The method has been used on transmission Kikuchi line patterns from the cubic crystal natural spinel, $MgAl_2O_4$. An enlarged section of one of the plates, containing some of the intersections used, is shown in Fig. 2.

From the lattice constant of $a_0(26\,°C) = 8{\cdot}0800$ Å (Wyckoff, 1965), the wavelength associated with the 100 kV switch on a JEM-7 electron microscope is determined. The results are given in Table 1.

The uncertainty in $\Delta R_3/R_3$ can for small ratios be allowed to be as high as 10%. Still the uncertainty in the calculated λ is less than 0·3% which is the estimated *maximum* uncertainty in a single determination. The deviation from the mean value gives a relative uncertainty in this quantity of less than 0·1%.

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Calculation of Absorption Corrections for Photographic Data

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An extension of the methods of Wells (*Acta Cryst.* (1960). **13**, 722) is described for calculating the direction cosines of incident and emergent rays for general camera geometry and for any standard setting of the crystal.

Wells (1960) gives methods for determining the directions of the incident and emergent rays for equi-inclination, normal-beam and precession geometry, with the crystal in a standard setting, with c as the principal axis. This paper generalizes his results (*a*) for any camera geometry, (*b*) for alternative settings of the crystal. Wells's notation is used throughout.

(*a*) *Generalization for any camera geometry*

In particular this covers data recorded by the inclined-beam oscillation technique (Milledge, 1963) and has two aspects

(1) to allow for l taking negative values,

(2) to calculate the sign of the direction cosine ($\cos \angle ZE$), between the principal axis and the emergent ray, when this angle lies in the range $0-\pi$, rather than $0-\pi/2$ (equi-inclination) or $\pi/2-\pi$ (precession).

Wells defines a set of orthogonal axes with $OX \equiv a^*$, OY in the a^*-b^* plane and OZ on the same side of the XY plane as c^* (Fig. 1). Then, considering a reflexion hkl (point P), he examines the lth layer of the reciprocal lattice [Fig. 2(*a*)] and derives the lengths and angles:

$$L_1 = lc^* \sin \omega_2\,,$$

L_2 and ω_3 (determined by the cell constants), ω_4 (a function of h and k only) and

$$\omega_5 = \pi + \omega_4 - \omega_3\,,$$

which determine

$$L_3 = (L_1^2 + L_2^2 - 2L_1L_2 \cos \omega_5)^{1/2}\,.$$

He does not consider the consequence of L_2 being zero, *i.e.* P lying on c^*. In this case ω_4 and ω_5 are both indeterminate, but $L_3 = L_1$ and $\omega_6 = \omega_2$, $\omega_7 = \omega_3$. If L_3 is also zero the reciprocal lattice point lies on OZ, and can never be recorded properly by photographic means.

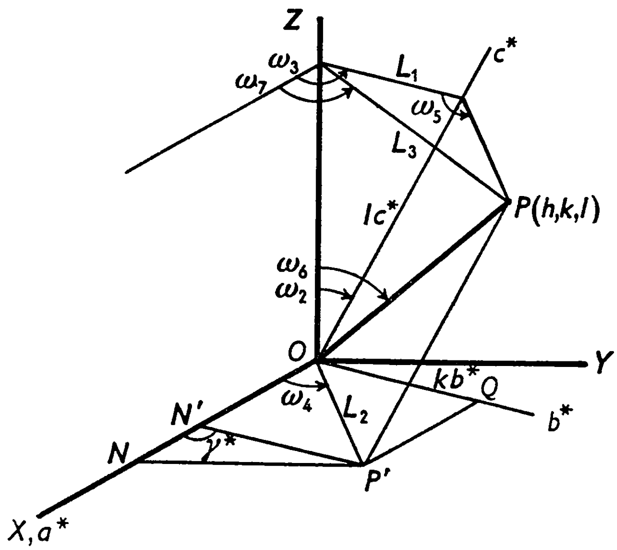


Fig. 1. The reciprocal lattice showing the angles and lengths referred to in the text (from Wells, 1960).

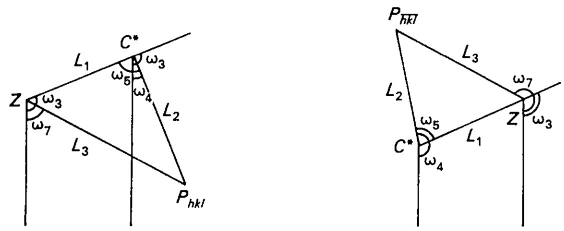
Further, the length OP is $2 \sin \theta$ and so

$$\sin \omega_6 = L_3/2 \sin \theta,$$
$$\cos \omega_6 = (1 - \sin^2 \omega_6)^{1/2}.$$

Then

$$\sin \omega_7 = (L_1 \sin \omega_3 + L_2 \sin \omega_4)/L_3,$$
$$\cos \omega_7 = (L_1 \cos \omega_3 + L_2 \cos \omega_4)/L_3,$$

determining the two angles ω_6 and ω_7 which define OP.



l positive (*a*) *l* negative (*b*)

Fig. 2. The lth layer of the reciprocal lattice. (*a*) l positive, (*b*) l negative.

