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A simplified Fly's Eye procedure.

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The Fly's Eye (Bragg, 1944; Stokes, 1946; de Vos, 1948) is now an accepted device for use in the initial stages of a crystal-structure determination, since it enables the user to decide rapidly whether or not a proposed atomic arrangement is approximately correct (Bunn, 1945; Crowfoot, Bunn, Rogers-Low & Turner-Jones, 1949). The aim of the present note is to point out that the experimental procedure can be considerably simplified by the use of the diffraction spectrometer (Taylor, Hinde & Lipson, 1951).

The Fly's Eye is a device for making diffraction gratings with a fine structure, which can be made to correspond to the projection of a crystal structure on to one face of a unit cell; the diffraction pattern obtained by illuminating this grating with a parallel beam of light should correspond to the appropriate zone of X-ray intensities. It is customary to produce diffraction gratings with several hundred elements, but this is not strictly necessary: if only four elements, corresponding to the projection of four adjacent unit cells, are used, a diffraction pattern is obtained which is crossed by two sets of parallel, equidistant fringes, which divide it into small areas corresponding to the reciprocal-lattice points.

A typical result is reproduced in Fig. 1 which shows (*a*) the diffraction pattern of a mask representing the (001) projection of a single unit cell of *p*-di-isocyanobenzene (Hulme, 1952), (*b*) a mask representing the projection of four adjacent unit cells, (*c*) the diffraction pattern of (*b*), and (*d*) the corresponding section of the reciprocal lattice weighted with the unitary structure factors (Harker & Kasper, 1948). Comparison of (*c*) and (*d*) constitutes a verification of the approximate correctness of the structure. It should be remarked, however, that the unit cell is the primitive one containing one molecule, and not the crystallographically preferable centred cell containing two molecules. The latter could be used, but it would involve making a mask with eight molecules.

The testing of a structure takes only a few minutes unless a permanent record is required; then the photographic processes take considerably longer than the rest of the operation. In addition to rapidity, however, the process has other advantages. First, it gives an undistorted representation of the reciprocal lattice, whereas the other devices quoted necessitate distortion to a square net. Secondly, it indicates which intensities are likely to be influenced by small changes in atomic position; if a reciprocal point lies in the middle of a region of zero intensity, like the point *A* in Fig. 1 (*d*), no small change will affect it appreciably, whereas if it lies on a steep gradient, like the point *B*, its intensity may be altered greatly. The disadvantage of the method—the fact that it gives diffuse areas in place of sharp spots—is likely to be of aesthetic importance only.

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A plea for the proper use of the Hermann–Mauguin space-group symbols.

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The Hermann–Mauguin symbols for space groups are explicit about the orientation of the essential symmetry elements present in the crystal. Thus† $Pca2_1$ shows not only that there are two glide planes present, but that one is perpendicular to **a** with glide component $\frac{1}{2}$**c**, and that the other is perpendicular to **b** with glide component $\frac{1}{2}$**a**. If for reasons of convenience (or because of the accidental order in which the crystal axes were measured!) the crystal were differently oriented, it would no longer be correct to represent its space group as $Pca2_1$; it would become one of $P2_1ab$, $Pc2_1b$, $Pb2_1a$, $Pbc2_1$ and $P2_1ca$. The appropriate symbols for space groups in non-standard orientations are set out in the *Internationale Tabellen* on pp. 34–44.

Unfortunately, the power of the Hermann–Mauguin symbols to show both the orientation and the type of a symmetry element is overlooked by some workers, and this has involved the Editors of *Structure Reports* in considerable correspondence. When the absent reflexions (or tables of observed reflexions) are explicitly quoted no great harm is done, but the following examples, all

* General Editor of *Structure Reports*.

† In the new *International Tables for X-ray Crystallography* Hermann–Mauguin symbols of the type $Pca2_1$ or $P4_2/nbc$ will be printed with the nature of the axis explicitly indicated. In the *Internationale Tabellen* these were abbreviated to *Pca* and *P4/nbc*. The new usage is followed in this note, except in quoting.

taken from recent issues of *Acta Crystallographica*, show what confusion might ensue from more compressed publication.

(1) A crystal of space group $P2_1$ is said to approximate to space group $P22_12_1$. The twofold screw axis present is parallel to **c**, and the appropriate symbol for the monoclinic space group is thus $P112_1$. [There is no suggestion in the paper that the **c**-unique monoclinic convention is adopted.]

