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Atomic resolution in generalized crystal-structure projections.

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Generalized crystal-structure projections (Cochran & Dyer, 1952) have now been used to advantage in several investigations (e.g. Clews & Cochran, 1949; Raeuchle & Rundle, 1952; Zussman, 1953) and some of their properties have been described. There has been no discussion, however, of the way in which the shapes of atomic peaks in such projections vary with the order of the projection. This variation can be especially important when the atoms are poorly resolved.

Cochran & Dyer (1952), whose results and notation are used here, have shown that the real and imaginary parts of the generalized projection

$$\varrho_L(x,y) = c\int_0^1 \varrho(x,y,z)\exp(2\pi iLz)dz$$
$$= C_L(x,y)+iS_L(x,y) \qquad (1)$$

can be built up quite simply from the contributions of the single atoms. Thus the contribution of the jth atom to $C_L(x,y)$ is given by $\sigma_{jL}(x,y)\cos 2\pi Lz_j$, where $\sigma_{jL}(x,y)$, if circularly symmetrical, can be evaluated at $(x, 0)$ from the relation

$$\sigma_{jL}(x,y) = \frac{1}{A}\sum_h^\infty\left\{\sum_k^\infty f_j(hkL)\right\}\cos 2\pi hx\ . \qquad (2)$$

The resolution of the atoms in the real and imaginary parts of upper-level generalized projections is often better than it is in the corresponding zero-level projection since adjacent atoms, having widely different coordinates in the direction of projection, may project as distinct positive and negative peaks. In addition to this effect, however, there may be improved resolution in the plot of

$$|\varrho_L(x,y)| = \{C_L(x,y)^2+S_L(x,y)^2\}^{\frac{1}{2}}\ . \qquad (3)$$

The peak shape in such a plot is given by equation (2); it depends only on the shape of the effective scattering factor curve.

The effective scattering factor curve generally becomes flatter in shape as the level of the projection is increased, so that the corresponding atomic peak becomes sharper though smaller. The increase in resolution is most pronounced for scattering factors in which a sudden drop in amplitude as $\sin\theta$ increases is followed by a long gradual decline. It is interesting to notice here that there would be no change at all if the atomic scattering factor could be represented by a relation of the form $f(s) = N\exp(-\pi^2s^2/p)$, where $s = 2\sin\theta$, corresponding to an atom with electron density distribution given by

$$\varrho(r) = N(p/\pi)^{3/2}\exp(-pr^2)\ .$$

Peak profiles, calculated for a carbon atom situated at the origin of a cubic unit cell of side 10 Å, are shown in Fig. 1(*a*). They correspond to generalized projections with $L = 0$, 2 and 4. Fig. 1(*b*) shows the corresponding effective scattering factor curves calculated from those given by McWeeny (1951) modified by a temperature factor with $B = 5\times10^{-16}$ cm.^{2}. As an example of the practical importance of this property, Fig. 2 shows the variation in peak shape observed in the generalized projections of two atoms in acridine III (Phillips, 1950) which are separated, in projection, by a distance of about 0·7 Å. The peak height falls rapidly as the level of the projection is increased, but the resolution is at first clearly improved. The shape of the peak observed for the fifth-level is, however, similar to that observed for the zero-level projection. This is apparently a diffraction effect. It has been assumed so far that sufficient orders of diffraction have been included for there to be no errors due to termination of the series. Thus the peaks of Fig. 1(*a*) were calculated using values of $\sin\theta/\lambda$ up to 1·4,

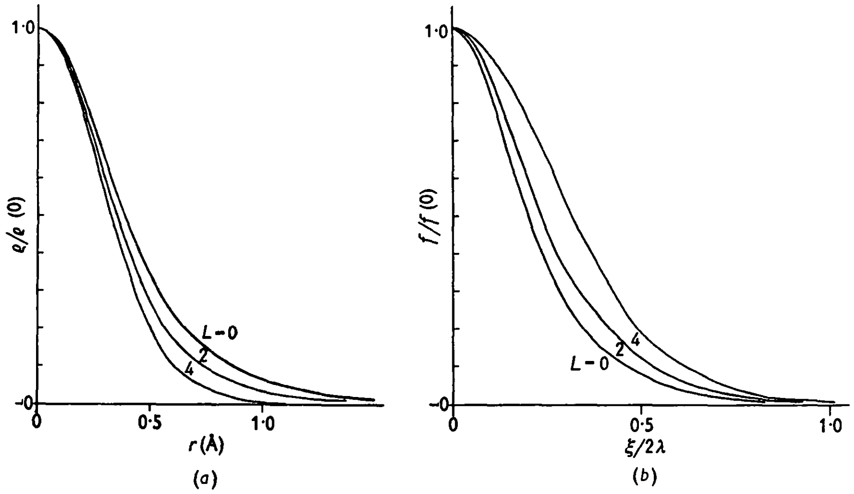

Fig. 1. (*a*) Carbon-atom profiles from generalized projections of a 10 Å cubic unit cell with (*b*) corresponding atomic scattering factor curves.

