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, W. 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 3A between 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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05.1–5 THE INFLUENCE OF HIGH PRESSURE ON THE JAHN-TELLER EFFECT OF Cu^{2+} IN $Cs_2PbCu(NO_2)_6$. By H. Sowa, H. Ahsbahs, E. Hellner, Institute for Mineralogy, and D. Reinen, Institute for Chemistry, University of Marburg, Lahnberge, 3550 Marburg, FRG

At 298K and 1bar $Cs_2PbCu(NO_2)_6$ crystallizes with an elpasolite-related structure. Caused by the Jahn-Teller effect in the ^2Eg ground state of Cu^{2+} ($\varepsilon \otimes E$ vibronic coupling) the lattice symmetry is reduced to orthorhombic (Fmmm: a=11.04(1)Å, b=11.01(1)Å, c=10.74(1)Å). The $Cu(NO_2)_6$ octahedra are tetragonally elongated; the cooperative order is antiferrodistortive, though there are planar dynamics in the (001) plane (Mullen et al., Solid State Comm. (1975) 17, 1249).

IR-spectroscopic and structural (X-ray and neutron diffraction) measurements at high pressure indicate that the temperature for the transition to the cubic high-temperature α-phase shifts to lower temperatures with increasing pressure. Also the extent of the local Jahn-Teller distortion decreases. At about 20kbar, $Cs_2PbCu(NO_2)_6$ becomes cubic (Fm3: a=10.72(1)Å). As may be deduced from the temperature ellipsoids of the N atoms, the Jahn-Teller distortion is now three-dimensional dynamic as in the α-modification (S. Klein and D. Reinen, J. Solid State Chem. (1978) 25, 295).

Presumably the potential barrier $2|\beta|$ in the lower potential surface of the "mexican hat" decreases with increasing pressure. At 20kbar and 298K the thermal energy kT ($\hat{=}200cm^{-1}$) reaches the warping energy $2|\beta|$ which determines the transition from the static to the dynamic Jahn-Teller effect.
We will also report on high-pressure results on $K_2SrCu(NO_2)_6$ with a ferrodistortive order of elongated $Cu(NO_2)_6$ octahedra.

05.1–6 SUPER-LATTICE MELTING IN $Ag_{0.35}TiS_2$. By J.L. de Boer, K.D. Bronsema and G.A. Wiegers, Laboratory of Inorganic Chemistry, Materials Sciences Center, University of Groningen, The Netherlands.

In the system Ag-TiS_2 there are two structurally related phases, being a first- and a second-stage intercalate of silver in the layered compound TiS_2. In both phases silver atoms are on part (≈1/3) of the sites of triangular lattice planes; which are 12.2 Å apart in the second-stage phase and 6.43 Å apart in the first-stage phase. Both phases show fast-ionic conduction of silver.

Single crystals of first-stage $Ag_{0.35}TiS_2$ were grown by vapour transport. The three-dimensional melting of the silver sublattice, as reported recently[1] to be of second-order nature, was studied by single crystal X-ray diffraction. A superstructure $a\sqrt{3} \times a\sqrt{3} \times 2c$, space group $P\bar{3}1c$ is present at 110 K; the order-disorder transition to the substructure with a = 3.428 Å, c = 6.398 Å, space group $P\bar{3}m1$, was studied by measuring the super reflections on a CAD-4 diffractometer as a function of temperature[2]. In this way the temperature dependence of the occupancy of the silver sites in $P\bar{3}1c$; 2a, 2c and 2d, could be determined, T_c = 301 K.

1) R.M. Suter, M.W. Shafer, P.M. Horn and P. Dymon, Phys. Rev. B 26 (1982) 1495.
2) J.L. de Boer and A.J.M. Duisenberg. This conference.

05.1–7 POLYTYPISM AND PHASE TRANSITION OF Sb_5O_7I. 1. THE INTERLAYER INTERACTIONS. By I. R. Jahn and W. Altenburger, Institut für Kristallographie der Universität Tübingen, and V. Krämer, Kristallographisches Institut der Universität Freiburg, Germany.

In the layer structure antimony (III)-oxide-iodide (SOI) the phenomena of polytypism and structural phase transition combine in an unique manner.
The polytypism of SOI shows special features. Neighbouring $Sb_2[Sb_3O_7]$-layers of pseudo trigonal symmetry are rotated by 180° against each other and coupled by the intermediate iodine ions. Since the Sb of the Sb_3O_7-prism can occupy two equivalent positions, neighbouring layers may be identical or enantiomorphic to another; therefore two basic structural units exist: the centrosymmetric type 2MC (modified Ramsdell notation) and the acentric 2MA (V. Krämer, Acta Cryst. (1975), B31, 234; (1978) B34, 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 antiferro-shifting 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 Sb-I-displacement patterns, realised in their pure form in 2MC, 2MA, and in the centrosymmetric 4-layered type 4TcC, respectively. The other polytypes of SOI can be interpreted as isolated points in a ternary diagram with the three basic types as the pure end members (Fig. 1).