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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.

The authors are indebted to the late Prof. Chr. Finbak for suggesting this work.

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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

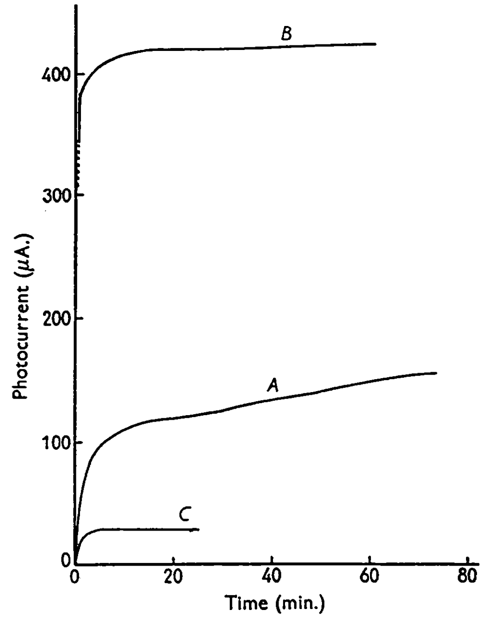

Fig. 1. Photoelectric currents in a ribbon-like CdS crystal after the irradiation with an electron beam of constant intensity. Curve *A*, for a fresh crystal; curve *B*, for a crystal previously irradiated with a strong electron beam (10^{-8}–10^{-9} A.); curve *C*, for a crystal kept in vacuum for 20 hr. The intensities of the irradiating electron beams are different in the three cases. The ratio of the ordinates of the curves does not mean the ratio of the sensitivities.

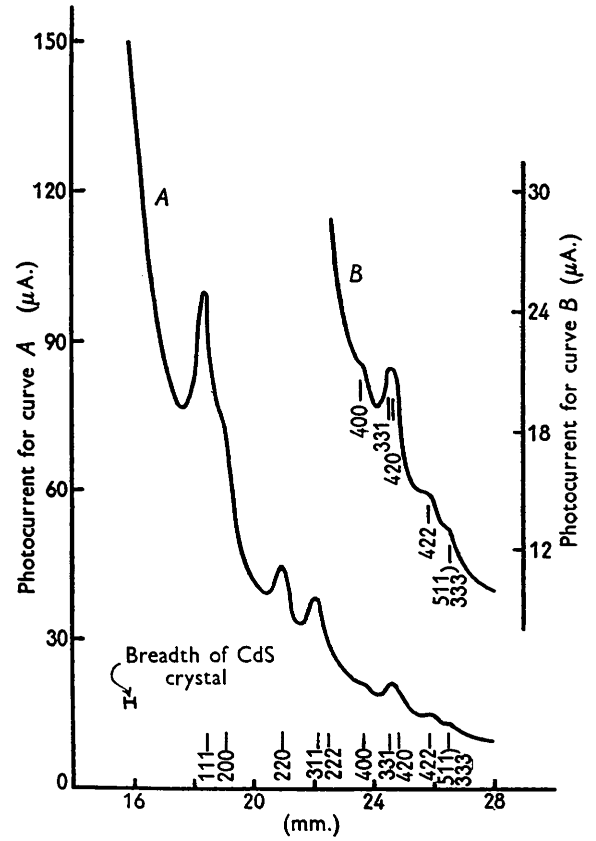

Fig. 3. Intensity curve of diffracted electrons by silver crystallites evaporated on collodion film. Right half of the curve *A* is shown magnified in curve *B*.

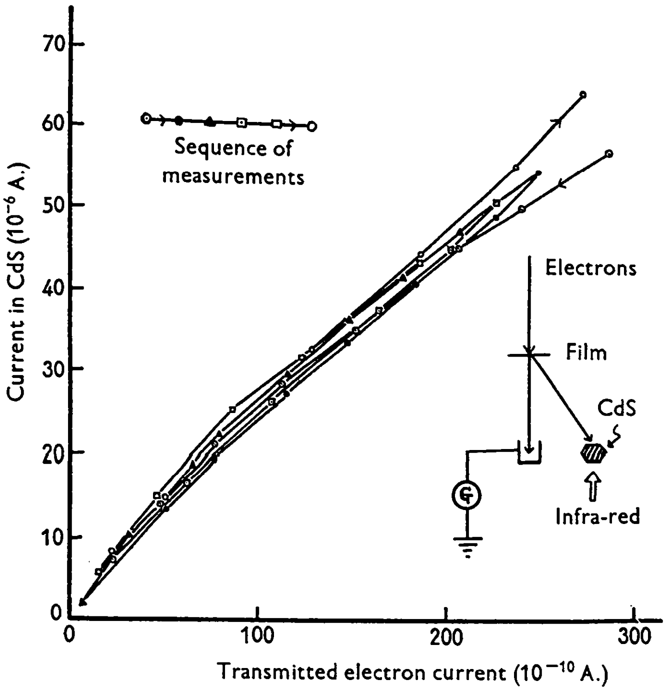

Fig. 2. Sensitivity curve. Current induced in CdS crystal by diffracted electrons is plotted against the current of the transmitted beam measured directly by a galvanometer. The arrangement of measurement is also shown schematically in the figure.

