



Fig. 1. The n -layered polytypes of $Sb_{507}I$ in the ternary diagram. Symbols for $n = 2$:+, 4 :◇, 6 :△, 8 :○, 10 :□. Crosses and filled symbols denote identified types.

To check the validity of this model, the transition temperatures of 2MC, 2MA, 4TcC were taken as a measure of the three different interlayer interactions. Then the T_C of the other types can be calculated. A very good agreement with the experimental transition temperatures is obtained.

In the case of the higher polytypes where T_C is not unambiguously related to a single stacking sequence, additional information can be gained by measurement of the optical extinction angle α ($0^\circ \leq \alpha \leq 13^\circ$). The value of α depends directly on the ratio n_f/n , where $n_f \leq n/2$ is the number of enantiomorphic layers in the n -layered polytype.

Using both the interlayer interactions and the extinction angle, a systematic treatment of all possible polytypes up to $n = 10$ will be given, from which we are able to predict T_C and α for a large number of new polytypes which have not been identified so far.

05.1-8 SHAPE CHANGE ASSOCIATED WITH PHASE SEPARATIONS ON AGING IN IN-PB AND IN-TL-PB ALLOY SYSTEMS. By Y. Koyama and O. Nittono, Faculty of Engineering, Tokyo Institute of Technology, Meguro-ku, Tokyo, Japan.

Some features of phase separations and shape changes during aging in In-(35-50)at%Pb and In-35at%Tl-13.5at%Pb alloys have been studied using X-ray diffractometry as well as electron microscopy. The In-Pb alloys undergo a phase separation from the fcc phase to a mixed (fcc+fct:c/a<1) phase on aging. With regard to the substructure, the {110} tweed structure develops in the early stage and finally the {110} twin forms inside the fct precipitates. The most interesting feature is that the precipitation of the fct phase proceeds by a bainitic mechanism, accompanying an appreciable surface relief. The surface relief indicates that the structural change in the separation is related to a cooperative atomic motion. On the other hand, the In-Tl-Pb alloys undergo first a phase separation from the fcc parent phase to a mixed (fct:c/a<1+fct:c/a>1) phase and subsequently from the mixed phase to the equilibrium (fcc+fct:c/a>1) phase. The former proved a spinodal decomposition by the appearance of the <100> modulated structure and a continuous change between the modulated and {100} banded structures during aging. The latter is characterized by the nucleation and growth of the fcc phase and also by the annihilation of the fct(c/a<1) phase. Moreover, all alloys, which were deformed in the fcc parent phase, showed an appreciable shape change when kept within a temperature range of the two-phase region and then heated to the fcc parent phase. The macroscopic shape change can be explained as a reversible shape memory effect in these separations on the analogy with that in a martensitic transformation. In the present study, the origin of the shape change is discussed in detail on the basis of the changes in substructures observed in both alloy systems.

05.1-9 HYDROGEN AND DEUTERIUM ORDERING IN β_1 - V_2H , β - V_2D AND β_2 - Ta_2D . By M. Hirabayashi,¹⁾ T. Kajitani,¹⁾ H. Kaneko,¹⁾ N. Niimura,²⁾ Y. Noda³⁾ and S. Sato⁴⁾, 1) The Research Institute for Iron, Steel and Other Metals, 2) Laboratory of Nuclear Science, 3) Faculty of Engineering, Tohoku University, Sendai, 4) The Institute for Solid State Physics, University of Tokyo, Tokyo, Japan

Transition metal hydrides (deuterides) V_2H , Ta_2H and Ta_2D undergo the order-disorder change of H (D) sublattice successively from β_1 through β_2 to α upon heating. X-ray and neutron diffraction studies were done to reveal the isotopic effect between V_2H and V_2D , and the successive disordering process in Ta_2D . As for β_1 - V_2H and β - V_2D , the crystal structures are found to be not isomorphic; symmetry and space group are respectively tetragonal, I41/amd and monoclinic, C2/m. The H (D) arrangement can be distinguished in the four-body correlation. The D arrangement in β_2 - Ta_2D , which is an intermediate phase at the temperature range of 40-60°C, was studied by neutron diffraction.* A proposed model is characterized with a statistical distribution of D atoms in tetrahedral sites of the sublattice with $\sqrt{2}a \times \sqrt{2}a \times a/2$ (a is the lattice parameter of bcc Ta). The results explain well the successive phase changes β_2 - β_1 - α of Ta_2H as well as Ta_2D .

* The work is progressing in cooperation with Drs. A. Schurtz and P. Leung at IPNS in Argonne Nat. Lab., Ill.

05.1-10 POTENTIAL ENERGY STUDY OF THE DISORDERED STRUCTURE OF INDOLE. By S. K. Talapatra, S. C. Biswas, S. B. Sarkar and Chitra Samanta, Department of Physics, Jadavpur University, Calcutta 700032, India

The pairwise nonbonded interaction potentials of the Buckingham 6-exp type were applied to the study of molecular reorientations in indole (C_8H_7N) crystals.

The variation of the intermolecular energy U (Kcal/mol) with rotation angle of the molecule about its best plane normal passing through the centre of gravity gave an interesting result. The indole molecule has no two-fold axis of symmetry about its plane normal, but two identical potential wells appeared in the energy curve and they were separated by an angle of 180°. This confirms the x-ray finding (Roychowdhury & Basak, Acta Cryst., B31, 1559, 1975) that indole has a disordered structure with molecules capable of assuming two alternative orientations.

Similar potential wells were also obtained from the energy study of 1:1 complex of indole with *s*-trinitrobenzene, in which the indole molecules are capable of assuming two alternative orientations (Hanson, Acta Cryst., 17, 559, 1964). The computations were made using the energy functions of Giglio (Nature, 222, 339, 1969) with our computer program (Talapatra et al., Ind. J. Phys. 55A, 281, 1981) with a summation radius of 15Å.