disordered sequence in any one tunnel. Crystals of the composition $Na_{0.5}V_6O_{15}$ give no diffuse spectra by which this may be assessed, but single crystals of $Ba_{2-x}Ti_8O_{16}$, which is isomorphous with hollandite, offer additional evidence which is being investigated both by X-ray diffraction and dielectric absorption measurements.

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Polarization Correction for Crystal-Monochromatized X-radiation*

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The polarization correction for diffraction of a crystal-monochromatized X-ray beam is derived. Suitable expressions for different experimental methods are also given. The polarization correction is first tabulated in parts so that the appropriate correction for any wavelength and monochromator crystal can be determined. Another table lists selected values of the polarization correction, in a final form, for different wavelength X-radiations reflected from $(10\bar{1}1)$ planes of a quartz monochromator. The maximum correction for Ag $K\alpha$ is a little more than 1%, whereas for Cr $K\alpha$ the maximum correction is 34%.

1. Polarization factor

The use of crystal-monochromatized X-radiation has many advantages over conventional methods using filters. Of greatest importance is the virtual elimination of background scattering due to non-characteristic radiation. Furthermore, it is possible to use a bent-crystal monochromator to obtain integrated intensities photographically, as will be shown in a subsequent communication. The chief objection to the use of crystal monochromators, the intensity decrease in the twice diffracted beam, can be minimized by suitable choice of monochromator crystal and X-radiation. Thus, single-crystal photographs of inorganic compounds made in the author's laboratory with Ag $K\alpha$ diffracted from $(10\bar{1}1)$ planes of a quartz monochromator have intensities directly comparable with similarly exposed photographs prepared with a conventionally filtered beam.

Whenever crystal-monochromatized X-radiation is used, the beam striking the specimen crystal is partially polarized owing to reflection by the monochromator crystal. The polarization factor for the twice diffracted beam is different, therefore, from the relation, $\frac{1}{2}(1+\cos^2 2\theta)$, normally used. In order to determine the appropriate polarization factor, consider Fig. 1. The intensity of an unpolarized X-ray beam

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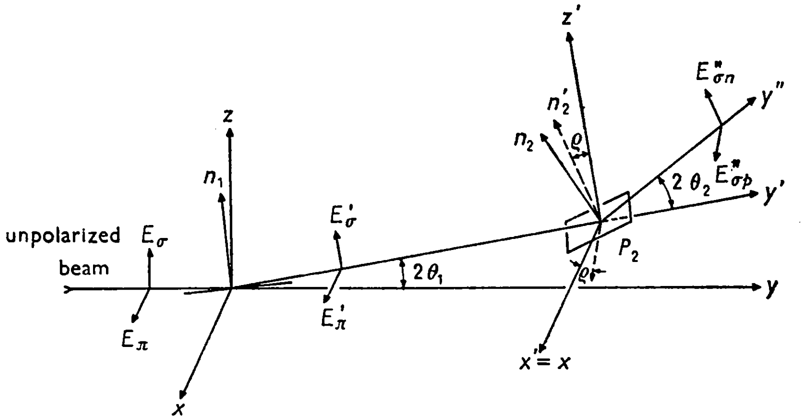

Fig. 1.

can be considered as the sum of two equal parts due to independent components in two orthogonal directions of polarization:

$$I_0 = I_\sigma + I_\pi\,, \tag{1}$$

or

$$\tfrac{1}{2}I_0 = I_\sigma = I_\pi\,,$$

where σ indicates the component in the plane of incidence, and π the component normal to it. Using the amplitudes of the optical field, equation (1) can be alternatively written

$$\tfrac{1}{2}E_0^2 = E_\sigma^2 = E_\pi^2\,. \tag{2}$$

The σ component can be considered first. This component is reflected by the monochromator planes, P_1, (whose normal, n_1, lies in the yz plane) along the y' direction (also lying in the yz plane) which is inclined by $2\theta_1$ to y. After reflection, the σ component becomes

$$E'_\sigma = kE_\sigma \cos 2\theta_1\,, \tag{3}$$

where $k = e^2/mc^2r$ and contains all the factors which are independent of the direction of polarization. Referring this component to the primed coordinates, it lies in the $y'z'$ plane and is parallel to z'.

