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STABILITY OF DIAMOND AND ZINC BLENDE STRUCTURES AT HIGH PRESSURES

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ABSTRACT

The ratio of the bond bending and bond stretching force constants is estimated for diamond, Si, Ge, GaAs and GaSb at high pressures. It is proposed that at high pressures these compounds transform into a metallic dense form when this ratio reaches a critical value, *i.e.* $\sim 0{\cdot}08$.

INTRODUCTION

THE group IV elements diamond, silicon, germanium and grey tin crystallize in open diamond structure, and most binary III-V and II-VI compounds in a related zinc blende structure, in which each atom is tetrahedrally bonded to the neighbouring atoms. The neighbouring atoms are held by covalent bonds in diamond, Si, Ge and grey tin; however, in III-V and II-VI compounds the bonds are partially ionic. At high pressures, these open structures transform into closely-packed structures. The transition pressures P_t, determined by the X-ray diffraction and resistance behaviour under pressures are summarised in Table I.

PRESSURE DEPENDENCE OF (β/α)

Bhagavantam and Bhimsenachar[1] and Musgrave and Pople[2] derived expressions for the shear elastic constants of diamond structures in terms of the bond stretching and bond bending constants α and β, and Martin[3] extended this work to partially ionic zinc blende structures. In this paper we estimate the value of (β/α) at high pressures, and correlate it with the stability of zinc blende structures.

(β/α) can be readily evaluated from equations (6), (8) and (11) in Martin's paper:

$$\frac{\beta}{\alpha} = \frac{C_{11} - C_{12} - 0{\cdot}053\,SC_0}{C_{11} + 3C_{12} + 0{\cdot}456\,SC_0} \qquad (1)$$

with

$$S = \frac{\Omega m}{4\pi e^2}(\omega_1^2 - \omega_t^2) \qquad (2)$$

and

$$C_0 = (e^2/r^4) \qquad (3)$$

where Ω is the unit cell volume, r the bond length, ω_1 and ω_t the frequencies of the longitudinal and transverse optic modes at $K = 0$, and S is related to the ionicity of the crystal, f_i. Differentiation of equation (1) at constant temperature (temperature suffix T is suppressed) gives:

$$(\beta/\alpha)' = \frac{d(\beta/\alpha)}{dP} = C + D \qquad (4)$$

$$C = (C_{11} + 3C_{12} + 0{\cdot}456\,SC_0)^{-1} \times \left\{\left(1 - \frac{\beta}{\alpha}\right)\frac{dC_{11}}{dP} - \left(1 + \frac{3\beta}{\alpha}\right)\frac{dC_{12}}{dP}\right\} \qquad (5)$$

$$D = -(C_{11} + 3C_{12} + 0{\cdot}456\,SC_0)^{-1} \times (0{\cdot}053 + 0{\cdot}491\,\beta/\alpha)\frac{d(SC_0)}{dP} \qquad (6)$$

$$\frac{d(SC_0)}{dP} = SC_0\left\{B_0^{-1} + (2\omega_1/\omega_1^2 - \omega_t^2)\frac{d\omega_1}{dP} - (2\omega_t/\omega_1^2 - \omega_t^2)\frac{d\omega_t}{dP}\right. \qquad (7)$$

where B_0 is the isothermal bulk modulus. The values of C_0, C_{11}, C_{12} and S tabulated by Martin[3],