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A method for structure determination in simple centrosymmetrical systems.

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The effect of replacing the structure factors and the cosine functions by their absolute values in the ordinary Fourier series for the electron density of a centrosymmetrical crystal has been investigated. The function thus obtained,

$$R(x, y, z) = \frac{1}{V} \Sigma\Sigma\Sigma |F(h, k, l)|\,|\cos 2\pi(hx+ky+lz)|\,,$$

shows some relationship to the electron-density function when the asymmetric unit contains a limited number of atoms.

In an area where the electron density equals zero, the function $R(x, y, z)$ will not deviate much from the mean value of the cosine functions

$$R_m = \frac{2}{\pi V} \Sigma\Sigma\Sigma |F(h, k, l)|$$

(except at some particular symmetry centers). At an atomic center, however, a peak may show up in $R(x,y,z)$ provided the electron density of the peak is comparable with R_m. When the unit cell contains only one atom in a general position, the peak electron density is larger than R_m. Peaks in $R(x, y, z)$ may, however, be distinguishable even if the corresponding electron-density peak is smaller than R_m. Thus, for simple systems, the calculation of $R(x, y, z)$ provides a direct way of determining approximate atomic positions, requiring no knowledge about the signs of the Fourier components.

By using the numerical values of the cosine functions, new symmetry elements are introduced, with the consequence that each peak is repeated at different symmetric positions in the cell. This obscures the interpretation of a $R(x, y, z)$ chart. On the other hand the symmetry elements reduce the calculation labour appreciably.

The method has been tried on a number of one- and two-dimensional examples. In the case of a two-dimensional projection of oxalic acid dihydrate, the $R(x, z)$ chart proved almost impossible to interpret. Some simpler systems, however, gave quite satisfactory results. Thus the method may be useful in favourable cases, for instance in connection with the heavy-atom technique.

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Intensity measurement in electron diffraction by means of a CdS single crystal.

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It has been confirmed by many experiments that a large photoconduction current is obtained when a CdS crystal is irradiated with X-rays and other radiations (e.g., Kallman & Warminsky, 1948; Frerichs, 1949, 1950). This crystal is now widely employed for the detection of these radiations. As far as we know, however, it has not yet been applied to the measurement of intensity in electron diffraction for which the electron-bombardment induced current could take the place of the photoconduction current. We have tried this application and obtained fairly satisfactory results.

The crystals used in this experiment were prepared by Frerichs' method (Frerichs, 1947). They have the shape of a hexagonal prism, about 0·3 mm. in diameter and 3 mm. in length. The crystal was set between two copper-plate electrodes separated by 1 mm. from each other, and the effective irradiated area was $0{\cdot}3 \times 1{\cdot}0$ mm.^{2}. The crystal was placed in the ordinary electron-diffraction camera instead of a photographic plate, and could be moved perpendicular to the incident beam by means of a micrometer head outside the camera; the specimen-crystal distance was 15 cm. The energy of the primary electron beam was about 40 keV.

On applying to the crystal an electric field of 22·5 V.mm.$^{-1}$ across the electrodes, a current of the order of 10^{-7}–10^{-4} A. was obtained from a diffracted electron beam that produced a photograph in an exposure of 1–2 sec. This is definitely larger than the dark current of the order of 10^{-8} A., and can be measured directly by an ordinary galvanometer of low sensitivity or even by a microammeter. In some crystals freshly placed in the diffraction camera, the current increases slowly and fails to reach a saturation value within an hour. However, when the crystal is kept in a vacuum for several hours or is previously irradiated with a direct electron beam (10^{-8}–10^{-9} A.), the current shows only a small after-effect. It reaches saturation in several minutes, as shown in Fig. 1 (c.f. Simon, 1953).

Sensitivity curves were obtained by holding the CdS crystal at a suitable fixed position and plotting the bombardment-induced current against the varying current of the transmitted direct beam. The latter was measured directly with a galvanometer and was assumed to be proportional to the current of the diffracted electron beam. Such sensitivity curves, obtained by increasing and decreasing the primary electron current, did not coincide. This hysteresis effect, however, was to some extent diminished by exposing the crystal to infra-red light during the measurement. The infra-red light was produced by a 1 W. miniature lamp with an infra-red filter, set closely behind the crystal. The curves obtained under infra-red illumination are shown in Fig. 2. The