This component is next reflected by the specimen crystal planes, P_2, along y'' which is inclined by $2\theta_2$ to y'. (The normal, n_2, of these planes may be inclined to x', y' and z'.) The effect on E'_σ of the second reflection can be studied best by resolving E'_σ along two mutually perpendicular directions, viz. one along the plane P_2, and one along n'_2, the projection of the normal n_2 on the $x'z'$ plane. If n'_2 lies at an angle ϱ away from the z' axis, the two components are:

$$\left.\begin{aligned} &\text{Along the normal: } E'_{\sigma n} = E'_\sigma \cos\varrho\,. \\ &\text{Along the plane: } \quad E'_{\sigma p} = E'_\sigma \sin\varrho\,. \end{aligned}\right\} \tag{4}$$

The normal component is attenuated by the cosine of the reflection angle, $2\theta_1$, while the component along the plane is not attenuated, i.e.

$$E''_{\sigma n} = k'E'_{\sigma n}\cos 2\theta_2 \tag{5}$$

and

$$E''_{\sigma p} = k'E'_{\sigma p}\,. \tag{6}$$

Similarly, the π component, after reflection by the planes, P_1, is not affected, i.e.

$$E'_\pi = kE_\pi\,. \tag{7}$$

Resolving E'_π along the same two perpendicular directions used for resolving E'_σ, the two components are:

$$\left.\begin{aligned} &\text{Along the normal: } E'_{\pi n} = E'_\pi \sin\varrho\,. \\ &\text{Along the plane: } \quad E'_{\pi p} = E'_\pi \cos\varrho\,. \end{aligned}\right\} \tag{8}$$

The normal component is changed and the component along the plane is not, so that

$$\left.\begin{aligned} &E''_{\pi n} = k'E'_{\pi n}\cos 2\theta_2 \\ \text{and} \quad & \\ &E''_{\pi p} = k'E'_{\pi p}\,. \end{aligned}\right\} \tag{9}$$

(k' has the same meaning for the second crystal as k had for the first.)

The resultant contribution of the σ component to the intensity

$$\overline{E''^2_\sigma} = \overline{E''^2_{\sigma n}} + \overline{E''^2_{\sigma p}}\,, \tag{10}$$

and of the π component,

$$\overline{E''^2_\pi} = \overline{E''^2_{\pi n}} + \overline{E''^2_{\pi p}}\,, \tag{11}$$

can be added to give the resultant contribution from both components:

$$\overline{E''^2} = \overline{E''^2_\sigma} + \overline{E''^2_\pi} = \overline{E''^2_{\sigma n}} + \overline{E''^2_{\sigma p}} + \overline{E''^2_{\pi n}} + \overline{E''^2_{\pi p}}\,. \tag{12}$$

After making appropriate substitutions for each term,

$$\overline{E''^2} = \tfrac{1}{2}k^2k'^2\overline{E_0^2}[(\cos^2 2\theta_1 \cos^2\varrho + \sin^2\varrho)\cos^2 2\theta_2 + (\cos^2 2\theta_1 \sin^2\varrho + \cos^2\varrho)]\,. \tag{13}$$

The final intensity is expressed in terms of the intensity just before the second reflection,

Table 1. *Bragg angles* (θ_1) *for* ($10\bar{1}1$) *planes of quartz*

Radiation†	Wavelength (Å)	θ_1 (°)	$\cos^2 2\theta_1$
Ag $K\alpha^*$	0·561	4·8	0·9722
Mo $K\alpha^*$	0·711	6·1	0·9553
Cu $K\alpha^*$	1·542	13·3	0·7995
Fe $K\alpha^*$	1·937	16·6	0·6905
Cr $K\alpha^*$	2·291	19·8	0·5937

† The wavelength of $K\alpha^*$ is computed according to the relation

$$K\alpha^* = \tfrac{1}{3}(2\,K\alpha_1 + K\alpha_2)\,.$$

Table 2. $\Sigma_1 = (\cos^2\varrho\cos^2 2\theta_2 + \sin^2\varrho)$ *and* $\Sigma_2 = (\sin^2\varrho\cos^2 2\theta_2 + \cos^2\varrho)$ *as a function of* θ_2 *and* ϱ