maximum difference of sensitivities on increasing or decreasing the incident electron current is about 10%. Probably it would be much diminished if the intensity of the electron current were restricted to a narrower range. Fig. 3 shows the intensity curve for electron diffraction by a polycrystalline silver film. The broadening of the diffraction lines seems to be due to the small size of the crystal grains; the estimated mean grain size is 20–30 Å. The integrated intensities obtained from Fig. 3 are compared with the values calculated by the kinematical theory. The results agree well, as shown in Fig. 4.

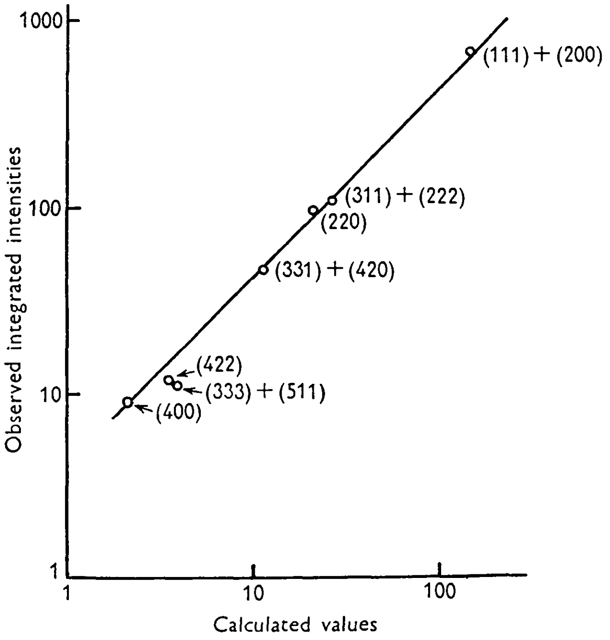

Fig. 4. Comparison of the integrated intensities obtained from Fig. 3 with the values calculated by the kinematical theory.

This agreement, however, must not be over-emphasized because the silver film used in this experiment was prepared by vacuum evaporation on collodion film and the influence of the base collodion film was only approximately taken into account. Owing to the presence of the hysteresis effect, it is too early at present to consider this method to give an accurate measurement of intensity. Still, considering the elaborate procedures needed for the photographic method and for d.c. amplification in the direct measurement of the diffracted electron current, the present simple method seems to be worthy of further investigation. Even at the present stage it can be applied for some purposes, e.g. the detection of weak halos, measurement of the widths of Debye–Scherrer rings and the rough estimate of their intensity, etc.

We express our hearty thanks to Assistant Prof. M. Eguchi of the Institute of Industrial Science, University of Tokyo, for his valuable advice and suggestions, and also for his kindness in supplying the crystals.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Thirteenth Annual Pittsburgh Diffraction Conference

The Thirteenth Annual Pittsburgh Diffraction Conference will be held on 3 and 4 November 1955 at the Mellon Institute in Pittsburgh, Pa., U.S.A. As in previous years, it is planned to hold sessions on 'Instrumentation and methods', 'Neutron diffraction', and 'Metals', with provisions also for papers on general diffraction subjects.

In so far as is possible, it is the practice at the Pittsburgh Conference to give ample time for the presentation and discussion of a limited number of papers. It is the desire of the Conference Committee this year to emphasize diffraction studies of imperfections and phase transformations, and papers pertaining to these subjects will be particularly welcome.

Titles of contributed papers should be sent to the Program Chairman, Mr W. L. Kehl, Gulf Research and Development Company, P. O. Drawer 2038, Pittsburgh 30, Pa., U.S.A., before 1 September 1955. Abstracts should be submitted by 20 September.

International Union of Crystallography

1. The Union has received a most generous donation of 10,000 Swedish crowns (approximately £700) as a contribution towards the expenses of its publications from the following Swedish Industrial firms:

Stora Kopparbergs Bergslags A. B., Falun.
Sandvikens Jernverks A. B., Sandviken.
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ASEA. Allmänna Svenska Elektriska Aktiebolaget, Västerås.
Georg Schönander A. B., Sjöbjörnsvägen 62, Gröndal.

2. With the approval of the Executive Committee, the Commission on Crystallographic Teaching has co-opted T. Watanabé (Japan).