11.2-11 THE MECHANISM OF POLYTYPE TRANSFORMATION IN CdI_2 CRYSTALS. By M.T. Sebastian, Regional Research Laboratory, Trivandrum 695019, India and Gladys Mathew, Physics Department, Cochin University, 682 022, India.

Single crystals of 2H CdI_2 on annealing undergo transformation (T. Minagawa, J. Appl. Cryst. 11 (1978) 243 and B. Palosz and S. Gierlotka, Set. Cryst. 340 (1984) 574) to the 4H structure. The transformation is found to occur through a disordering process as revealed by the broadening of certain x-ray reflections indicating the involvement of stacking faults in the process. Such a 2H → 4H solid state transformation can occur by the non-random insertion of stacking faults at certain layer spacings to create the new 4H structure and can occur by three distinct types of faults as shown below:

(i) Deformation stacking fault:

2H: A B A B A B A B ....
C A C A C A ....
B A B A B ....
C A ....
B ....

4H: A B C B A B C B ....

(ii) Layer displacement stacking fault:

2H: A B [A] B A B [A] B ....

4H: A B [C] B A B [C] B ....

The displaced layers are shown inside the rectangles.

(iii) Extrinsic stacking faults:

2H: A B A B A B .....

4H: A C B C A C B C A C B C .....

The inserted layers are underlined. Following our earlier work on the 2H-6H and 3C-6H transformations (M.T. Sebastian and P. Krishna, Phys. Stat. Sol. A79 (1983) 271, A84 (1984) 401, Progr. Cryst. Growth Charact. 1987), we develop the theory of x-ray scattering by the 2H crystals undergoing transformation to the 4H structure by the above three processes and predict the different diffraction effects. A comparison of the theoretically computed intensity profiles with the experimentally recorded profiles shows clearly that the layer displacement stacking faults are involved in the 2H-4H transformation in CdI_2. The observed intensity profiles are in very good agreement with those calculated for the layer displacement faults.

11.2-12 THE MECHANISM OF THE 2H-3C SOLID STATE TRANSFORMATION IN SILICON CARBIDE. M.T. Sebastian, Regional Research Laboratory, CSIR, Trivandrum 695 019, India; K. Narayanan, Cochin University, and P. Krishna, Physics Department, Banaras Hindu University, Varanasi, India.

Single crystals of 2H SiC on annealing around 1400°C transform to a disordered twinned 3C structure [P. Krishna and R.C. Marshall, J. Cryst. Growth 9 (1971) 319, Adv. in x-ray analysis 14 (1971) 67.] The 2H→ 3C solid state transformation can occur by the non-random insertion of stacking faults by two different processes as shown below:

(i) Layer displacement faulting

initial structure: A B [A B A B] A B [A B A B] A B

resulting structure : A B [C A B C] A B [C A B C] A B

where the layers shown inside the rectangles have been transposed as a single event during the course of the transformation.

(ii) Deformation faulting:

initial structure (2H): A B | A B A B A B ....
C A | C A C A ....
B C | B C ...
A B ...

resulting structure (3C): A B C A B C A B ....

The theory of x-ray diffraction from 2H crystals undergoing transformation to the 3C structure has been developed for both the above processes. Different diffraction effects like peak broadening and peak shift are predicted as a function of the fault probability. A comparison of the experimentally observed diffraction effects with those computed theoretically shows that the transformation in SiC occurs by the non-random insertion of layer displacement faults.