

TABLE II. Comparison of predicted and experimental isotropic pressure derivatives of polycrystalline elastic moduli for Al, Cu,  $\alpha$ -Fe, and MgO ( $\sim 300^\circ\text{K}$ ).

|              | Material and reference <sup>a</sup> | Isothermal pressure derivatives of adiabatic moduli |                               |                               |
|--------------|-------------------------------------|---|-------------------------------|-------------------------------|
|              |                                     | $(\partial K^*/\partial p)_T$                       | $(\partial G^*/\partial p)_T$ | $(\partial L^*/\partial p)_T$ |
| Al           | Calculated (49LI) <sup>a</sup>      | 3.95  | 2.71                          | 7.56                          |
|              | Calculated (59SI)                   | 5.22  | 2.01                          | 7.90                          |
|              | Measured (61VI) <sup>b</sup>        | 4.75  | 2.00                          | 7.42                          |
|              | Measured (66BI) <sup>c</sup>        | 3.9   | 2.2                           | 6.8                           |
| Cu           | Calculated (49LI)                   | 4.44  | 0.86(?)                       | 5.59(?)                       |
|              | Calculated (58DI)                   | 5.59  | 1.36                          | 7.40                          |
|              | Calculated (66HI)                   | 5.28  | 1.45                          | 7.21                          |
|              | Measured (66 BI) <sup>c</sup>       | 4.9   | 1.4                           | 6.8                           |
| $\alpha$ -Fe | Calculated (66RI)                   | 5.96  | 1.91                          | 8.50                          |
|              | Measured (61VI) <sup>b</sup>        | 5.13  | 2.16                          | 8.01                          |
|              | Measured (66BI) <sup>c</sup>        | 4.0   | 1.9                           | 6.5                           |
| MgO          | Calculated (65BI)                   | 4.14  | 2.47                          | 7.43                          |
|              | Measured (66BI) <sup>c</sup>        | 3.9   | 2.6                           | 7.4                           |

<sup>a</sup> See Table I for the complete reference.<sup>b</sup> 61VI: F. F. Voronov and L. F. Vereshchagin, *Fiz. Metal Metalloved.* **11**, 443 (1961).<sup>c</sup> 66BI: F. Birch, *Handbook of Physical Constants*, S. P. Clark, Jr., Ed (Geological Society of America, 1966), Memoir 97, p. 124.

is

$$C_p - C_v = TV\beta^2 K^T = T\beta\gamma_G C_v. \quad (28)$$

It may be seen from Eqs. (25) and (28) that the two bulk moduli and the two specific heats have the same ratio:

$$K^*/K^T = C_p/C_v = 1 + TV\beta^2 K^*/C_p = 1 + T\beta\gamma_G = A. \quad (29)$$

Therefore,

$$K^T = K^* A^{-1}, \quad (30)$$

and this is a convenient relation to be used in the following.

Differentiating Eq. (30), with respect to pressure, yields

$$\begin{aligned} (\partial K^T/\partial p)_T = (\partial K^*/\partial p)_T + [(A-1)/A][1 - (2/\beta K^T)(\partial K^T/\partial T)_p - 2(\partial K^*/\partial p)_T] \\ + [(A-1)/A]^2[(\partial K^*/\partial p)_T - (1/\beta^2)(\partial\beta/\partial T)_p - 1]. \end{aligned} \quad (31)$$

The quantity  $(\partial K^T/\partial T)_p$  can be obtained from the experimental  $(\partial K^*/\partial T)_p$  by differentiating Eq. (30), with respect to temperature. Thus

$$(\partial K^T/\partial T)_p = (1/A)(\partial K^*/\partial T)_p - (K^T/A)(\partial A/\partial T)_p, \quad (32)$$

where

$$\begin{aligned} (\partial A/\partial T)_p = A[(A-1)/A]\{1/T + (1/\beta)(\partial\beta/\partial T)_p + (1/K^*)(\partial K^*/\partial T)_p \\ + \beta[1 + (1/\beta^2)(\partial\beta/\partial T)_p] - (1/C_p)(\partial C_p/\partial T)_p\}. \end{aligned} \quad (33)$$

Equation (31) is the desired relation from which one can calculate the isothermal pressure derivative of the isothermal bulk modulus from the experimentally measured  $(\partial K^*/\partial p)_T$ , the isothermal pressure derivative of the adiabatic bulk modulus. Equation (31) was given first by Overton.<sup>10</sup> Equation (32) is the relation through which one can convert the isothermal temperature derivative of the isothermal bulk modulus from the experimental  $(\partial K^*/\partial T)_p$ , the isothermal temperature derivative of the adiabatic bulk modulus.

It can be shown that, although Eqs. (25) and (26) are referred to the zero-pressure condition, these relations hold also for all the other pressures. Differentiating Eq. (25), with respect to pressure, yields

$$(\partial c_{11}^T/\partial p)_T - (\partial c_{11}^*/\partial p)_T = (\partial c_{12}^T/\partial p)_T - (\partial c_{12}^*/\partial p)_T = (\partial K^T/\partial p)_T - (\partial K^*/\partial p)_T = B, \quad (34)$$

where an expression for  $B$  may be found from Eq. (31):

$$B = [(A-1)/A][1 - (2/\beta K^T)(\partial K^T/\partial T)_p - 2(\partial K^*/\partial p)_T] + [(A-1)/A]^2[(\partial K^*/\partial p)_T - (1/\beta^2)(\partial\beta/\partial T)_p - 1]. \quad (35)$$

<sup>10</sup> W. C. Overton, Jr., *J. Chem. Phys.* **37**, 116 (1962).