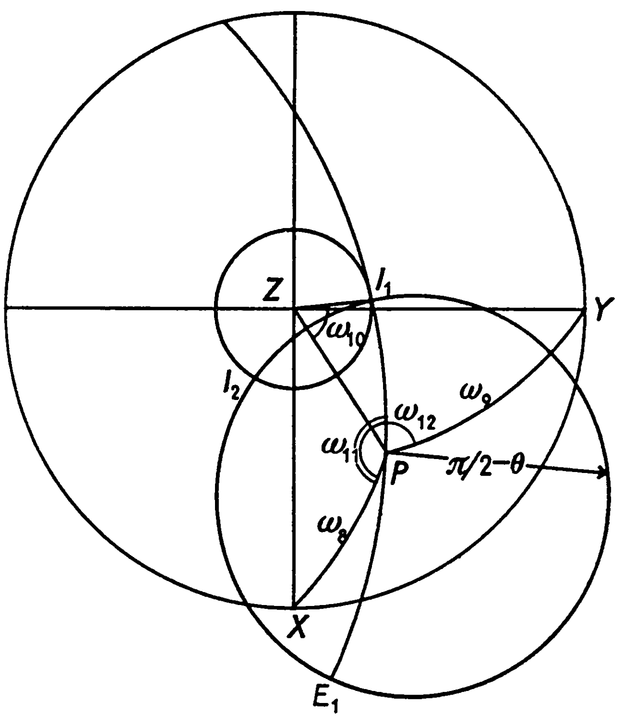


Fig. 3. The reflexion geometry of the precession camera (from Wells, 1960).

If l is negative, then the $-l$th layer of the reciprocal lattice must be considered [Fig. 2(*b*)].

In this case ω_3 no longer has the same relationship to P and c^* as before, and the formulae need modification:

$$L_1 = |lc^* \sin \omega_2|,$$
$$\omega_5 = \omega_4 - \omega_3,$$
$$\sin \omega_7 = (L_2 \sin \omega_4 - L_1 \sin \omega_3)/L_3,$$
$$\cos \omega_7 = (L_2 \cos \omega_4 - L_1 \cos \omega_3)/L_3,$$

and $\cos \omega_6$ is negative:

$$\cos \omega_6 = -(1 - \sin^2 \omega_6)^{1/2}.$$

To determine the direction cosines of the incident and emergent rays, Wells then considers a special condition for each camera geometry, but in fact all these conditions are equivalent to specifying the angle between the principal axis and the incident ray ($\angle IZ$) which is constant for a given block of data for all methods, including general inclination. Thus the formulae for precession geometry (when $\angle IZ = \mu$, stated explicity) can be used for all cases with the appropriate value of $\angle IZ$ as in Table 1.

The incident ray lies on a small circle about Z and its position is given by the intersection of this circle with a small circle of radius $\pi/2 - \theta$ about P (Fig. 3). There are in general two intersections, unless the reflexion is unobservable, when the two circles do not cross.

These two intersections correspond to different reflexion positions for the normal-beam and general inclination method (upper or lower sides of the film); for the precession method the two different positions record at the same spot on the film and the corrections must be averaged; for equi-inclination the two positions correspond to exchange of the incident and reflected rays and only one need be considered.

The sign of l has no effect on Wells's formulae for calculating the direction cosines of the incident and emergent rays, and in the general case, only the formula for $\angle ZE$ must be changed, as his method does not give its sign. The angle ω_{13} (I_1PZ) is given by

$$\cos \omega_{13} = (\cos \mu - \cos \omega_6 \sin \theta) / \sin \omega_6 \cos \theta,$$

and using its supplement (E_1PZ) we have

$$\cos \angle ZE = \cos \omega_6 \sin \theta - \sin \omega_6 \cos \theta \cos \omega_{13}$$
$$= 2 \cos \omega_6 \sin \theta - \cos \mu.$$

This in fact only depends on l, as is required physically.

Table 1.

Method	Nature of angle $\angle IZ$	Value
Precession	Precession angle (μ)	μ
Equi-inclination	Complement of inclination angle (different for each l value)	$90 - \sin^{-1} (\zeta_l/2)$
General inclination	Complement of inclination angle (μ). (Constant for all l values)	$90 - \mu$
Normal beam	90° (constant for all l values)	90°

The results of the whole calculation are the direction cosines of two rays which are treated symmetrically, *i.e.* reflected and reversed incident rays both leaving the crystal.

