TABLE I. The adiabatic elastic constants of CdS, and their logarithmic pressure derivatives at 23°C. The acoustic waves were propagated parallel to, perpendicular to, and at 45° from the crystallographic c axis for the crystals A, B, and C, respectively.

| Crystal | Type of wave | Wave velocity in m/sec | Related constant | Value of elastic constant calculated C_{ij} in Mbar | | | | Pressure Derivative $d \ln C_{ij}/dp$ in Mbar^{-1} |
				Jaffe[a]	Bolef[b]	McSkimin[c]	Present study	
A	Longitudinal	4408	C_{33}	0.938	0.9397	0.9370	0.9361	$+3.44$
B	Longitudinal	4216	C_{11}	0.907	0.8432	0.8581	0.8565	$+3.56$
C	Longitudinal	4146	C_{13}	0.510	0.4638	0.4615	0.4616	$+9.92$
A	Transverse	1756	C_{44}	0.1504	0.1489	0.1487	0.1487	-4.28
B	Transverse	1756	C_{44}	0.1504	0.1489	0.1487	0.1486	-4.16
B	Transverse	1835	C_{66}	0.1630	0.1610	0.1623	0.1622	-4.97
C	Transverse	2122	C_{13}	0.510	0.4638	0.4615	0.4612	$+10.10$
C	Transverse	1794	$\frac{1}{2}(C_{66}+C_{44})$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$-4.65 (\rho v^2)$

[a] H. Jaffe, D. Berlincourt, H. Krueger, and L. Shiozawa, in Proceedings of the Fourteenth Annual Symposium on Frequency Control, 1960 (unpublished).
[b] D. I. Bolef, N. T. Melamed, and M. Menes, Westinghouse Research Labs. Scientific Paper No. 6-40301-1-P5 (unpublished). Also, Bull. Am. Phys. Soc. 5, 169 (1960).
[c] H. J. McSkimin, T. B. Bateman, and A. R. Hutson, J. Acoust. Soc. Am. 33, 856 (1961).

calculated from the room-pressure measurements using the thermal expansivity data of Jost and Shiozawa[3]

$$(\beta = 11.02 \times 10^{-6}/°C, \beta_a = 4.25 \times 10^{-6}/°C,$$
$$\beta_b = 2.50 \times 10^{-6}/°C)$$

and assuming[4] c_p to be 4 cal/mole-g°C. The isothermal changes in length $(1/L)(dL/dP)$ and in orientation $d\theta/dP$ of the crystals as a function of pressure were calculated in a similar manner.

$$(1/L)(dL/dP) = -(0.5441 \sin^2\theta + 0.5335 \cos^2\theta) \text{ Mbar}^{-1},$$
$$d\theta/dP = 0.0106 \sin\theta \cos\theta \text{ Mbar}^{-1}.$$

The effective elastic constants and their pressure derivatives listed in Table I are defined by the acoustic wave equation $C = \rho v^2$. These effective elastic constants may be converted to the elastic constants defined as the derivatives of the internal energy in the manner discussed by Wallace.[5]

DISCUSSION

The above elastic-constant pressure data open the possibility of a pressure-induced shear instability of the wurtzite structure as the mechanism of the transformation in CdS. A rough extrapolation of the data (assuming that $d^2C_{ij}/dP^2 = 0$) suggests that a macroscopic shear instability $(C_{ij} \to 0)$ would occur at pressures greater than 200 kbar. A shear instability mechanism is consistent with the rapid nature[6] of the transformation, but is inconsistent with the experi-

mental observations of the occurrence of the transformation at pressures (20–25 kbar) an order of magnitude lower than the predicted macroscopic shear instability. The object of the following discussion is to correlate these aspects and suggest a mechanism for the transformation.

The wurtzite structure may be deformed into the rocksalt structure by a combination of a compression along the crystallographic c axis and a shear about this axis. The wurtzite-to-rocksalt phase transformation is depicted in Fig. 1 as it would occur by this type of deformation. The stresses corresponding to this type of deformation are shown as broad arrows acting on the faces of the hexagonal unit cell in Fig. 1(a). In Fig. 1(b) the cell is shown slightly distorted and the logical (spring-model) motions of the atoms with respect to the cell are indicated by the small arrows. In Fig. 1(c), the distortion is completed, and the atoms have become the body-centered tetragonal arrangement of the rocksalt structure. The normal representation of the rocksalt structure, a face-centered cubic arrangement, is indicated by the dashed lines for clarity. The lightly shaded atom in the base of the rocksalt arrangement in Fig. 1(c) would be the atom from the cell directly below corresponding to the atom labeled 2.

By considering the distortion to take place at constant volume, we may calculate the strain energy (per unit volume) associated with small distortions from the wurtzite structure. This calculation follows the procedure suggested by Huntington[7] for c/a variation of hexagonal crystals at constant volume. The second derivative of this strain energy with respect to strain yields a combination of the effective elastic constants characteristic of the distortion. The calculation (see Appendix) of the characteristic elastic constant C_t for the distortion shown in Fig. 1 yields

$$C_t = (C_{11} + C_{33} + 3C_{66} - 2C_{13}) = +1.3564 \text{ Mbar}.$$

[3] J. M. Jost and L. R. Shiozawa, Clevite Corporation Engineering Memorandum No. 64-28, 1964 (unpublished).
[4] The specific heat of CdS is reported to be in a paper by A. N. Krestovnikov, M. S. Vendrikh, and E. I. Feigina [Sb. Nauchn. Tr., Mosk. Inst. Tsvetn. Metal i Zolota 26, 233 (1957)]. This paper was not available to the author. The uncertainty in the calculation introduced by a rather large error in c_p is unimportant, therefore the value used was estimated from known values of similar compounds.
[5] D. C. Wallace, Rev. Mod. Phys. 37, 57 (1965).
[6] During static pressure experiments in which the wurtzite-to-rocksalt structural change in a single-crystal CdS sample is observed by monitoring the resistance of the sample, at the onset of the transition, the resistance will drop several orders of magnitude in less than the reaction time of most recorders.

[7] H. B. Huntington, in Solid-State Physics, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1958), Vol. 7, p. 237.

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