

It was established that the frequencies of occurrence of layers o and t (representing here structures 2H and 4H) in a polytype cell are correlated with relative stabilities of basic structures 2H and 4H in given conditions. It was observed that in some specific conditions pure large polytypes form, in others disordered structures occur frequently. The mechanism of formation of polytype structures in CdI₂ is in case (i) the competition between 2H- and 4H-type stackings of molecular layers and in case (ii) the competition between differently oriented domains of 4H-type stackings (e.g. a slip along [11.0] direction and generation of fault sequences f4f5). The present study do not allow us to decide in which way the inter-phase boundaries created during growth are repeated periodically and form large period polytypes.

20.3-5 SOME ASPECTS OF SYMMETRY OF POLYTYPE STRUCTURES MX₂. By B.Pałosz and S. Gierlotka

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Determination of the symmetry of a polytype may be performed directly on the basis of X-ray pattern, while the determination of the space group is possible only after complete determination of the layer stacking of a polytype cell. The information of a space group of a polytype is practically useless in the analysis of the reasons for polytypism and in the description of the structural behaviour of the crystals. For the characterization of polytype structures we suggest the use of the t-o-f molecular layer notation [Pałosz, B. Z. Krist. (1980) 155, 51-72] where the sequences which form polytypes may be divided into hexagonal- and rhombohedral-type stackings. In this notation it is clearly seen that hexagonal and rhombohedral structures are fully equivalent structures: a hexagonal cell may in some cases be constructed only of rhombohedral-type arrangements of layers of which a rhombohedral cell may also be composed. Similarly, hexagonal-type arrangements of layers may form hexagonal as well as rhombohedral polytypes. The existence of such semi-hexagonal and semi-rhombohedral structures have been confirmed experimentally in a tens of identified polytypes of CdI₂ and SnS₂; Pałosz, B. Acta Cryst. C39 (1983) 1160-1165, Pałosz, B., Pałosz, W. and Gierlotka, S. Acta Cryst. (1984) submitted.

20.3-6 POLYTYPISM, SUBGROUP RELATIONS AND SUPERPOSITION STRUCTURES. By O. Jarchow, Mineralog.-Petrogr. Inst. der Universität Hamburg, Grindelallee 48.

A new method of derivation and description of polytype structures will be presented. All space groups of the hexag. and tetragonal system and their subgroups are decomposed in layer groups parallel and perpendicular to the symmetrical directions and arranged to the a₁b₁ plane of layer dimensions. For space groups and their subgroups of the 6mm and 4mm point groups existing only one kind of layer groups in every space group. In all the other space groups their exist two maximum and one minimum layer groups, with the minimum group as common subgroup in the both max. groups. All in all we find 409 different sequences with maximum and 212 with a minimum symmetry of the layers.

As known from disordered polytypes, pseudo-translations a/2; a/4; (-a+b)/3 etc. between adjacent layers give rise to sharp and diffuse spots in diffraction images. The sharp spots belong to a superposition structure (SPS) with a regular space group (Dornberger-Schiff, 1964), that means, they belong to one of the regular sequences. The transition from SPS to polytypes may be described by transformations like ma, nb, pc. These transformation matrices together with the symmetry of the SPS give the entrance of tables, which allow to determine the different classes of polytypes. From other tables, containing the transformed symmetry operators, we get the informations about space group and partial operators. To avoid a description by partial symmetry operators, we take in account the strong relations between polytypes and their SPS.

Above all the MDO concept of Dornberger-Schiff (Abh. Dt. Akad. Wiss. 1964) about polytypes with maximum degree of order has given new advances in structure determination of polytypes. It will be shown, that these MDOs are in close relationship to twin- and antiphase domains defined by Wondratschek & Jeitschko (Acta Cryst. A 32, 664) and that the use of group-subgroup relations have also many advantages in derivation and description of polytypes.

By generalisation of the procedure in a simple way it is also possible to include polytypes without SPS and also with different kind of layers.

The usefulness and practical application of the method will be demonstrated on some examples.