dispersion correction applied. This is to be expected as the dispersion corrections have spherically symmetric contributions in the analysis. However, significant deviations from spherical symmetry in the electron distribution of the fluorine ion may introduce some directional dependence of the dispersion correction. Hence, on the basis of the above analysis it remains uncertain to what extent the observed asphericity originates in the asphericity of the dispersion correction.

Disregarding any possible asphericity, a few additional remarks on the theoretical dispersion corrections should be made. The theoretical calculations require knowledge of the oscillator strengths and the manner in which the photoelectric absorption coefficient varies with the wavelength. The main limitation of the accuracy of these calculations is the uncertainty in the wavelength dependence of the absorption coefficients. Further, the values of Cromer (1965) and Cromer & Liberman (1968) are based on the oscillator strengths calculated from free atom wave functions. However, changes induced in the free atom wave functions when the atom is placed in a solid may manifest themselves in significant changes in the oscillator densities and thus in the dispersion corrections. In particular, this is the case for fluorine where the L-electrons are valence electrons and the probability of multiple excitations produced by X-rays is large (Åberg, Graeffe, Utriainen & Linkoaho, 1970).

On the basis of the above considerations further direct measurements of the dispersion corrections and calculations based on the solid state wave-functions are readily suggested.

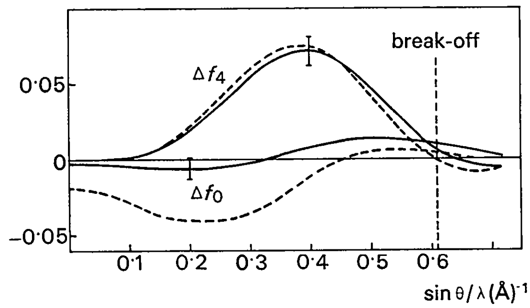

Fig. 1. The radial scattering amplitudes Δf_0 and Δf_4 for fluorine in lithium fluoride obtained by the application of the theoretical (solid curves) and experimental (broken curves) values of the dispersion correction. The remarkable Δf_4 component indicates electron transfer from the [111] to the [100] direction. The number of electrons necessary to produce this deformation has been calculated to be 0·08 (Kurki-Suonio, 1970).

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Setting a rhombohedral crystal to its trigonal axis.

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Double oscillations at 120° intervals are used to set a rhombohedral crystal to its trigonal axis, using the separation of non-equatorial pairs of equivalent spots at $\theta = 45°$. The two exposures are made each at 30° to the directions usually used for double oscillation photographs at 180° intervals; arc corrections are derived in the usual way but are here increased by the factor sec 30° = 1·155.

We have found by experience that when an oscillation photograph shows equatorial symmetry, non-equatorial pairs of equivalent spots can be used for setting the crystal to its axis by double oscillation photographs, provided that the spots are on a reasonably linear pait of the ζ-scale, say $\zeta < 0{\cdot}5$. Oscillation photographs of rhombohedral crystals taken around their trigonal axes show row-lines in which only every third layer-line is occupied by a spot. The majority of row-lines are asymmetrical about the equator and only about one-third of them show equatorial symmetry and an equatorial spot; the latter are difficult to recognize and are usually too few to be useful for crystal setting. The spots are however repeated at 120° intervals, and double oscillation photographs at 120° intervals show all spots as equivalent pairs from which convenient pairs can be selected for use, whether or not they lie on the equator.

Crystallographers vary as to whether they prefer to take 180° double oscillation photographs with the mean beam directions parallel to, or at 45° to an arc. In either case, if the directions usually chosen are at 0 and 180° of azimuth, for 120° double oscillation photographs the exposures are made with the mean beam directions at 30 and 150°. Arc corrections are derived from measured pairs of equivalent spots at $\theta = 45°$ in the usual way, but are here increased by the factor sec $30° = 1{\cdot}155$.

We have verified this finding experimentally using a crystal of aerugite (Davis, Hey & Kingsbury, 1965), now known to be rhombohedral. The crystal was set to its trigonal axis on arcs graduated to read to $0{\cdot}1°$, using fortunately-placed equatorial spots, with the beam parallel to an arc. The crystal was then displaced by three known amounts and in each case 120° double oscillation photographs were used to determine the known arc corrections, with the following results:

	Observed		True	
(i)	T	1·3°L	T	1·4°L
	B	0·0°	B	0·0°
(ii)	T	$1{\cdot}4_5$°L	T	1·4°L
	B	$1{\cdot}4_5$°R	B	1·6°R
(iii)	T	1·5°R	T	1·8°R
	B	3·7°R	B	3·8°R

These results achieve our usual degree of accuracy, and the method has since proved useful in setting crystals of rhombohedral perryite (Reed, 1968) to their trigonal axes.

