

Effect of Pressure on the Elastic Parameters and Structure of CdS†

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The effective elastic constants of CdS have been measured by the ultrasonic pulse-echo method as a function of hydrostatic pressure to 4 kbar. The logarithmic pressure derivatives determined were $d\ln C_{11}/dP=3.56$, $d\ln C_{33}/dP=3.44$, $d\ln C_{13}/dP=10.0$, $d\ln C_{44}/dP=-4.22$, $d\ln C_{66}/dP=-4.97$ (in Mbar^{-1}). A continuous-deformation model of the wurtzite-to-rocksalt pressure-induced transformation in CdS is presented. A combination of elastic constants characteristic of this deformation is derived and the transformation discussed in terms of a microscopic shear mechanism based on these results.

INTRODUCTION

THIS paper proposes a mechanism for the well-known pressure-induced structural transformation in CdS based on the possibility of microscopic instabilities in the wurtzite structure developing under high applied stresses. The ability of a material to resist a given deformation is a direct function of the elastic parameters of the material, and the measurements reported in this paper were undertaken to determine how these parameters (and hence the structural stability) are affected by external pressures.

The mechanism proposed is a continual deformation from the wurtzite structure to the rocksalt structure on a microscopic scale which propagates throughout the crystal when initiated at points of stress concentration. The required deformation of the wurtzite structure into the rocksalt structure is described, and an elastic constant C_i characteristic of this deformation is developed. The data reported in the experimental section show the pressure derivative of this characteristic elastic constant C_i to be negative, indicating that with increasing pressure the wurtzite structure becomes less stable with respect to this type of deformation.

EXPERIMENTS AND RESULTS

The sound velocities used to determine the effective elastic constants of CdS were measured by the ultrasonic pulse-echo method. The techniques of ultrasonic pulse-echo experiments are well known,¹ and the details pertinent to this experiment are as follows. A 10-Mc pulse, approximately 1 μsec in duration from a gated oscillator, was used to activate the quartz transducer. This pulse and the subsequent echos were displayed on one trace of a dual trace oscilloscope. A timing comb and a 10-Mc wave from a time mark generator were displayed on the other trace to calibrate the oscilloscope screen. Photographic records of the traces were made and the transit-time measurements taken from these photographic records with the aid of a telereader. By

this method the time positions of the cycles within the pulses were determined to better than $\pm 5 \times 10^{-9}$ sec.

It can be shown² that for low-resistivity crystals, the piezoelectric coupling may be ignored and the sound velocities directly correlated to the elastic constants. The crystals used in these experiments were purchased from Harshaw Chemical Company and had dark resistivities of less than $1 \Omega\text{-cm}$. The crystals were in the form of right parallelepipeds ($1 \text{ cm} \times 1 \text{ cm} \times 2 \text{ cm}$) with the square faces of the crystals oriented at 0° , 90° , and 45° from the crystallographic c axis. The crystals were denoted as crystal *A*, crystal *B*, and crystal *C*, respectively, and the orientations substantiated by x-ray analysis to be within $\pm 0.2^\circ$. The three orientations permitted eight separate velocity measurements. Cadmium sulfide, being hexagonal, has five independent elastic constants; therefore, the eight velocity measurements provided several internal crosschecks.

The 10-Mc quartz transducers were bonded to the crystals with polyethylene. The pressure experiments were limited to 4 kbar by failures of the polyethylene bonds at higher pressures. Several other bonding materials, including epoxy, were also tried. In all cases the bond failed at pressures less than 5 kbar, and the crystals were eventually destroyed in attempts to obtain data at higher pressures. The pressure apparatus was a simple piston-cylinder device. Prior pressure experiments in this apparatus involving the change in resistance of a manganin wire coil and the solidification of Hg at room temperature (taken to be 12.30 kbar at 23°C) have shown the friction in the apparatus to be small and quite reproducible. The pressure on the sample was calculated from these prior calibrations and the load applied to the piston. The uncertainty introduced by this method of pressure calculation was less than 1% at 4 kbar. The experiments were performed at room temperature (23°C) and data recorded at pressure intervals of approximately $\frac{1}{2}$ kbar.

The effective adiabatic elastic constants C_{ij} and their logarithmic pressure derivatives, $d \ln C_{ij}/dP$, calculated from the velocity measurements of these experiments are listed in Table I. The reduction of the pressure data required the knowledge of several physical parameters. The isothermal compressibility ($k_t=1.625 \text{ Mbar}^{-1}$) was

² A. R. Hutson and D. L. White, *J. Appl. Phys.* **33**, 40 (1962).

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¹ W. B. Daniels and C. S. Smith, in *The Physics and Chemistry of High Pressures* (Society of the Chemical Industry, London, 1963), p. 50.