equilibrate. There are indications for the existence of a mixed phase in this temperature range between 190K and 150K. All the phase changes in this system have been found to have hysteresis.

Single crystal neutron diffraction data have been collected at 190K, 178.5K, 168K and 150K (upto $\sin\theta/\lambda = 0.50A^{-1}$, $\lambda = 1.036A$). The kinetics of the phase transitions and the structural details of various phases will be presented.

Landau theory and the symmetry of the 2MA lattice, both point to a Potts-type interaction as in the case of $Pb_3(PO_4)_2$ (E. Salje, B. Wruck, Phys. Rev. (1983) B28, 6510). We, therefore, have to consider a term of third order in the Landau theory.

During these experiments, the results were often affected by multiple light beam reflection within the sample. In SOI the phenomenon occurs in a pronounced manner because of the ideal cleavage and the very high refractive indices, and it shows up as a wavyness of the monotonic birefringence curves. To get a feeling for the multiple reflection effects in birefringent plates, we performed calculations for the given experimental conditions and were able to reproduce the observations.

05.1–36 POLYTYPISM AND PHASE TRANSITION OF Sb_5O_7I. 2. THE ORDER PARAMETER. By W. Altenburger, G. Bosch, I.R. Jahn, W. Prandl and M. Verhein, Institut für Kristallographie der Universität Tübingen; and V. Krämer, Kristallographisches Institut der Universität Freiburg, Germany.

In this paper we report on birefringence measurements performed at the antiferrodistortive phase transitions of all polytypes of Sb_5O_7I (SOI) identified up to now. Details of the structure, polytypism and notation are given in the accompanying contribution (I.R. Jahn, W. Altenburger and V. Krämer, this conference). The phase transitions ranging between 438 K and 481 K can be described by a zone boundary soft mode. Consequently, the birefringence follows the square of the order parameter.

The most common centrosymmetric basic type 2MC has been studied as a function of temperature and hydrostatic pressure (up to 0.5 GPa). Furthermore, in the mixed system $[Sb_{1-x}As_x]_5O_7I$ the antimony ions have been replaced by arsenic ions up to x = 0.13.

We find the following results: In 2MC the ferroelastic phase transition is weakly of first-order, the order parameter can be well described by the classical Landau formalism with a negative 4^{th} order term. Hydrostatic pressure increases the transition temperature of pure 2MC by 10 K / 0.1 GPa, whereas the discontinuity is practically not affected by pressure. In the mixed system, however, the As content leads to a drastic lowering of T_C and a remarkable increase of the discontinuity.

The 2MA and the higher polytypes all of which contain the acentric 2MA behave completely different from the 2MC compound: the birefringence cannot be interpreted in terms of a free-energy expansion with even powers of the order parameter only. This deviation from the "normal"

05.1–37 STRUCTURAL PHASE TRANSITION IN $Ni(NH_3)_6Cl_2$. By A. Hoser and J. Ihringer, Institut für Kristallographie der Universität Tübingen, West-Germany.

Hexammine nickel chloride $Ni(NH_3)_6Cl_2$ was studied with a focusing x-ray powder diffractometer between 297 and 35 K. The room temperature phase has Fm3m space group (CaF_2-type). The low temperature phase, which exists below 78 K has a monoclinic symmetry with a = 9.2982(7), b = 6.8819(5), c = 7.6985(5) Å, β = 92.36(1)°, Z = 2, (35 K). The phase transition deforms the cubic unit cell strongly. The change of the cell constants $a \sim a_{cub}$ and $c \sim a_{cub} \cdot \sqrt{2}$ at T_C amount to -6 % and + 9 % respectively. We found the contraction of the unit cell volume at 78 ± 1 K to be 0.5 %. We cannot confirm the suggestion (e.g. Jenkins & Bates, J. Phys. C: Sol. State Phys. (1981), 14, 817) that the primitive volume of the unit cell doubles at the transition. In $Fe(NH_3)_6Cl_2$ this doubling does not occur either: it can easily be demonstrated that the powder pattern reported by Aseh (Aseh et al., J. Chem. Phys (1975), 62, 6, 2335) may be refered to a cell which is similar to the cell we find for the Ni-compound. Nevertheless, if hydrogen ordering should play a role, the definitive unit cell parameters can be determined from a neutron experiment only.

The profile refinement (Rietveld, J. Appl. Cryst. (1969), 2, 65) was made in the space group I2/m (R_{nuc} = 0.096) rather than C2/m because of the close relation to the cubic cell. The hexammine nickel octahedron remains essentially undistorted, and the bond distances Ni - N stay within their expected values. The octahedra are rotated by 11° around the monoclinic b-axis (≙[110] direction is the cubic phase). - A neutron diffraction investigation is in progress.