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the limit of observation for Mo $K\alpha$ radiation, at which value the f considered becomes negligibly small. If, however, the series are sharply terminated the effect under discussion may be masked. Single-atom peaks are then less sharp and are also surrounded by diffraction ripples; peaks due to unresolved atoms are correspondingly more complicated. Such diffraction effects become more serious as the level of the projection is increased since the value of f at which the series are terminated becomes an increasingly large fraction of the maximum value.

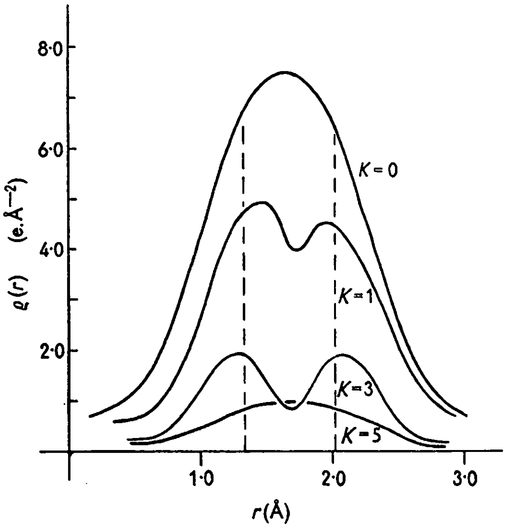

Fig. 2. Profiles of peaks due to two carbon atoms in generalized projections of acridine III. Atomic positions are indicated by broken lines.

The variation in the termination-of-the-series errors, apparent in Fig. 2, has been remarked upon by Clews & Cochran (1949). If the atoms are resolved, however, such errors can be corrected by the use of Fourier techniques (e.g. Booth, 1946) which are not so readily applicable when the atoms are unresolved. The increased resolution in upper-level generalized projections may, therefore, be useful. It must be noticed, however, that similar increases in resolution can be obtained in the zero-level projection by the use of suitable sharpening functions and, furthermore, that the resolution available by this means will be better in the zero-level than in upper-level projections because higher-order reflexions generally will be observed.* The accuracy with which the atomic positions can be determined, being dependent on the peak curvatures and hence on the peak heights, also will be greatest for the zero-level projection.

References

Booth, A. D. (1946). *Proc. Roy. Soc.* A, **188**, 77.
Clews, C. J. B. & Cochran, W. (1949). *Acta Cryst.* **2**, 46.
Cochran, W. & Dyer, H. B. (1952). *Acta Cryst.* **5**, 634.
McWeeny, R. (1951). *Acta Cryst.* **4**, 513.
Phillips, D. C. (1950). *Research, Lond.* **3**, 578.
Raeuchle, R. F. & Rundle, R. E. (1952). *Acta Cryst.* **5**, 85.
Züssman, J. (1953). *Acta Cryst.* **6**, 504.

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* I am indebted to a referee for this observation.

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The intermetallic phase $NpBe_{13}$.

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Neptunium–beryllium alloys have been prepared by the reduction of neptunium fluoride with powdered beryllium metal in vacuum at 1100–1200° C. At these temperatures the beryllium fluoride product readily distilled, leaving a fluoride-free alloy.

X-ray diffraction patterns, taken with Cu $K\alpha$ radiation (λ = 1·5418 Å) on a 14·3 cm. powder camera, showed that only one intermediate phase exists between the limits α-Np and Be at room temperature. This phase has a composition approximating to $NpBe_{13}$, and was not melted by heating to 1400° C. The alloy produced at the latter temperature was crystalline and loosely sintered. The compound is face-centred cubic, with X-ray reflections comparable in intensity to those from UBe_{13}. The lattice constant decreases from 10·266 ± 0·001 Å on the Be-rich side to 10·256 ± 0·001 Å on the Np-rich side, indicating some small range of solid solubility.

The compound UBe_{13} has been found to be isomorphous with $NaZn_{13}$ and is described by the space group O_h^6–$Fm3c$ (Baenziger & Rundle, 1949). The parameter values for $NaZn_{13}$ reported by Zintl & Hauche (1937) have been refined by Shoemaker, Marsh, Ewing & Pauling (1952). These refined parameters, $y = 0{\cdot}1806$ and $z = 0{\cdot}1192$, were used in fixing the atom positions (Fig. 1)

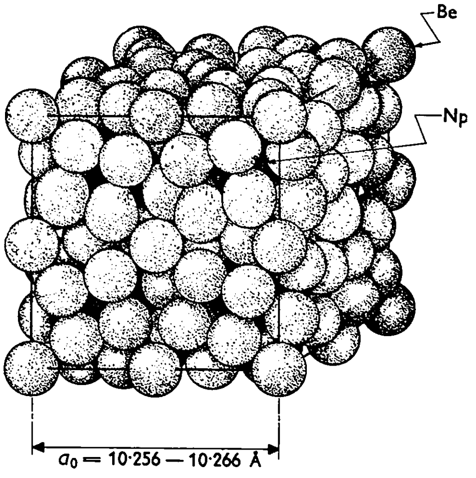

Fig. 1. The $NpBe_{13}$ unit cell.