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

			Isc	othermal press			
×,	Material and reference <sup>a</sup>		(6	$(K^*/\partial p)_T$	( <i>∂G</i> */ <i>∂p</i> ) <sub>T</sub>	$(\partial L^*/\partial p)_T$	
	Al	Calculated (49Ll)	· · ·	3.95	2.71	7.56	
		Calculated (59Sl)		5.22	2.01	7.90	
		Measured (61Vl) <sup>b</sup>		4.75	2.00	7.42	
		Measured (66Bl)°		3.9	2.2	6.8	
						· · · · ·	
	Cu	Calculated (49Ll)		4.44	0.86(?)	5.59(?)	
		Calculated (58Dl)		5.59	1.36	7.40	
		Calculated (66Hl)	1. S.	5.28	1.45	7.21	
		Measured (66 Bl)°		4.9	1.4	<b>6.8</b>	
	o Fe	Calculated (66R1)		5.96	1 01	8 50	
	u-i c	Measured (61VI)b		5 13	2.16	8 01	
		Measured (66Pl)		4.0	1.0	6.5	*
		Measured (00DI)		4.0	1.9	0.5	
	MgO	Calculated (65Bl)		4.14	2.47	7.43	
		Measured (66Bl)°		3.9	2.6	7.4	

Therefore,

following.

yields

<sup>a</sup> See Table I for the complete reference.

<sup>b</sup> 61Vl: F. F. Voronov and L. F. Vereshchagin, Fiz. Metal Metalloved. 11, 443 (1961).

<sup>6</sup> 66Bl: F. Birch, Handbook of Physical Constants, S. P. Clark, Jr., Ed (Geological Society of America, 1966), Memoir 97, p. 124.

 $K^T = K^* A^{-1}$ 

and this is a convenient relation to be used in the

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

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$$C_p - C_v = TV\beta^2 K^T = T\beta\gamma_G C_v. \tag{28}$$

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

$$K^{*}/K^{T} = C_{p}/C_{v} = 1 + TV\beta^{2}K^{*}/C_{p} = 1 + T\beta\gamma_{g} = A.$$
 (29)

$$(\partial K^{T}/\partial p)_{T} = (\partial K^{s}/\partial p)_{T} + [(A-1)/A][1 - (2/\beta K^{T})(\partial K^{T}/\partial T)_{p} - 2(\partial K^{s}/\partial p)_{T}]$$

$$+ [(A-1)/A]^{2}[(\partial K^{s}/\partial p)_{T} - (1/\beta^{2})(\partial \beta/\partial T)_{p} - 1].$$
(31)

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

$$(\partial K^T / \partial T)_p = (1/A) (\partial K^s / \partial T)_p - (K^T / A) (\partial A / \partial T)_p, \tag{32}$$

where

$$(\partial A/\partial T)_p = A[(A-1)/A]\{1/T + (1/\beta)(\partial\beta/\partial T)_p + (1/K^{*})(\partial K^{*}/\partial T)_p$$

 $+\beta [1+(1/\beta^2)(\partial\beta/\partial T)_p] - (1/C_p)(\partial C_p/\partial T)_p]. \quad (33)$ 

Equation (31) is the desired relation from which one can calculate the isothermal pressure derivative of the isothermal bulk modulus from the experimentally measured  $(\partial K^s/\partial p)_T$ , 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  $(\partial K^s/\partial T)_p$ , 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

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

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

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

n, Jr., J. Chem. Phys. 37, 116 (1962)