$2\theta_2$ (°)	ϱ (°)	Σ_1	Σ_2
0, 180	0, 180	1	1
	10, 170	1	1
	20, 160	1	1
	30, 150	1	1
	40, 140	1	1
	50, 130	1	1
	60, 120	1	1
	70, 110	1	1
	80, 100	1	1
	90, (270)	1	1
10, 170	0, 180	0·9698	1
	10, 170	0·9707	0·9991
	20, 160	0·9733	0·9965
	30, 150	0·9774	0·9924
	40, 140	0·9823	0·9875
	50, 130	0·9875	0·9823
	60, 120	0·9924	0·9774
	70, 110	0·9965	0·9733
	80, 100	0·9991	0·9707
	90, (270)	1	0·9698
20, 160	0, 180	0·8830	1
	10, 170	0·8865	0·9965
	20, 160	0·8967	0·9863
	30, 150	0·9122	0·9708
	40, 140	0·9313	0·9517
	50, 130	0·9517	0·9313
	60, 120	0·9708	0·9122
	70, 110	0·9863	0·8967
	80, 100	0·9965	0·8865
	90, (270)	1	0·8830
30, 150	0, 180	0·7500	1
	10, 170	0·7576	0·9925
	20, 160	0·7792	0·9708
	30, 150	0·8125	0·9375
	40, 140	0·8533	0·8967
	50, 130	0·8967	0·8533
	60, 120	0·9375	0·8125
	70, 110	0·9708	0·7792
	80, 100	0·9925	0·7576
	90, (270)	1	0·7500
40, 140	0, 180	0·5868	1
	10, 170	0·5993	0·9875
	20, 160	0·6351	0·9517
	30, 150	0·6901	0·8967
	40, 140	0·7575	0·8293
	50, 130	0·8293	0·7575
	60, 120	0·8967	0·6901
	70, 110	0·9517	0·6351
	80, 100	0·9875	0·5993
	90, (270)	1	0·5868
50, 130	0, 180	0·4132	1
	10, 170	0·4309	0·9823
	20, 160	0·4819	0·9313
	30, 150	0·5599	0·8533
	40, 140	0·6557	0·7575
	50, 130	0·7575	0·6557
	60, 120	0·8533	0·5599
	70, 110	0·9313	0·4819
	80, 100	0·9823	0·4309
	90, (270)	1	0·4132
60, 120	0, 180	0·2500	1
	10, 170	0·2726	0·9774
	20, 160	0·3378	0·9122
	30, 150	0·4375	0·8125
	40, 140	0·5599	0·6901
	50, 130	0·6901	0·5599
	60, 120	0·8125	0·4375
	70, 110	0·9122	0·3378
	80, 100	0·9774	0·2726
	90, (270)	1	0·2500
70, 110	0, 180	0·1170	1
	10, 170	0·1436	0·9733
	20, 160	0·2203	0·8967
	30, 150	0·3377	0·7792
	40, 140	0·4818	0·6351
	50, 130	0·6351	0·4818
	60, 120	0·7792	0·3377
	70, 110	0·8967	0·2203
	80, 100	0·9733	0·1436
	90, (270)	1	0·1170
80, 100	0, 180	0·0302	1
	10, 170	0·0595	0·9707
	20, 160	0·1437	0·8865
	30, 150	0·2727	0·7576
	40, 140	0·4309	0·5993
	50, 130	0·5993	0·4309
	60, 120	0·7576	0·2727
	70, 110	0·8865	0·1437
	80, 100	0·9707	0·0595
	90, (270)	1	0·0302
90	0, 180	0	1
	10, 170	0·0302	0·9698
	20, 160	0·1170	0·8830
	30, 150	0·2500	0·7500
	40, 140	0·4132	0·5868
	50, 130	0·5868	0·4132
	60, 120	0·7500	0·2500
	70, 110	0·8830	0·1170
	80, 100	0·9698	0·0302
	90, (270)	1	0

$$I = KI' \times \left\{\frac{(\cos^2 2\theta_1\cos^2\varrho + \sin^2\varrho)\cos^2 2\theta_2 + \cos^2 2\theta_1\sin^2\varrho + \cos^2\varrho}{1+\cos^2 2\theta_1}\right\}, \tag{14}$$

where the quantity in brackets is the polarization factor for a twice diffracted X-ray beam.

2. Polarization correction

The final expression for the polarization correction depends on the experimental arrangement used. For

Table 3. *Polarization factor p', and polarization correction p/p', as a function of θ_2 and ϱ, for selected X-radiations*

($\cos^2 2\theta_1$ values as listed in Table 1.)

