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RECOVERY OF ROCKSALT STRUCTURE CdS TO ROOM PRESSURE

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Abstract—The high pressure phase of CdS has been recovered to room pressure at 77°K. The starting material was single crystal CdS, and the recovered material varied from powder to single crystal NaCl structure CdS. The annealing temperature of the reverse transformation of the NaCl phase was measured as was the annealing temperature of the zincblende to wurtzite phase transformation. E_g of the high pressure phase is 2·04 ± 0·02 eV.

1. INTRODUCTION

A CRYSTAL structure transformation in CdS with pressure was first reported by EDWARDS, SLYKHOUSE and DRICKAMER[1] in the range 20–30 kb. A shift in the fundamental absorption edge was measured optically. The band gap of the high pressure phase was reported to be 1·7 eV. A value of $E_g = 2{\cdot}50$ eV for normal CdS at atmospheric pressure was the reference. The structure of the high pressure phase was investigated by KALBALKINA and TROITSKAYA[2] using a high pressure X-ray camera. They reported a transformation of the original wurtzite structure to a NaCl phase in the pressure range 18–35 kb. Upon release of the pressure, the NaCl structure transforms to a cubic zincblende structure with a small admixture of the wurtzite structure. CORLL[3] reported the recovery of the high pressure phase to room pressure at room temperature. His starting material was CdS powder, precipitated from CdCl with H_2S. The powder was a strained mixture of the zincblende and wurtzite phases. X-ray diffraction patterns showed that the crystals were heavily strained. The recovered NaCl structure transformed to the zincblende phase when annealed at 125°K over night or at 250°C for less than a minute. The wurtzite structure was obtained on further annealing at 700° for several hours. SAMARA and GIARDINI,[4] using electrical measurements, have determined values of 2·3 eV and 1·3 eV, respectively, for the band gaps of the wurtzite and NaCl phases.

In this paper, we report the recovery of the high pressure phase of CdS to room pressure at 77°K using single crystal CdS as the starting material. The recovered material contains relatively large single crystal regions along with regions of relatively unstrained powder. We also report results on the annealing temperature of the NaCl and zincblende phases and on the absorption edge of the NaCl phase.

2. EXPERIMENTAL

The starting materials were Li-doped single crystals grown in this laboratory by vapor phase deposition. Li-doped CdS crystals can be subjected to uniaxial stresses up to three times greater than pure crystals without being crushed, and were used in this work for their higher strength characteristics. The samples were cut into plates perpendicular to the *c*-axis and lapped to thicknesses varying from 2·5 to 36 mil.

The high pressure bomb was modeled after Drickamer's high pressure optical bomb except that it had no optical windows. The high pressure chamber was $\frac{3}{16}$ in. dia. by $\frac{1}{8}$ in., and the working fluid was single crystal NaCl. A standard Sheffer HH Series 2000 hydraulic cylinder was used to pressurize the bomb.