Theory

Fig. 1 shows a stereographic projection of a crystal with rotation axis S at $(0, 0°)$ and a reciprocal lattice point (relp) at R given by (ξ, ζ, φ) in cylindrical polar coordinates. The radius of the stereogram is chosen to make $SR = \xi$. The crystal is now tilted so that S is displaced to S'

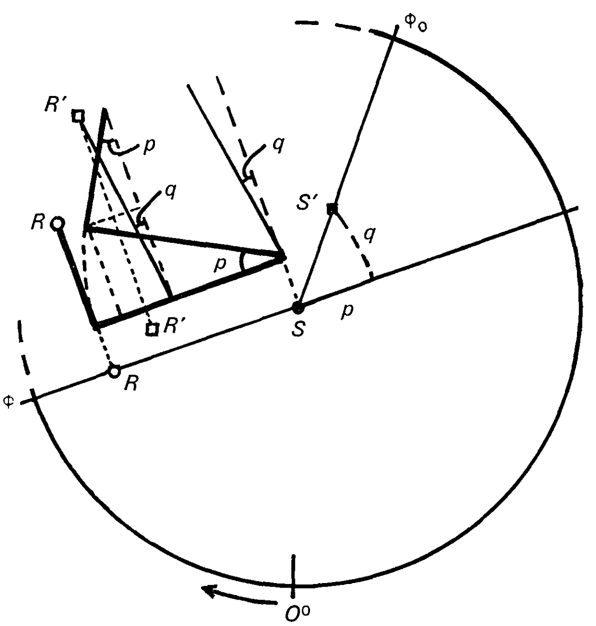

Fig. 1. Stereoscopic projection of a crystal with rotation axis S at (0·0°) and reciprocal lattice point at $R(\xi, \zeta, \varphi)$.

at (ϱ, φ_0) and R is thus displaced to R' at (ξ', ζ', φ'). The tilt angle, ϱ, can be resolved into components p and q, respectively parallel and perpendicular to SR, and given by:

$$\tan p = -\tan \varrho \,.\, \cos(\varphi_0 - \varphi) \qquad (1)$$

$$\sin q = \sin \varrho \,.\, \sin(\varphi_0 - \varphi) \qquad (2)$$

where the minus sign is inserted in (1) to make p positive away from R (see below). Inset in the stereogram is an elevation along SR; from this it can be seen that the effect of p is to increase ζ to $(\xi \sin p + \zeta \cos p)$ and the additional effect of q is to make

$$\zeta' = (\xi \sin p + \zeta \cos p) \cos q \,. \qquad (3)$$

ϱ is normally a small angle ($< 5°$ say) and to this approximation $\cos p = \cos q = 1$, $\tan \varrho = \sin \varrho = \varrho$, $\tan p = \sin p$; for $\theta = 45°$, $\xi = \sqrt{2}$. (1) and (3) then reduce to

$$d\zeta' = \zeta' - \zeta = -\sqrt{2}\varrho \,.\, \cos(\varphi_0 - \varphi)$$

which is independent of ζ to the approximations assumed. The minus signs here and in (1) arise from measuring $d\zeta$ positive upwards.

In a conventional double oscillation photograph, the exposure at 0° records the measured spot at $\theta = 45°$ on the left of the photograph, arising from a relp at azimuth $\varphi = \varphi_1 = 45°$, whence $d\zeta_1 = -\sqrt{2}\varrho \,.\, \cos(\varphi_0 - 45°)$. For the exposure at 180°, the relp for the equivalent measured spot on the left is at azimuth $\varphi = \varphi_2 = 225°$, whence $d\zeta_2 = -\sqrt{2}\varrho \,.\, \cos(\varphi_0 - 225) = +\sqrt{2}\varrho \,.\, \cos(\varphi_0 - 45°)$. Hence

$$\Delta\zeta_L = d\zeta_2 - d\zeta_1 = 2\sqrt{2}\varrho \,.\, \cos(\varphi_0 - 45°) \,.$$

Similarly the reflexions on the right of the photograph have $\varphi_1 = -45°$, $\varphi_2 = 135°$, and $\Delta\zeta_R$ reduces to

$$\Delta\zeta_R = 2\sqrt{2}\varrho \,.\, \cos(\varphi_0 + 45°) \,.$$

Arc corrections are then derived from $\Delta\zeta_L$ and $\Delta\zeta_R$ in the usual way, according to the position chosen for the arcs.

For the 120° case, the first exposure at 30° gives $\varphi_1 = 75°$ on the left, and for the exposure at 150°, $\varphi_2 = 195°$. Thus

$$\begin{aligned}\Delta\zeta_L &= -\sqrt{2}\varrho \,.\, \cos(\varphi_0 - 195°) + \sqrt{2}p \,.\, \cos(\varphi_0 - 75°)\\ &= +\sqrt{2}\varrho \,.\, \cos(\varphi_0 - 45 + 30°)\\ &\quad + \sqrt{2}\varrho \,.\, \cos(\varphi_0 - 45 - 30°)\\ &= 2\sqrt{2}\varrho \,.\, \cos(\varphi_0 - 45°) \,.\, \cos 30° \,.\end{aligned}$$

Similarly by considering reflexions on the right of the photograph for which $\varphi_1 = -15°$, $\varphi_2 = 105°$ one obtains:

$$\Delta\zeta_R = 2\sqrt{2}\varrho \,.\, \cos(\varphi_0 + 45°) \,.\, \cos 30° \,.$$

Thus $\Delta\zeta_L$ and $\Delta\zeta_R$ now give arc corrections in the correct sense but underestimated by a factor cos 30°. It may be noted that while for 180° double oscillation photographs the two equivalent spots are displaced symmetrically from their true position, in the 120° case the displacements are asymmetrical.

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