Short Communications

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Identification of the rhombohedral lattice in CdI_2 crystals.

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A new method is described by which a rhombohedral lattice may be distinguished from a hexagonal lattice in CdI_2 crystals. Two rows of spots, $10.l$ and $20.l$, from the same crystal of a polytype are recorded side by side on the same photograph, are compared and the lattice identified.

Hitherto, distinguishing between a rhombohedral lattice and a hexagonal lattice in CdI_2 crystals has been done by comparing a Weissenberg or an oscillation photograph of any polytype with a corresponding photograph of a basic polytype $2H$ or $4H$. This involves two photographs of two different crystals having different central spots and maybe with different shrinkage factors and therefore makes the method impracticable for higher polytypes. In the present paper a new method in which, instead of comparing two photographs, two rows of spots, *i.e.* $10.l$ and $20.l$, from the same crystal of a polytype are recorded side by side on the same photograph, are compared and the lattice identified.

In principle it is simple to distinguish a rhombohedral lattice from a hexagonal lattice. One can observe the symmetry of spots either about the zero layer line in a c-axis oscillation photograph or about the central Laue streak in an a-axis Weissenberg photograph. But these simple methods could not be used in most of the cadmium iodide crystals. In CdI_2, c-axis oscillation photographs usually show streaking and smearing of the diffraction spots (Trigunayat & Verma, 1962), rendering it almost impossible to scrutinize the distribution and symmetry of spots about the zero layer line. Secondly cadmium iodide crystals grow as platelets and owing to heavy absorption the spots near the central Laue streak, which are the transmission spots, generally do not appear. Besides, most of these crystals consist of two or more polytypes occurring in syntaxic coalescence; these transmission spots consist of a mixture from the various types. Therefore, in order to identify the polytype it is compared with a standard $4H$ polytype. For all hexagonal polytypes of the compound the range 10.0 to $10.n_1$ for a n_1H type coincides exactly with the range 10.0 to $10.n_2$ for a second n_2H type. On the other hand, if the polytype has a rhombohedral cell and is indexed on hexagonal axes the reciprocal axes are those for which the algebraic sum $(-h+k+l)$ is divisible by 3. The reflexions which should have coincided with $2H$ or $4H$ are missing. Therefore for a rhombohedral lattice none of its spots coincide with those of hexagonal type $4H$ (Chadha & Trigunayat, 1967). Higher polytypes give small spacings between the $10.l$ spots; it then becomes impossible to say whether the spots coincide or not and it is difficult to identify the polytype.

Instead of comparing two different photographs, if we compare the different rows of spots in the same photograph we can identify the polytype more easily. From the spacing of the spots alone the polytype can be nH or $3nR$. Assuming the type to be hexagonal we can find the set of points in two different rows, *i.e.* $10.l$ and $20.l$, which have the same angle of diffraction and therefore should be recorded at the same point on the photograph. Out of the set we can choose one l_1 and l_2 which could be recorded on the same side of the photograph. Therefore, a photograph is taken in the range 25–40° to record $10.l$ spots. Then the film is moved slightly along the a axis (in a Weissenberg Camera) and another exposure is given in the range 5–20° which will record $20.l$ spots on the same side of the photograph. If we calculate the angle of diffraction, θ_{hkl}, from

$$\sin \theta_{hkl} = \tfrac{1}{2}[(h^2+hk+k^2)a^{*2}+l^2c^{*2}]^{1/2}$$

we can find which l_1 in $10.l$ has the same angle as l_2 in $20.l$. Therefore, by indexing the two rows of the photograph (assuming the type to be hexagonal) we can look for l_1 and l_2. If they coincide (lie side by side) the type is hexagonal and if they do not coincide it is rhombohedral. In a rhombohedral lattice the l_1th spot in the $10.l$ row is not $3l_1$ but $3l_1+1$, since $-h+k+l=3n$, and the spots which appear in the $10.l$ row are $l=1,4,7,\ldots$. Similarly the spot l_2 is $3l_2-1$ since the spots which appear in the $20.l$ row are $l=2,5,8,\ldots$. The angles for rhombohedral spots are not the same for l_1 and l_2, therefore they will not coincide. In this way, we can decide if the lattice is rhombohedral or hexagonal.

Example. For a type $16H$ with $a=b=4{\cdot}24$, $c=54{\cdot}68$ and $\lambda=1{\cdot}54$ Å, the l_1 and l_2 which have the same angle of diffraction are ($l_1=45$, $l_2=37$); ($l_1=51$, $l_2=44$); ($l_1=58$, $l_2=52$) in the above-mentioned range of oscillations. In Fig. 1(*a*) the 51st spot in $10.l$ coincides with the 44th spot in $20.l$; therefore the type is hexagonal. In Fig. 1(*b*) the 51st spot is shifted from the 44th by about 2/3 of the spacing between the spots, therefore the type is rhombohedral and is $48R$.

References

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Trigunayat, G. C. & Verma, A. R. (1962). *Acta Cryst.* **15**, 499–504.

(a)

(b)

Fig. 1. X-ray oscillation photograph in the range 25–40° (upper row) and 5–20° (lower row) of the polytype (a) 16*H* (b) 48*R*. Cu $K\alpha$ radiation; camera diameter 5.73 cm; the *l* value of one spot in each row is marked on the photograph.

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