Identification of the rhombohedral lattice in CdI$_2$ crystals. By G. K. CHADHA, Department of Physics and Astrophysics, University of Delhi, Delhi-110007, India

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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, 10.0 and 20.0, 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. 10.0 and 20.0, 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 syntactic 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$_1$H type coincides exactly with the range 10.0 to 10.n$_2$ for a second n$_2$H 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 10.0 spots; it then becomes impossible to say whether the spots coincide or not and it is difficult to identify the polytype.

Example. For a type 16H with a = b = 4.24, c = 54.68 and $\lambda$ = 1.54 Å, the 1$_1$ and 2$_2$ 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 10.0 coincides with the 44th spot in 20.0; 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


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