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.

*Acta Cryst.* (1952). **5**, 146

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

By H. J. Grenville-Wells, *University College, London W.C. 1, England*

(*Received* 16 *July* 1951 *and in revised form* 16 *September* 1951)

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.

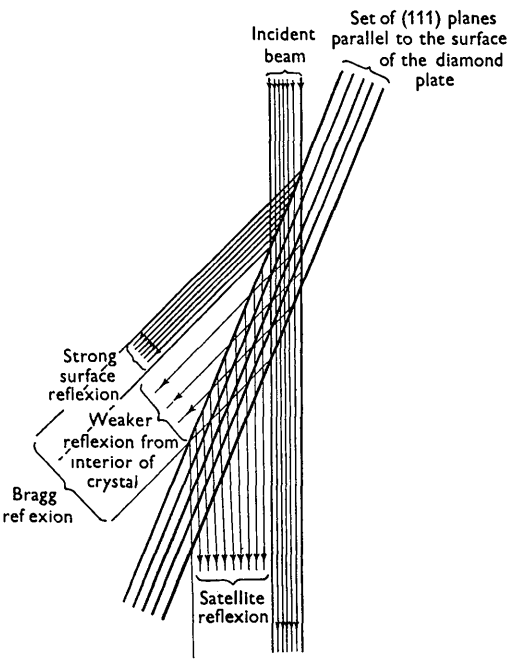


Fig. 1. Explanation of satellite reflexion.

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

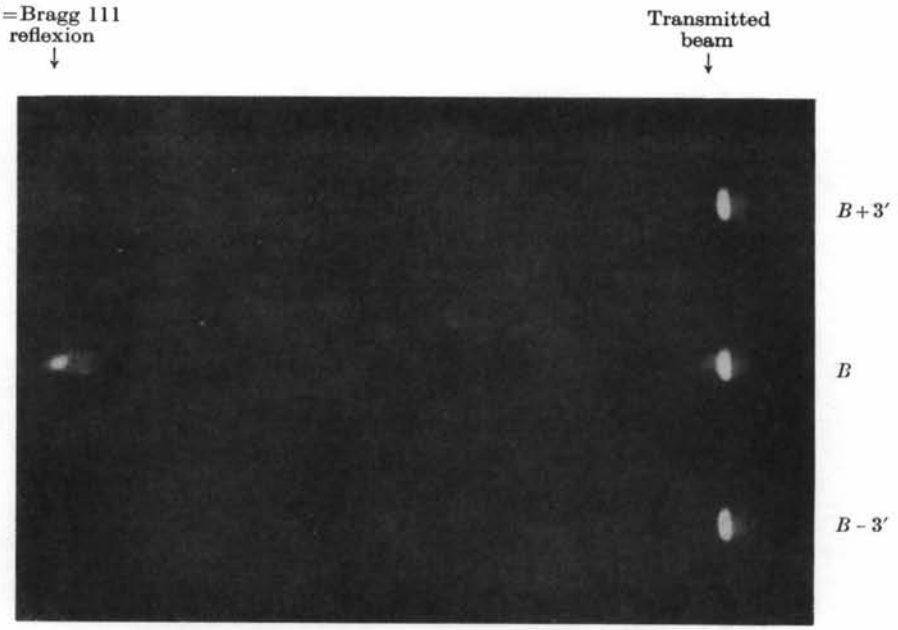


Fig. 2. Diamond. Cu $K\alpha$ radiation (monochromatized); [1$\bar{1}$0] vertical.

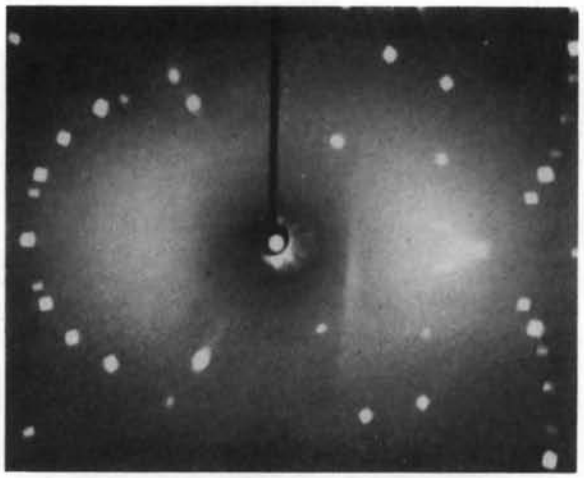

Fig. 3. Diamond plate. Cu $K\alpha$ radiation (Ni filter); 30 kV.; 15 mA.; 4½ hr.; [1$\bar{1}$0] vertical.

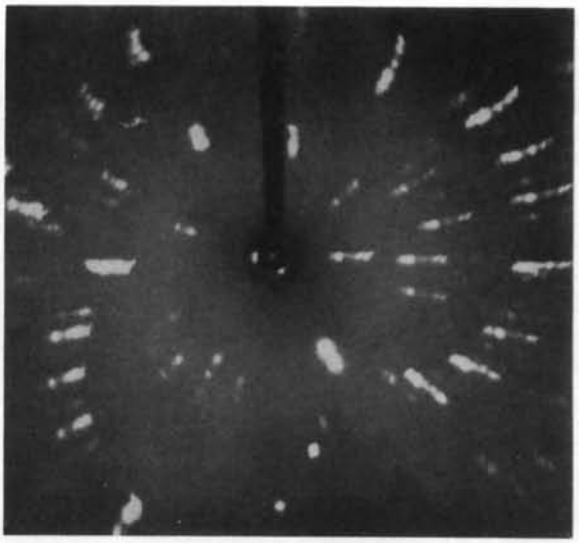

Fig. 4. Diamond No. 227. (Cu+Zn) radiation (unfiltered); 40 kV.; 10 mA.; 1½ hr.

