constants have been already tabulated in Table I. The elastic and thermal properties of each solid used in the construction of Table I are summarized in Tables V and VI. The computed values of polycrystalline acoustic data corresponding to three thermodynamic boundary conditions are illustrated in Table VII with crystalline MgO as an example. In Table VII, also entered are two other values of pressure derivative of the bulk modulus; one is a theoretical value based on the Dugdale–MacDonald relation,[12] and the other is derived from the Murnaghan equation of state[13] by a curve-fitting procedure using experimental compression data.[14–17] It is seen here that these values compare very well with the corresponding quantities resulting from the ultrasonic-pressure experiments made on both the single-crystal and polycrystalline materials.

5. CALCULATION OF THE POLYCRYSTALLINE ACOUSTIC DATA FROM THE SINGLE-CRYSTAL THIRD-ORDER ELASTIC CONSTANTS

The pressure-dependent second-order elastic constants can be written in a form[11,18]

$$C^s_{ijkl}(p)=(\lambda/V^0)[\partial^2U(V^0,S,\tilde{\eta})/\partial\eta_{ij}\partial\eta_{kl}]_{V^0,S=\mathrm{const.},\eta=\epsilon 1}+pD_{ijkl} \tag{50}$$

where

$$D_{ijkl}=\delta_{ij}\delta_{kl}-\delta_{il}\delta_{jk}-\delta_{ik}\delta_{jl}.$$

V denotes the volume of crystal at a reference state characterized by the hydrostatic pressure p, and $\tilde{\eta}$ is the strain tensor corresponding to an arbitrarily deformed state characterized by that pressure p. V^0 is defined by the relation $(V/V^0)=\lambda^3$, where λ is a factor given by the coordinates of a material point in two reference states a_i and a_i^0 according to $(a_i/a_i^0)=\lambda$. The Lagrangian strain tensors[19] corresponding to these two reference states η_{ij} and η_{ij}^0 are then related by

$$\eta_{ij}^0=\lambda^2\eta_{ij}+\epsilon\delta_{ij},$$

where $\epsilon=\frac{1}{2}(\lambda^2-1)$. Keeping in mind the relations $(\partial/\partial p)_{s,T}=-(V/K^{s,T})(\partial/\partial V)_{s,T}$ and $(\partial\lambda/\partial V)_0=(\partial\epsilon/\partial V)_0=1/3V^0$, one finds by differentiating Eq. (50) that

$$(\partial C^s_{ijkl}/\partial p)_S=-(1/3K^s)\{(1/V^0)[\partial^2U(V^0,S,\tilde{\eta})/\partial\eta_{ij}\partial\eta_{kl}]_{V^0,S=\mathrm{const.},\eta=0}+(1/V^0)[\partial^3U(V^0,S,\tilde{\eta})/\partial\eta_{ij}\partial\eta_{kl}\partial\eta_{mn}]_{V^0,S=\mathrm{const.},\eta=0}\}+D_{ijkl}, \tag{51}$$

and

$$(\partial C^s_{ijkl}/\partial p)_T=-(1/3K^T)((1/V^0)[\partial^2U(V^0,S,\tilde{\eta})/\partial\eta_{ij}\partial\eta_{kl}]_{V^0,S=\mathrm{const.},\eta=0}+(1/V^0)\{(\partial/\partial\eta_{mn})[\partial^2U(V^0,S,\tilde{\eta})/\partial\eta_{ij}\partial\eta_{kl}]_{V^0,S=\mathrm{const.},\eta=0}\}_{V^0,S=\mathrm{const.},\eta=0})+D_{ijkl}. \tag{52}$$

Note that the first terms in Eqs. (51) and (52) are by definition the zero-pressure second-order elastic constants. The second term in Eq. (51) is the zero-pressure third-order elastic constants, whereas that in Eq. (52) is by definition thermodynamically "mixed" third-order elastic constants at $p=0$. Hence, from these, we obtain the familiar expressions[11]

$$(\partial C^s_{ijkl}/\partial p)_S=-[(C^s_{ijkl}+C^s_{ijklmm})/3K^s]+D_{ijkl}, \tag{53}$$

and

$$(\partial C^s_{ijkl}/\partial p)_T=-[(C^s_{ijkl}+C_{ijklmm})/3K^T]+D_{ijkl}, \tag{54}$$

where

$$C_{ijklmm}=(1/A)\{C^s_{ijklmm}+T\gamma_G[-\beta C^s_{ijkl}+3(\partial C^s_{ijkl}/\partial T)_p]\}. \tag{55}$$

Similarly, we find

$$(\partial C^T_{ijkl}/\partial p)_T=-[(C^T_{ijkl}+C^T_{ijkimm})/3K^T]+D_{ijkl}. \tag{56}$$

The quantities specified by Eq. (55) are certain linear combinations of the third-order elastic constants C_{ijklmn}, and they are the primary experimental quantities when ultrasonic-pressure experiments are made with hydrostatic pressure. Thus, for cubic crystals, C_{ijklmm} reduces to the following:

$$C_I=C_{1111ii}=c_{111}+2c_{112}=-[3K^T(\partial c_{11}^s/\partial p)_T+3K^T+c_{11}^s], \tag{57}$$

$$C_{II}=C_{1122ii}=2c_{112}+c_{123}=-[3K^T(\partial c_{12}^s/\partial p)_T-3K^T+c_{12}^s], \tag{58}$$

$$C_{III}=C_{1212ii}=c_{144}+2c_{166}=-[3K^T(\partial c_{44}/\partial p)_T+3K^T+c_{44}]. \tag{59}$$

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