20. X–1 INTERRELATING CBED GROUPS AND SPACE GROUPS; A CASE FOR I.T. INCLUSION?

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The symmetries of zero-layer CBED zone-axis patterns form groups isomorphous with the Alexander and Hermann space groups of 2-dimensional layers (Zeits.Krist.(1929) 70,328) . These groups in turn are lattice ("klassengleich") subgroups of specific 3-dimensional space groups.

This suggests a 2-step logic in space group identification from CBED data.

International Table listings have so far not included "sub-periodic" groups. In the case of the layer groups this may have been advantageous in that, in the absence of any over-riding necessity, this has permitted experimentation with notations suited to different specialist applications (e.g. Wood,E, Bell Sys.Tech.Journ.(1964); Pond R.C. and Valchavis,D.S. Proc.Roy.Soc.(1983) A 386 ,95).

Recent experience suggests that, as with the 3-dimensional space groups (Hall,S.R.Acta Cryst. (1981) A37 517), an explicit, generator-based listing can provide a valuable aid to identification of space groups and their subgroup relationships.

20. X–2 MODULATED STRUCTURES IN ALLOYS.

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A survey is given of the X-ray diffraction and electron microscopy and diffraction studies on the modulated structures in ordered alloys. The long-period structures in alloys often show incommensurate character. The well-known examples are seen in the one-dimensional antiphase domain structures (1d-APS) based on the $L1_0$ or $L1_2$ structure. Antiphase domain sizes M's estimated from the diffraction patterns are in general non-integral multiples of the basic cell. The fractional property of M value is interpreted in terms of the uniform mixture of domains with different sizes, and actual mode of domain mixing revealed by high resolution electron microscopy study agrees with this prediction. In the two-dimensional antiphase structures (2d-APS), on the other hand, it is very difficult to visualize the actual domain configurations in real space from the diffraction study alone: the M's in the two directions are generally not equal and vary with composition. However, high resolution structure images can reveal the incommensurate structures in an atomic scale, and the technique has been applied successfully to several alloys, Au-Zn, Au-Mg, Au-Mn, Cu-Zn-Au, etc. It is particularly interesting that incommensurate structures of the Au-Zn alloys containing 16-19 at.% Zn consist of two types of "domains" with commensurate structures of the same unit cell size and they are arranged in such a characteristic way that the incommensurate periods are produced in the two directions, [100] and [001]. The high resolution images give information on the density modulations as well existing in the incommensurate structures. However, the details of the modulation waves including displacement modulation are obtained only from the analyses of diffraction data.

20. X–3 POLYTYPISM AND THE OD THEORY

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The phenomenon of polytypism was discovered by Baumhauer (Z. Krist. (1912) 50, 33; (1915) 55, 249). The chief concern of those investigating this phenomenon was to find a correct answer to the generation of almost limitless number of polytypes of a substance, some of which possess giant-sized unit cells. A great number of polytypic substances has since been found, numerous polytypes have been discovered and notation systems to describe their structures proposed. Recently also physical properties of polytypes attracted attention since these depend on the actual stacking of layers (e.g. Brafman and Steinberger, Phys. Rev. (1966) 143, 501), and thus a "fine tuning" of properties in a purely structural way, without admixtures, might well be possible. There is also growing tendency to use polytypes of some phyllosilicates as indicators of their genesis (typomorphism). Although polytypists were aware of the peculiar geometry of their structures, the symmetry of polytypes was virtually never investigated in detail.

Independent on polytypism, Dornberger-Schiff (Acta Cryst. (1956) 9, 593) developed her theory of OD structures to explain the disorder phenomena exhibited by β-wollastonite and Madrell salt since it became evident that the behavior of these structures cannot be adequately described in terms of space-group crystallography. The OD structures consist of 2D-periodic disjunct parts of crystal space a) all geometrically equivalent or relative few in kind, b) with identical translation groups or with a common subgroup, c) stacked so that the layer pairs of the same species remain equivalent in structures of the same substance (family), and d) with ambiguity of stacking at every layer boundary. The letters OD mean that these structures can be periodic (ordered) as well as aperiodic (disordered), but the possibility of being disordered is inherent to them. In contrast to fully ordered structures, the set of relevant coincidence operations expressing their symmetry does not form a group, but only a groupoid, since some of these operations are partial. The apparatus of the OD theory contains classification schemes, the list of all OD groupoid families for structures of equivalent layers, the methods to calculate the number of equivalent positions of any OD layer relative to its predecessor, the procedures for systematic derivation of all structures of maximum degree of order (MDO structures), for the choice of OD layers, and procedures to determine the symmetry principle from diffraction patterns (for references see Dornberger-Schiff, Cryst. Res. and Technol. (1979) 14, 1027).

An analysis of dozens of structures described as polytypic revealed that all of them are OD structures. Hence the OD theory can be considered as the theory of symmetry of polytypes. The recognition of these facts can bring advantages for the study of polytypes in an analogy to those brought by the space-group theory for the traditional crystallography. Among others, it makes it possible to correlate the physical properties of polytypes with their full symmetry, it suggests a new definition of crystalline substances and thus it opens the way for the development of a generalized crystallography.