[*To face p.* 146

3·0 cm.) using a 1·0 mm. collimator. Here the pattern is rather irregular, and does not show very obvious association of the central beam pattern with strong Laue spots. This diamond is one which shows the anomalous X-ray reflexions (Lonsdale, 1942) very strongly, but a central-beam pattern is also observed for diamonds which do not do so.

Fig. 4, however, which was obtained with a brown diamond from Premier Mine, South Africa (British Museum (Natural History); 1910, no. 227) shows a marked correlation between the Laue pattern and the central-beam pattern. Presumably in this position the strong Laue spots really do correspond to the most strongly reflecting planes.

It should perhaps be mentioned that this pattern is not due in any way to the beam-trap itself. For precisely the same experimental arrangement, the pattern is quite different for different diamonds, and alters for the same diamond when the orientation is altered. It remains the same, however, for the same diamond in the same setting with a different beam-trap.

For the diamond plate used in Fig. 3, a slight improvement in the clarity of the pattern resulted when the radiation was filtered with nickel foil, which suggests that the pattern is due to the characteristic Cu $K\alpha$ radiation, whereas on a Laue photograph multiple reflexion would result for any wavelength actually producing a Laue spot (though of course filtering also reduces the continuous radiation to some extent). This question might be cleared up by taking comparative photographs with the crystal in the Bragg position and a few degrees away from it, or by using the same setting and different radiations. Further experiments with monochromatic radiation are also required, but it is not possible for the author to continue this work, and these preliminary results are therefore placed on record.

I am indebted to the British Museum (Natural History), Mr B. W. Anderson and Mr P. Grodzinski for the loan of diamonds used in this investigation. It is a pleasure to thank Prof. Kathleen Lonsdale, F.R.S., for the interest she has taken in this work, and for helpful discussions.

## References

Bragg, W. H. (1914). *Nature, Lond.*, **43**, 31.
Grenville-Wells, H. J. (1951). Thesis, London.
Lonsdale, K. (1942). *Proc. Roy. Soc.* A, **179**, 315.
Lonsdale, K. (1947). *Philos. Trans.* A, **240**, 219.

*Acta Cryst.* (1952). **5**, 147

## A method of deriving crystal geometry from random rotation photographs.

By H. J. Grenville-Wells, *University College, London W.C.* 1, *England*

(*Received* 16 *July* 1951)

In the course of investigations of the nature of crystalline inclusions in diamond (where it is often difficult to obtain rotation photographs of the inclusion orientated with a prominent zone axis as rotation axis) an attempt was made to interpret rotation photographs of a crystal in a random orientation by a method analogous to the general solution of powder photographs from crystals of any symmetry applied by Ito (1949).

The values of $1/d^2_{hkl}$ for all the reflecting planes in the crystal can be obtained from random rotation photographs just as they can be found from a powder photograph. The reflexions can in general be indexed in terms of an arbitrary unit cell defined by the three planes of largest spacing. If these are unsuitable for some reason, such as that they are all orders of the same reflexion, or that all three planes lie in the same zone, then combinations involving the next one or two planes will be necessary. The unit cell obtained in this way will not, however, necessarily exhibit the symmetry of the Bravais lattice of the crystal, and the problem is now to discover what that symmetry really is. This can be done graphically from the arbitrary cell, but can also be done—in terms of an elegant reduction process devised by Delaunay (1933)—quite mechanically by means of a tetrahedral diagram (a paper on this subject is in the course of preparation).

If a single crystal of the substance, and not merely a powder, is available, a very powerful modification of this method can be employed by making use of multiplicities. When a rotation photograph is taken of a single crystal in a random orientation, each spot will in general be produced by reflexion from one side of one set of planes, and thus the number of spots on any Debye ring of constant $\theta$ will be equal to (or less than) the multiplicity of the form of planes $\{hkl\}$ producing them. Theoretically it should be possible to obtain the multiplicities of various reflexions by comparing the intensities on a rotation photograph and on a powder photograph of the same crystal.

The system, and indeed the Laue group, to which a crystal belongs can be determined almost by inspection. On a rotation photograph of the usual type, recorded on a cylindrical film whose axis coincides with the axis of rotation, any plane $(hkl)$ produces two spots above the equator, while $(\bar{h}\bar{k}\bar{l})$ produces two spots below the equator. Hence the multiplicities on one half of the film (the division being taken in practice parallel to the rotation axis) correspond to those conventionally listed in tables. Accidental coincidences of spacing can usually be detected by differences of intensity among the spots on a single Debye ring, due allowance being made for the increase of intensity on moving away from the equator (Cox & Shaw, 1930).

If there is no multiplicity greater than two, then the crystal is triclinic. For the monoclinic system there will only be multiplicities of two and four, whereas in the orthorhombic system, eight will appear, and so on. If the planes are then arranged in groups of the same multiplicity, relationships can be found much more easily than when all the reflexions from the crystal are considered together.

This method has an advantage over the general powder