

20.4-10 SUPERSTRUCTURES IN WURTZITE AND SPHALERITE LATTICES BY CONVERGENT BEAM ELECTRON DIFFRACTION AND LATTICE IMAGING

by A.F.Moodie and H.J.Whitfield CSIRO Division of Chemical Physics, P.O.Box 160, Clayton, Victoria, Australia 3168.

A combination of X-ray diffraction, convergent beam electron diffraction and high resolution electron microscopy has been employed in the determination of the structures of a number of materials which exhibit a high degree of polytypism.

These materials are of Grimm-Sommerfeld type with lattices of mixed sphalerite-wurtzite character, typically having stoichiometries 26, 156,  $1_2 246_4$ , 245<sub>2</sub> or 23<sub>2</sub>45<sub>4</sub>.

Some of the key structural elements identified using convergent beam diffraction and lattice images are clearly revealed in color-encoded electron micrograph images. Color encoding was done using a two-channel (red and green) parallel processing operation in a long focal length incoherent optical processor.

20.5-2 CRYSTAL-SETTING AMBIGUITIES, THEIR RELATION TO CRYSTAL ORIENTATION AND TWINNING BY MEROHEDRY. By Y. Le Page, Solid State Chemistry, NRC of Canada, Ottawa KIA OR9, J.D.H. Donnay and Gabrielle Donnay, Geological Sciences, McGill University, Montreal, Canada H3A 2A7.

Any crystal whose point group is a subgroup of index  $p$  of its lattice symmetry (merohedral crystals,  $p=2,4$  or 8) can be referred to  $p$  non-equivalent possible settings of the coordinate axes. These settings, together with the relevant transformation operation, are given for the 44 oriented point groups in terms of the triplet of indices  $\underline{h\ k\ l}$  into which the original  $\underline{hkl}$  transforms. If one such set of reflection intensities is published with a structure determination of a merohedral crystal, the chosen setting can be identified. Reflections unsuitable for orientation use are tabulated. If crystallographers could agree to place the most intense reflection into a specified asymmetric domain of reciprocal space for the point group associated with the lattice symmetry, a unique orientation of co-ordinate axes would be obtained at the start of any investigation and no intensities would have to be published. The Table of transformation operations is also a Table of twin laws in twinning by merohedry: each transformed symbol  $\underline{h\ k\ l}$  represents the reflection which, on the diffraction pattern of the twin, contributes its intensity to that of  $\underline{hkl}$ . The reflections unsuitable for orientation purposes are 'twin-proof' in that their intensities are not affected by twinning; they are of the greatest help in structure determinations based on twin data.

20.5-1 KINETIC AND STRUCTURAL GROUNDS OF GROWTH TWINNING. By O.G.Kozłowa, Crystallography and crystallochemistry chair, Moscow University, USSR.

Kinetic, morphological and structural studies of diphenyl, silica, mica and plagioclase crystals gave the possibility of finding kinetic and structural grounds of their growth twinning. For different crystals crystallographic zones and coalescence faces are different. Twinning is contributed by conditions stabilizing twinning zone faces.

The symmetry element produced must be localized on twin borders.

Germination twin's generation is connected with small atomic displacements near the twinning zone faces. A highly symmetric transition layer is formed in this way. The atomic displacements are caused by mechanical and isomorphous admixtures, external forces and tensions, modification and temperature changes.