05. PHYSICAL PROPERTIES AND STRUCTURE

05.1-4 HIGH RESOLUTION TEM STUDY OF 2H-TaSe 2 AT LOW TEMPERATURES. By T. Onozuka,* N. Otsuka and H. Sato, School of Materials Engineering, Purdue University, West Lafayette, IN 47907, U.S.A.

The hexagonal incommensurate phase of 2H-TaSe 2 has been investigated by means of high resolution transmission electron microscopy with the resolution of 3Å at 85K and 120K. The temperature dependence of the orientation, the intensity and the width of stripe patterns (with the width of around 300 Å at 97K) which appear in the incommensurate phase has been investigated along with the lattice fringes of around 9 Å. These results can be summarized as follows: The stripe patterns are proven to be interference fringes due to the primary and secondary diffraction beams from the incommensurate phase. The incommensurate phase is hexagonal at higher temperatures but at least one of Q (modulation) vectors shift slightly as the temperature is lowered and the structure deviates from the hexagonal symmetry. The distortion is observed magnified as the rotation of the interference fringes. The fringes do not have any relation to the discommensuration as confirmed by the observation of the lattice fringes. The double honeycomb model for the incommensurate hexagonal phase can be denied definitely.

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05.1-6 SUPER-LATTICE MELTING IN AgO.35Ti 2.

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In the system Ag-Ti 2 there are two structurally related phases, being a first- and a second-stage intercalate of silver in the layered compound Ti 2 . In both phases silver atoms are on part (or all) of the sites of triangular lattice planes; which are 12.2 Å apart in the second-stage phase and 6.4 Å apart in the first-stage phase. Both phases show fast-ionic conduction of silver.

Single crystals of first-stage AgO.35Ti 2 were grown by vapour transport. The three-dimensional melting of the silver sublattice, as reported recently, has to be of second-order nature, was studied by single crystal X-ray diffraction. A superstructure a = a/3 = 2c, space group P31c is present at 110 K; the order-disorder transition to the substructure with a = 3.428 Å, c = 6.398 Å, space group P31m, was studied by measuring the super reflections on a CAD-4 diffractometer as a function of temperature). In this way the temperature dependence of the occupancy of the silver sites in P31c; 2a, 2c and 2d, could be determined, T c = 301 K.

2) J.L. de Boer and A.J.M. Duijnsenburg. This conference.

05.1-7 POLYTOPISM AND PHASE TRANSITION OF Sb 2 O 7.

I. THE INTERLAYER INTERACTIONS. By H. Ahsbahs, E. Hellner, Institute for Mineralogy, and D. Reinen, Institute for Chemistry, University of Marburg, Lahnberge, 3550 Marburg, FRG.

At 298K and Ibar Cs 2 PbCu(NO 2 ) 6 crystallizes with an elpasolite-related structure. Caused by the Jahn-Teller effect in the 'Eg ground state of Cu * (eE vibrionic coupling) the lattice symmetry is reduced to orthorhombic (Pnma: a=11.04(1), b=11.01(1), c=10.74(1)). The Cu(NO 2 ) 6 octahedra are tetragonally elongated; the co-operative order is antiferrodistortive, though there are three dimensional as in the a-modification (S. Kramer, Thesis, Freiburg (1978)) and found three basic types of pseudo trigonal symmetry are possible against each other and coupled by the intermediate iodine ions. Since the Sb of the SbOy-prism can occupy two equivalent positions, neighboring layers may be identical or enantiomorphic to another; therefore two basic structural units exist: the centrosymmetric type 2MC (modifed Ramsdell notation) and the centric 2MA (V. Kramer, Acta Cryst. (1978), B31, 254; (1978) B36, 2695). Eight higher polytypes, combinations of both, are identified till now, and among these there are three types with eight layers as the maximum stacking period.

The ferroelastic room temperature phase of all polytypic modifications is characterized by an antiferroshifting of the iodine ions perpendicular to the stacking axis. However, the large spread of their transition temperatures (438 K ≤ T c ≤ 481 K) clearly points to a well-defined influence of the stacking sequence. We analysed the structural data of 2MC, 2MA and 4MA (A. Bussmann, Thesis, Freiburg (1978)) and found three basic SbOy-displacement patterns, realised in their pure forms in 2MC, 2MA, and in the centrosymmetric 4-layered type 4Tc, respectively. The other polytypes of 501 can be interpreted as isolated points in a ternary diagram with the three basic types as the pure end members (Fig. 1).