

20.3-2 STUDY OF SUBSTITUTIONAL SOLID SOLUTIONS IN MELT-GROWN CRYSTALS OF CADMIUM IODIDE. By U. P. Tyagi and G. C. Trigunayat, Department of Physics & Astrophysics, University of Delhi, Delhi-7, India.

The past investigations carried out on various polytypic compounds in the last four decades or so have shown that the presence of impurities during crystal growth affects the formation of polytypes. However, so far this work has remained very broadly qualitative in nature. In order to assess the role of impurities on polytype growth in a definite manner, it was decided to dope well purified crystals of a polytypic compound with such impurities that would interact with the atoms of the host material, e.g. form a substitutional solid solution. Thus, the richly polytypic compound cadmium iodide was chosen for the purpose and the impurities were carefully selected according to their known physical and chemical properties. Cadmium iodide being an ionic compound, both cations (lead, tin, indium, gallium) and anions (bromine, chlorine) were used as dopants. Zone refining and Bridgman-Stockbarger techniques were employed for the purification/growth of the doped single crystals. For all the dopant impurities, the doping has been found to lead to the formation of substitutional solid solutions. The crystals have been examined by x-ray diffraction and physical methods and the following significant results have been obtained. (i) All the doped crystals are harder than the crystals of pure, undoped cadmium iodide. (ii) The exposure times for the crystals doped with lead iodide and gallium far exceed those for the pure, undoped crystals. (iii) All the tin-doped crystals show arcing of reflections on their x-ray photographs, whereas none of the other doped crystals show any such arcing. (iv) Cleavage in the tin-doped crystals becomes very difficult and remains highly localized, unlike the other doped crystals, which could be smoothly cleaved over their entire basal planes with relative ease. (v) The x-ray diffraction photographs of the crystals show absence of streaking of the reflections. (vi) Although melt-grown crystals are generally expected not to show any polytypism, a few higher polytypes have been observed in the lead-doped crystals. The results have been interpreted in terms of the properties of the dopant atoms (atomic radius, ionisation potential, etc.), crystal structures of the halides of the dopants and interatomic forces.

20.3-3 EFFECT OF DOPING ON THE POLYTYPIISM AND ELECTRICAL CONDUCTIVITY OF  $\text{CdBr}_2$  SINGLE CRYSTALS

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$\text{CdBr}_2$  has been purified using the zone-refining technique. The purified material has been used to grow undoped and Zn-doped single crystals of  $\text{CdBr}_2$  by the Bridgman-Stockbarger method. X-ray diffraction studies showed the crystals are of the 6R polytype.

D.C. conductivity studies were made on these crystals at room temperature. Thermoelectric measurements show that the doped and undoped single crystals to be n-type. An increase in the value of  $\sigma$  has been observed. Typical values of  $\sigma$  for the undoped and doped single crystals are  $2.2 \times 10^{-11} \text{ohm}^{-1} \text{cm}^{-1}$  and  $1.3 \times 10^{-10} \text{ohm}^{-1} \text{cm}^{-1}$  respectively.

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20.4-1 ELECTRON MICROSCOPIC EVIDENCE FOR "DISCOMMENSURATIONS" AND METAL ATOM TRIMER FORMATION IN THE PSEUDO ONE-DIMENSIONAL COMPOUNDS  $\text{MTe}_4$  (M = Nb, Ta). By J. Mahy, J. Van Landuyt, S. Amelinckx, RUCA (University of Antwerp) 2018-Antwerpen (Belgium).

The deformation modulated structures of  $\text{TaTe}_4$  and  $\text{NbTe}_4$  reveal a commensurate and an incommensurate diffraction pattern respectively. Below 50K,  $\text{NbTe}_4$  "locks-in" into a commensurate superstructure, which is assumed to be isostructural with that of  $\text{TaTe}_4$ . Moreover, X-ray structure refinement indicated a tendency to form "trimers" of metal atoms displaced longitudinally along the pseudo-one-dimensional chain axis.

It was demonstrated by means of low temperature EM techniques that above 50K "discommensurations" nucleate and propagate in  $\text{NbTe}_4$ . These planar defects are characterized and described as a quasi-periodic array of antiphase boundaries, perpendicular to the chain axis (Mahy, J., Van Landuyt, J., Amelinckx, S., Bronsema, K. and Van Smaalen, S., J. Phys. C : Solid State Physics 19, 5049, (1986)). At room temperature, the modulation has acquired a harmonic profile, which is consistent with the incommensurate structure refinement results.

Direct evidence for the formation of metal atom trimers was obtained from the comparison of high resolution EM images with calculated images of  $\text{TaTe}_4$ . The latter were obtained from the commensurate structure refinement data. This evidence demonstrates the use of HREM techniques to observe weak modulation phenomena in CDW type deformed crystal structures.