(*b*) *Alternative settings of the axes*

If data have been recorded using only one principal axis, it is immaterial whether this is a, b or c, as the axes and reflexion indices can readily be renamed. If however data have been recorded using two different axes (say b and c) for the same crystal, it is inconvenient (and productive of error) to have to define the crystal on two different sets of orthogonal axes. It is preferable to calculate the ray direction cosines for reflexions recorded with b as principal axis ($Z' \equiv b$) on the orthogonal axes $X'Y'Z'$, using Wells's formulae and then to convert these cosines to those for the same rays on the axes XYZ ($Z \equiv c$) used for definition of the crystal.

This may readily be done if the direction cosines of X, Y, and Z are known on the axes $X'Y'Z'$, as then

$$\cos \angle IX = \cos \angle IX' \cos \angle XX' + \cos \angle IY' \cos \angle XY' + \cos \angle IZ' \cos \angle XZ', \; etc.$$

These direction cosines may be determined in the following way. Define a set of unit vectors $\mathbf{a},\mathbf{b},\mathbf{c}$ along a^*,b^*,c^*. Then unit vectors $\mathbf{X},\mathbf{Y},\mathbf{Z}$ along X, Y, Z may be found in terms of these:

$$\mathbf{X}=\mathbf{a}$$
$$\mathbf{Y}=k\mathbf{a}+\mathbf{b}$$
$$\mathbf{Z}=m\mathbf{a}+n\mathbf{b}+p\mathbf{c}\,.$$

$\mathbf{a}$ and $\mathbf{Y}$ are orthogonal, so

$$k\mathbf{a}\,.\,\mathbf{a}+l\mathbf{b}\,.\,\mathbf{a}=0\,,$$

and $\mathbf{Y}$ is a unit vector, so

$$(k\mathbf{a}+l\mathbf{b})^2=1\,,$$

i.e.

$$k^2\mathbf{a}\,.\,\mathbf{a}+l^2\mathbf{b}\,.\,\mathbf{b}+2kl\mathbf{a}\,.\,\mathbf{b}=1\,,$$

giving

$$k=-\mathbf{a}\,.\,\mathbf{b}/D\,,\quad l=1/D\,,$$

where

$$D=[1-(\mathbf{a}\,.\,\mathbf{b})^2]^{1/2}\,,$$

for $\mathbf{Y}$ on the same side of $\mathbf{a}$ as $\mathbf{b}$.

Similarly, as $\mathbf{Z}$ is orthogonal to both $\mathbf{a}$ and $\mathbf{b}$ we get

$$m=[(\mathbf{b}\,.\,\mathbf{c})\,(\mathbf{a}\,.\,\mathbf{b})-\mathbf{c}\,.\,\mathbf{a}]/DE$$
$$n=-m/(\mathbf{a}\,.\,\mathbf{b})-D(\mathbf{c}\,.\,\mathbf{a})/E(\mathbf{a}\,.\,\mathbf{b})$$
$$p=D/E$$

where

$$E=\mathbf{a}\,.\,\mathbf{b}\times\mathbf{c}\,.$$

If $\mathbf{a}\,.\,\mathbf{b}=0$, the expression for n is indeterminate and it is given by

$$n=-p(\mathbf{b}\,.\,\mathbf{c})\,.$$

In a similar way the components of the unit vectors $\mathbf{X}',\mathbf{Y}',\mathbf{Z}'$ may be found, for whichever permutation is required. Then if

$$\mathbf{X}=a_1\mathbf{a}+a_2\mathbf{b}+a_3\mathbf{c}$$

and

$$\mathbf{X}'b={}_1\mathbf{a}+b_2\mathbf{b}+b_3\mathbf{c}\,,$$

the required cosine $\angle X'X'$ is given by

$$\mathbf{X}\,.\,\mathbf{X}'=a_1b_1\mathbf{a}\,.\,\mathbf{a}+a_1b_2\mathbf{a}\,.\,\mathbf{b}+a_1b_3\mathbf{a}\,.\,\mathbf{c}+\ldots\,,$$

and similarly for the remaining angles.

These methods have been incorporated in a general absorption correction program written in Fortran for the Atlas Computer, using the method of De Meulenaer & Tompa (1965).

I would like to thank Dr R. E. Gaskell for the solution of the problem outlined in part (*b*).

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On the Bragg Reflexion from Ideal Absorbing Crystals

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The general analytic expression is given for the integral reflexion coefficient of X-rays from thick ideal absorbing crystals.

Introduction

In order to calculate the integral reflexion of X-rays from thick ideal crystals in the presence of an absorption, one has to utilize, in accord with the Prins method, the numerical integration of the well-known formula for the reflexion coefficient, in which the absorption is taken into account by adding the imaginary terms to the atomic scattering amplitudes. However, a simple analytic expression of the integral reflexion can be