

and

$$C_h = C_a c_{44} - 2c_{14}^2.$$

$K_V$  is given by Eq. (13) and its first pressure derivative is given by Eq. (8) and

$$dC_h/dp = C_a(dc_{44}/dp) + c_{44}(dC_a/dp) - 4c_{14}(dc_{14}/dp).$$

(d) *Tetragonal Crystals:*

$$dK_V/dp = \text{Eq. (8)}, \quad (20)$$

and

$$dK_R/dp = \text{Eq. (9)}. \quad (21)$$

$$dG_V/dp = \frac{1}{30}[3(dC_a/dp) + 12(dc_{44}/dp) + 6(dc_{66}/dp) + dC_b/dp], \quad (22)$$

where

$$dC_b/dp = dc_{11}/dp + dc_{12}/dp + 2(dc_{33}/dp) - 4(dc_{13}/dp)$$

and

$$dC_a/dp = dc_{11}/dp - dc_{12}/dp.$$

$$dG_R/dp = \frac{1}{3}[2(G_R/C_a)^2(dC_a/dp) - 6(G_R/C_c)^2(dK_V/dp) + 6K_V(G_R/C_c)^2(dC_c/dp) + 2(G_R/c_{44})^2(dc_{44}/dp) + (G_R/c_{66})^2(dc_{66}/dp)], \quad (23)$$

where

$$G_R = C_i/C_j \quad (24)$$

where

$$C_i = 5C_a C_c c_{44} c_{66},$$

and

$$C_j = [2C_c c_{44} c_{66} + 6K_V C_a c_{44} c_{66} + C_a C_c c_{44} + 2C_a C_c c_{66}].$$

$K_V$  and its first pressure derivative are given by Eqs. (13) and (8), respectively, and

$$dC_c/dp = (c_{11} + c_{12})(dc_{33}/dp) + c_{33}(dc_{11}/dp + dc_{12}/dp) - 4c_{13}(dc_{13}/dp).$$

### 3. COMPARISON OF THE PREDICTED ISOTROPIC ACOUSTIC DATA WITH EXPERIMENTAL POLYCRYSTALLINE ACOUSTIC DATA

Having presented theoretical expressions for isotropic (polycrystalline) acoustic data in terms of anisotropic (single-crystal) acoustic data, we proceed in this section to compare the computed values of the isotropic acoustic data with experimental polycrystalline acoustic data. Comparison is made here for crystalline Al, Cu,  $\alpha$ -Fe, MgO, and Mg, since for these solids, results on ultrasonic-pressure experiments are reported in the literature individually for both single-crystal and polycrystalline materials.

#### 3.1. Cubic Crystals

Table I lists values of the first pressure derivatives of single-crystal elastic constants for Al,<sup>2,3</sup> Cu,<sup>2,4,5</sup>  $\alpha$ -Fe,<sup>6</sup> and MgO.<sup>7</sup> The values listed under  $(\partial c_{\mu\nu}/\partial p)_T$  are the experimental quantities resulting from the usual ultrasonic-pressure experiments. Other quantities entered are computed results according to thermodynamic re-

lations to be presented in Sec. 4, and they are discussed there. Using the values of  $c_{\mu\nu}^*$  and  $(\partial c_{\mu\nu}^*/\partial p)_T$ , the isotropic values of  $(\partial B^*/\partial p)_T$  and  $(\partial G^*/\partial p)_T$  are computed according to the relations given in the preceding section, and these are compared with experimental polycrystalline acoustic data in Table II. Here the quantity  $(\partial L^*/\partial p)_T$  is the isothermal pressure derivative of adiabatic longitudinal modulus calculated from  $(\partial B^*/\partial p)_T$  and  $(\partial G^*/\partial p)_T$  in the usual way (i.e.,  $L^* = K^* + 4G^*/3$ ). The polycrystalline acoustic data entered in Table II are those compiled by Birch<sup>8</sup> and also by Voronov and Vereshchagin.<sup>9</sup> Note that for every solid, the values of the pressure derivatives for the bulk, shear, and longitudinal moduli calculated from the single-crystal acoustic data are in essential agreement with the corresponding values measured on actual polycrystalline specimens. The observed discrepancies between the predicted and measured values for the pressure derivatives of isotropic elastic moduli are always within the scatter in both the single-crystal and polycrystalline acoustic data themselves. The kind of agreement seen here lends support to the validity of the theoretical relations presented in Sec. 2.

<sup>2</sup> D. Lazarus, Phys. Rev. **76**, 545 (1949).

<sup>3</sup> R. E. Schmunk and C. S. Smith, J. Phys. Chem. Solids **9**, 100 (1959).

<sup>4</sup> W. B. Daneils and C. S. Smith, Phys. Rev. **111**, 713 (1958).

<sup>5</sup> Y. Hiki and A. V. Granato, Phys. Rev. **144**, 411 (1966).

<sup>6</sup> C. A. Rotter and C. S. Smith, J. Phys. Chem. Solids **27**, 267 (1966).

<sup>7</sup> E. H. Bogardus, J. Appl. Phys. **36**, 2504 (1965).

<sup>8</sup> F. Birch, *Handbook of Physical Constants* S. P. Clark, Jr., Ed. (Geological Society of America, Inc., New York, 1966), Memoir No. 97, p. 124.

<sup>9</sup> F. F. Voronov and L. F. Vereshchagin, Fiz. Metal Metalloved **11**, 443 (1961).