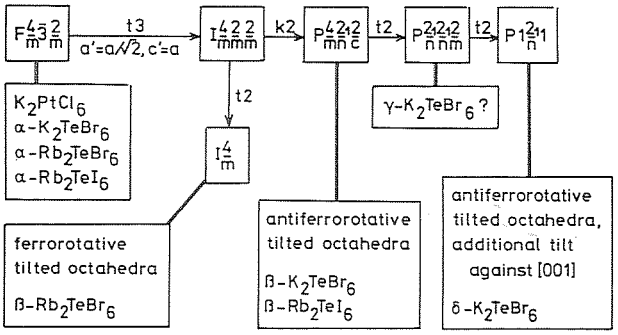

Fig. 1: Group-subgroup relations of the spacegroups of the corresponding A_2TeX_6 phases.

05.1–22 MECHANISM OF PHASE TRANSFORMATION IN ZnS, $Zn_xCd_{1-x}S$ AND $Zn_xMn_{1-x}S$: A THREE PARAMETER MODEL. By M.T. Sebastian and P. Krishna Physics Department, Banaras Hindu University, Varanasi 221005, India.

Single crystals of 2H ZnS when annealed at an elevated temperature undergo solid state transformation to a disordered twinned 3C structure by the non-random insertion of deformation faults preferentially at two layer spacings. Many of the resulting 3C structures show an enhancement of intensity near the 6H positions and some 2H crystals even transform to 3C through an intermediate 6H phase. It is observed that solid solutions of ZnS with small amounts of CdS or MnS predominantly display the 2H-6H transformation. The mechanism of polytype transformations and the type of faults involved were studied by quenching the crystals in an intermediate state and examining the structure by X-ray diffraction methods. One obtains a one-dimensionally disordered structure containing a non-random distribution of faults. The theory of X-ray diffraction from one-dimensionally disordered close-packed structures is highly developed, but assumes a random distribution of faults and a small fault probability. Both these assumptions breakdown when studying polytype structures undergoing phase-transformation.

The 2H-6H transformation in $Zn_xCd_{1-x}S$ and $Zn_xMn_{1-x}S$ is found to occur by the non-random insertion of deformation faults with a high probability (β) of occurrence at three layer separations and a low probability (α) of occurrence at larger separations. The resulting 6H structure, however, shows an enhancement of diffracted intensity in positions corresponding to 3C reflections, indicating that the probability (γ) of faulting at two-layer separations is not negligible. The 2H-3C transformation in these materials occurs by the non-random insertion of deformation faults with $\gamma >> \alpha$ and $\beta > \alpha$. We have therefore developed a three-parameter theoretical model to compute the diffracted intensity along the 10.L row of crystals undergoing such transformations and predict the diffraction effects for various values of α, β and γ. These theoretically predicted intensity profiles are compared with those experimentally recorded on a single crystal diffractometer from (i) 2H $Zn_x Cd_{1-x}S$ and $Zn_x Mn_{1-x}S$ crystals partially transformed to 6H and (ii) 2H ZnS crystals partially transformed to 3C.
It is found that the observed intensity profiles correspond to a suitable addition of the intensities calculated separately for the 2H-3C and 2H-6H transformations indicating that these occur simultaneously in different regions of the same single crystal.

05.1–23 THE EFFECT OF d-ELEMENTS ON THE STRUCTURAL TRANSFORMATIONS IN TiNi. By A.G. Khundzhua and M.I.Zakharova, Faculty of Physics, Moscow State University, Moscow, USSR.

High temperature phase of $Ni_{50}Ti_{50-x}M_x$ (x= 3-5; M = Zr, Hf, Nb, Mo, Mn) has been studied by means of transmission electron microscopy and monocrystal X-ray analysis. The martensitic transformation B2→B2 + B19'→B19' was observed in the $Ni_{50}Ti_{46}Zr_4$ and $Ni_{50}Ti_{46,5}Hf_{3,5}$ alloys. Zr and Hf substituted for Ti lead to M_s point decrease to 300 K and 270 K correspondingly. Nb, Mo, Mn substituted for Ti stabilize the high temperature B2-phase and martensitic transformation was not observed on cooling from 300 K to 120 K. The annealing of alloys $Ni_{50}Ti_{46}Nb_4$, $Ni_{50}Ti_{46}Mo_4$, $Ni_{50}Ti_{46}Mn_4$ at 623 K leads to the formation of X-phase. Contrary to previous results, however, the crystal structure of X-phase is interpreted as rhombohedral with lattice constants a=6.7 A, α=114°. The orientation relationships between B2- and X-phase was found to be

$$\{110\}\langle 111\rangle_X \parallel \{321\}\langle 111\rangle_{B2}.$$