(2) In two papers there is a discussion whether a crystal belongs to *Pnma* or *Pna*. The alternatives that maintain the orientation of the axes are *Pnma* and $Pn2_1a$.

(3) The space group of a crystal is given in the abstract as *Pna*, and in the body of the paper as *Pmnc* or *Pnc*, the latter being chosen on the basis of Patterson projections. Reference to the table of observed reflexions shows, however, that the space group is correctly designated as $P2_1cn$ (or *Pmcn*). This is a possible orientation for $Pna2_1$, but not for *Pnc*2, a quite different space group (Schoenflies symbols C_{2v}^9 and C_{2v}^8 respectively).

I appeal, therefore, to authors to be careful in their use of space-group symbols, and to referees to make sure that authors' symbols are in accordance with the orientation of the observed symmetry elements. An explicit statement of the systematic absences is well worth the space it occupies.

I feel sure that accuracy in the use of space-group symbols will be appreciated by the whole body of crystallographers, and not merely by the Editors of *Structure Reports*, whose selfish interest is my excuse for raising the matter.

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Diffraction effects observed in diamond in the vicinity of the collimated incident beam.

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The presence of strong absorption conics on divergent-beam photographs of diamond (Lonsdale, 1947; Grenville-Wells, 1951) indicates that there should be a diminution in the intensity of the transmitted beam when the crystal is in the Bragg position, an effect which was demonstrated by early ionization spectrometer measurements (Bragg, 1914). An attempt to observe this photographically with Cu $K\alpha$ radiation, monochromatized by reflexion from a calcite crystal, was made for the 111 reflexion from a diamond plate.

The experimental technique involved setting the crystal plate with the (111) plane in question vertical, and taking a series of equal exposures of the transmitted beam on the same film for rotation of the crystal through the Bragg position, the unit of rotation being 3 min. of arc. Using suitable exposures (about 10 sec. with the experimental arrangement used) a slight diminution of intensity was observed.

For exposures about twenty times as long, however, the effect shown in Fig. 2 was obtained. When the Bragg reflexion flashed out, a satellite reflexion appeared at the side of the transmitted beam on the side on which the Bragg reflexion occurred, and this was similar in shape to the Bragg reflexion apart from the fact that one side of the satellite overlapped the central spot. (There is a small tail of white radiation also to be seen on the other side of the central spot. By re-orientation of the crystal the satellite observed in the Bragg position can be obtained overlapping this 'white radiation' tail and extending beyond it.)

The most probable explanation of the appearance of the satellite reflexion seems to be in terms of multiple reflexion, as shown in Fig. 1. Such an effect must in fact occur, but its intensity would presumably be strongly dependent on the shape, size and texture of the crystal, and for the small crystals customarily used in X-ray diffraction work, which are completely bathed in the incident beam, the whole reflexion would lie within the incident beam itself, and could not be separately detected. One might, however, expect to find such an effect for large, rather monolithic crystals, particularly when these are in the form of plates, so that there could be a considerable extension of the area available for this multiple reflexion without a corresponding increase in thickness.

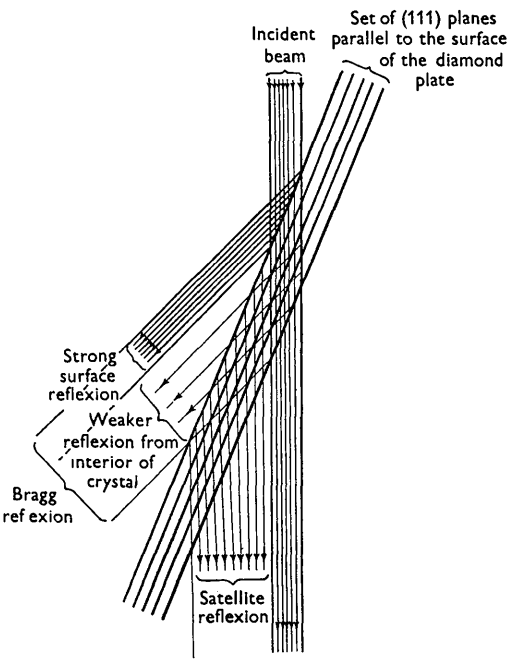

Fig. 1. Explanation of satellite reflexion.

In the course of an extended investigation on diamond, many large crystals of suitable type were examined, and quite complex patterns were found in the immediate vicinity of the undeviated beam, using copper radiation. Fig. 3 shows such a pattern from a polished diamond plate, approximately 1·5 mm. thick and about 5 mm. in diameter, on a cylindrical Laue photograph (radius