		Ag $K\alpha$*		Mo $K\alpha$*		Cu $K\alpha$*		Fe $K\alpha$*		Cr $K\alpha$*	
$2\theta_2$ (°)	ϱ (°)	p'	p/p'	p'	p/p'	p'	p/p'	p'	p/p'	p'	p/p'
0, 180	90	1	1	1	1	1	1	1	1	1	1
30, 150	90	0·8732	1·0021	0·8721	1·0033	0·8611	1·0161	0·8521	1·0268	0·8431	1·0378
60, 120	90	0·6197	1·0085	0·6164	1·0139	0·5832	1·0716	0·5563	1·1234	0·5294	1·1805
90, (270)	90	0·4929	1·0144	0·4885	1·0235	0·4443	1·1253	0·4085	1·2240	0·3725	1·3423

the powder method, $\varrho = 0$ provided that the intensities are measured along the plane of incidence, and that the specimen rotation axis is parallel to the reflecting planes of the monochromator crystal. In this case, the correct expression for the polarization factor is

$$\frac{1+\cos^2 2\theta_1 \cos^2 2\theta_2}{1+\cos^2 2\theta_1} . \qquad (15)$$

If the rotation axis is inclined, the more general equation (14) must be used.

The correct expression for the normal-beam method (rotation, oscillation or Weissenberg arrangements) is given by equation (14) where $\varrho = \nu$ (constant for any level). For the zero level $\varrho = \nu = 0$ and equation (14) reduces to equation (15). For the equi-inclination method the determination of ϱ is more complicated and would have to be made, individually, for each reflection of every crystal.

Since ϱ is the angle between the projection of the normal to the reflecting plane (on to a plane perpendicular to the incident monochromatized X-ray beam) and the plane of incidence, it can be measured directly on the film in the Buerger precession method. Furthermore, θ_2 varies radially on the film, and also can be measured directly. Owing to these simple geometrical relations between ϱ, θ_2 and the position of the reciprocal lattice points photographed by the Buerger precession method, it is convenient to prepare a chart of the polarization correction on the same scale as the film.

There is one other unknown in (14), viz. the angle (θ_1) of the first reflection of the X-ray beam. This angle is a function of the monochromator crystal and the wavelength of the radiation selected. Quartz crystals cut parallel to $(10\bar{1}1)$ make satisfactory monochromators for most wavelengths. Table 1 lists values of the Bragg angle, θ_1, for the wavelengths commonly used.

The expression for the polarization factor is the bracket in equation (14).

Let

$$(\cos^2 \varrho \cos^2 2\theta_2+\sin^2 \varrho) = \Sigma_1 \quad \text{and}$$
$$(\sin^2 \varrho \cos^2 2\theta_2+\cos^2 \varrho) = \Sigma_2 ;$$

then the polarization factor becomes

$$\frac{1}{1+\cos^2 2\theta_1} (\cos^2 2\theta_1 \Sigma_1+\Sigma_2) . \qquad (16)$$

Since the polarization factor depends on the value of θ_1 selected, but Σ_1 and Σ_2 are independent of θ_1, Table 2 lists the values of Σ_1 and Σ_2 separately. This table can be used, therefore, to compute the polarization correction for any experimental arrangement.

The magnitude of the structure factors is related to the experimentally determined intensity by the relation

$$|F|^2 = I(1/Lp) . \qquad (17)$$

Since charts plotting $1/Lp$ for the Buerger precession method have been published (Waser, 1951; Grenville-Wells & Abrahams, 1952) it is convenient to prepare similar charts by plotting the reciprocal of (16) multiplied by the conventional polarization factor. If the polarization factor for a twice diffracted beam is denoted by p', equation (17) can be written

$$|F|^2 = I \times \frac{1}{Lp} \times \frac{p}{p'} = I \times \frac{1}{L} \times \frac{1}{p'} . \qquad (18)$$

Table 3 lists the polarization correction, p/p', for selected values of θ_2 and ϱ, for several X-radiations monochromatized by reflection from the $(10\bar{1}1)$ planes of quartz. This table is included to indicate the magnitude of this correction, which is negligible for Ag$K\alpha$ but attains a maximum value of 34% for Cr$K\alpha$. Complete tables for the radiations listed in Table 3 are in preparation.

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