

TABLE I. Pressure derivatives of crystalline Al, Cu, α -Fe, and MgO at different thermodynamic boundary conditions ($\sim 300^\circ\text{K}$).

Material	dC_{11}/dp			dC_{12}/dp			dC_{44}/dp			dK/dp		
	$(\partial C_{11}^s/\partial p)_T$	$(\partial C_{11}^s/\partial p)_s$	$(\partial C_{11}^T/\partial p)_T$	$(\partial C_{12}^s/\partial p)_T$	$(\partial C_{12}^s/\partial p)_s$	$(\partial C_{12}^T/\partial p)_T$	$(\partial C_{44}^s/\partial p)_T$	$(\partial C_{44}^s/\partial p)_s$	$(\partial C_{44}^T/\partial p)_T$	$(\partial K^s/\partial p)_T$	$(\partial K^s/\partial p)_s$	$(\partial K^T/\partial p)_T$
Al(49LI) ^a	8.40	8.02	8.83	1.80	1.58	2.23	2.10	1.99	3.95	3.69	4.37	4.37
Al(59SI) ^b	7.38	7.00	7.71	4.14	3.92	4.47	2.31	2.20	5.22	4.94	5.55	5.55
Cu(49LI) ^a	5.23	5.06	5.35	4.04	3.96	4.16	1.04	0.93	4.41	4.33	4.56	4.56
Cu(58DI) ^c	6.37	6.20	6.42	5.21	5.13	5.26	2.36	2.24	5.59	5.48	5.65	5.65
Cu(66HI) ^d	5.93	5.76	6.00	4.95	4.87	5.02	2.77	2.66	5.28	5.17	5.35	5.35
α -Fe(66RI) ^e	7.51	7.39	7.54	5.19	5.13	5.22	2.66	2.63	5.96	5.88	5.99	5.99
MgO(65BI) ^f	8.90	8.74	8.94	1.76	1.78	1.80	1.19	1.16	4.14	4.10	4.18	4.18

^a 49LI: D. Lazarus, Phys. Rev. 76, 545 (1949).^b 59SI: R. E. Schmunk and C. S. Smith, J. Phys. Chem. Solids 9, 100 (1959).^c 58DI: W. B. Daniels and C. S. Smith, Phys. Rev. 111, 713 (1958).^d 66HI: Y. Hiki and A. V. Granato, Phys. Rev. 144, 411 (1966).^e 66RI: C. A. Rotter and C. S. Smith, J. Phys. Chem. Solids 27, 267 (1966).^f 65BI: E. H. Bogardus, J. Appl. Phys. 36, 2504 (1965).

3.2. Hexagonal Crystals

In the literature, experimental acoustic data on both single-crystal and polycrystalline materials of Mg are reported. The single-crystal acoustic data are due to Schmunk and Smith²; for polycrystalline data, we use the acoustic data reported by Voronov and Vereshchagin.⁹ Table III summarizes the single-crystal acoustic data. In Table IV, we compare the isotropic acoustic data resulting from the present calculations with the corresponding values measured on polycrystalline specimens. The agreement is good as may be seen from the table.

4. THERMODYNAMIC RELATIONS FOR THE ADIABATIC AND ISOTHERMAL ACOUSTIC DATA

Typical ultrasonic experiments, in which pressure is a variable, involve measurements of the behavior of an elastic wave propagating in a statically stressed crystal. Thermodynamically, the ultrasonic velocity measurements in the crystal (specimen) involve an adiabatic process; on the other hand, the application of pressure to the specimen is an isothermal process. Thus, the acoustic data resulting from such experiments are neither thermodynamically "pure" adiabatic nor thermodynamically "pure" isothermal quantities, but are "mixed" quantities. How, then, can one calculate (a) isothermal pressure derivatives of the isothermal elastic moduli and (b) adiabatic pressure derivatives of the adiabatic elastic moduli from the experimentally determined isothermal pressure derivatives of the adiabatic elastic moduli? In the following discussion, the thermodynamic relations applicable for cubic crystals are presented for (a) and (b) in terms of the measured quantities resulting from the usual ultrasonic-pressure experiments.

At the absence of pressure, it is well-known that the relationships between the adiabatic and isothermal values of the second-order elastic constants are given by the following:

$$\begin{Bmatrix} c_{11}^s - c_{11}^T \\ c_{12}^s - c_{12}^T \\ K^s - K^T \end{Bmatrix} = \frac{T\beta^2}{\rho C_p (s_{11}^s + 2s_{12}^s)^2} = T\beta\gamma_G K^T, \quad (25)$$

and

$$c_{44}^s = c_{44}^T = c_{44}. \quad (26)$$

Where β is the coefficient of volume expansion, ρ is the density, T is the temperature, and γ_G is the Grüneisen constant given by

$$\gamma_G = \beta K^s / \rho C_p = \beta V K^T / C_v = \beta V K^s / C_p. \quad (27)$$

The superscripts s and T denote the adiabatic and the isothermal values, respectively. C_p and C_v are the specific heats at constant pressure and that at constant volume, respectively, and the difference between them