

dislocations, vacancies, interstitials, or impurities. When the microscopic regions become unstable, the transformation would spread rapidly from these regions, similar to the motion of dislocations. Once the mechanism was initiated, the change in structure would spread throughout the crystal if the rocksalt phase were the thermodynamically stable phase. The large pressure hysteresis¹⁰ (~12 kbar) of the structural transformation in CdS indicates that the rocksalt structure becomes the thermodynamically stable phase below 20 kbar at room temperature.

In conclusion, the effective elastic-constant data reported in this paper provide the basis for a plausible mechanism for the pressure-induced phase transformation in CdS.

APPENDIX

In this Appendix we give the derivation of the characteristic elastic constant for the deformation of the wurtzite structure to the rocksalt structure at constant volume.

For simplicity of calculation the coordinate system is chosen such that the 1 axis is parallel to the longer diagonal of the rhombic base of the hexagonal unit cell, the 2 axis is parallel to the shorter diagonal of the rhombic base of the hexagonal unit cell, and the 3 axis is parallel to the *c* axis of the hexagonal unit cell. This choice is equivalent to rotating the usual hexagonal coordinate system 30° about the *c* axis. The symmetry of the structure requires the elastic-constant matrix to be unvaried by this rotation. The required distortion can now be described as a compression along the 1 and 3 axes combined with an extension along the 2 axis. Since we consider the distortion to take place at constant volume, the sum of the strains must be zero, i.e.,

$$\epsilon_1 + \epsilon_2 + \epsilon_3 = 0. \quad (1)$$

¹⁰ J. A. Corll, J. Appl. Phys. 35, 3032 (1964).

The constant-volume stipulation also requires that the edge lengths of the base remain constant [$\frac{1}{2}\sqrt{3} \times (\sqrt{8/\sqrt{3}})X^3 = \sqrt{2}X^3 = \frac{1}{2}(\sqrt{2}X)^3$] which in turn requires that

$$\epsilon_2 = -\tan^2 60^\circ \epsilon_1 = -3\epsilon_1. \quad (2)$$

Combining Eqs. (1) and (2), we may write

$$\epsilon_1 = -\epsilon, \quad \epsilon_2 = 3\epsilon, \quad \epsilon_3 = -2\epsilon. \quad (3)$$

Now, the strain energy W_d of the distortion is merely the sum of the work associated with the various strains W_i . The work associated with a given dilation strain may be written as

$$W_i = T_i \epsilon_i V_0, \quad (4)$$

where T_i is the stress in the *i*th direction, ϵ_i is the strain in the *i*th direction, and V_0 is the volume of the structure. Thus

$$W_d = \sum_i W_i = \sum_i T_i \epsilon_i V_0 = V_0 \sum_i T_i \epsilon_i. \quad (5)$$

The T_i may be calculated from the effective elastic constant matrix and the ϵ_i , to yield the strain energy per unit volume

$$(1/V_0)W_d = (10C_{11} + 4C_{33} - 6C_{12} - 8C_{13})\epsilon^2. \quad (6)$$

In hexagonal crystals, $C_{66} = \frac{1}{2}(C_{11} - C_{12})$. Thus, substituting for C_{12} and differentiating twice with respect to ϵ , we obtain

$$(1/V_0)(d^2W_d/d\epsilon^2) = 8(C_{11} + C_{33} + 3C_{66} - 2C_{13}). \quad (7)$$

The constant in front of the right side relates only to the arbitrary definition of the magnitude of ϵ in Eq. (3), and may be ignored in defining the characteristic elastic constant of the deformation

$$C_t = (C_{11} + C_{33} + 3C_{66} - 2C_{13}). \quad (8)$$

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