5·0	200
	A'	45	4·8	216
IV	A	—	—	—
	A'	47	4·2	197
V	A	44	2·78	122
	A'	43	2·74	118
VI	B	15	19·5	292
	B'	19	19·5	370
VII	B	26	9·5	247
	B'	26	9·2	239
VIII	B	24	6·6	158
	B'	27	6·8	184
IX	B	47	5·5	258
	B'	45	5·4	248
X	B	45	4·2	189
	B'	47	4·5	212
XI	B	51	2·44	124
	B'	46	2·45	113

$$TOT' = \text{arc tan } \frac{R \sin \Upsilon}{z}$$

about CO and towards the vertical. Finally, rotate the crystal through an angle $(90° - \alpha)$ about AA', again towards the vertical.

Conclusion

Prime coordinate points have been defined and shown to be uniformly distributed throughout an n-dimensional lattice. Application of the two-dimensional case to Laue photographs gives a practical method of identifying relplanes by their relative relpoint packing densities, whenever the Laue ellipses generated by the relplanes are complete on the photograph. Use of the 'extreme point' of a Laue ellipse also enables one to calculate roughly the angular corrections required to swing the corresponding relplane into the horizontal. The applicability of the method is at present limited

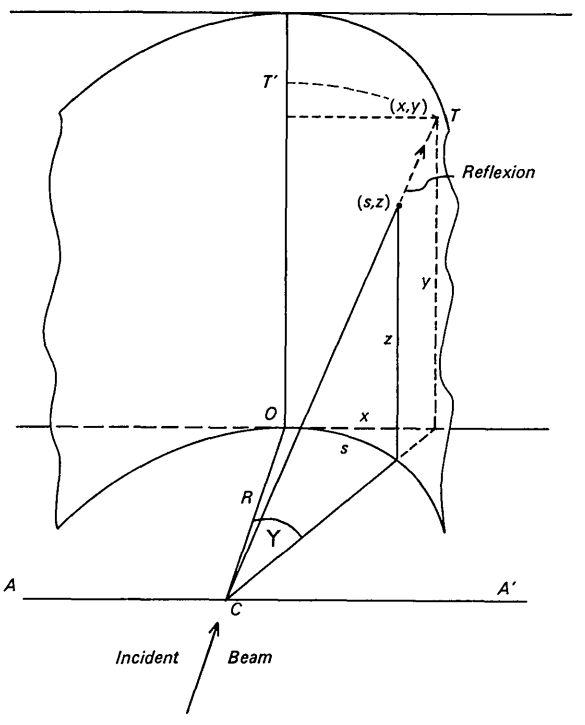

Fig. 5. Laue reflexion coordinates on a plane and a cylindrical film.

by the comparatively small angular ranges of both the cylindrical camera and the type of goniometer normally employed.

Application of the three-dimensional case to Laue photographs leads us to expect the same average number of Laue reflexions into the solid angle 4π, no matter what the orientation of the crystal may be. This offers a method, in principle, of determining the volume of the primitive unit cell of a crystal mounted in random orientation, from a knowledge of the minimum wavelength of the X-rays used, and of the total number of Laue reflexions obtained.

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