

3. Preliminaries

The various relations used in the iterative procedure to be described originate either in the theory of elastic wave propagation in a solid or in thermodynamics theory. These general relations are presented with brief introductory remarks drawn from the two theories and appended only to clarify the material of this paper.

3.1 Relations obtained from the theory of elastic wave propagation

The elastic constants of a solid are determined by measuring the velocities with which elastic waves are propagated along several directions in the solid. The number of velocity measurements needed to understand the elastic property of the solid depends on the crystallographic class to which it belongs. Christoffel's equations (e.g. equation (2)) which are applicable to any crystalline system give the relationship between measured velocities and elastic constants. In general, for a plane wave propagated in a crystal having direction cosines l, m, n , the three possible wave velocities V may be found in terms of the elastic constant C_{pq} from the roots of Christoffel's equations.

$$\begin{vmatrix} A_{11} - \rho V^2 & A_{12} & A_{13} \\ A_{12} & A_{22} - \rho V^2 & A_{23} \\ A_{13} & A_{23} & A_{33} - \rho V^2 \end{vmatrix} = 0, \quad (2)$$

where

$$A_{ij} = l^2 C_{1i1j} + m^2 C_{2i2j} + n^2 C_{3i3j} + l m (C_{1i2j} + C_{2i1j}) + \\ + l n (C_{1i3j} + C_{3i1j}) + m n (C_{2i3j} + C_{3i2j}). \quad (3)$$

It follows that ρV^2 is related to C_{ijkl} in a manner determined by the direction in which a wave is propagated. Three different velocities of propagation imply that the three displacement vectors associated with these velocities are mutually perpendicular and hence independent. Usually the three waves are mixed; one is predominantly longitudinal and the other two are predominantly shear. Pure waves may be propagated only in a few special crystallographic directions. The location of the pure mode directions in crystals of various symmetries have been investigated exhaustively by Borgnis [4] and Brugger [5].

3.2 Thermodynamic relations

These relations serve two purposes:

(i) To evaluate the pressure derivatives of the specific heat and the linear thermal expansions in the three principal directions of the solid at pressure P and temperature T ; and

(ii) To convert the adiabatic quantities into their isothermal counterparts at pressure P and temperature T .

The adiabatic and isothermal elastic compliances are related by

$$S_{ijkl}^S(P, T) - S_{ijkl}^T(P, T) = -\beta_{ij}(P, T) \beta_{kl}(P, T) T [C_P(P, T) \rho(P, T)]^{-1}. \quad (4)$$

When expressed in our notation the following relation between $\chi^S(l, m, n, P, T)$ and $\chi^T(l, m, n, P, T)$ results:

$$\chi^T(l, m, n, P, T) = \chi^S(l, m, n, P, T) + \Delta(l, m, n, P, T), \quad (5)$$

where

$$\chi(l, m, n, P, T) = (S_{11} + S_{12} + S_{13}) l^2 + (S_{12} + S_{22} + S_{23}) m^2 + (S_{13} + S_{23} + S_{33}) n^2, \quad (6)$$

$$\Delta(l, m, n, P, T) = \frac{\beta(P, T) T}{\varrho(P, T) C_P(P, T)} \{ \beta(1, 0, 0, P, T) l^2 +$$

and

$$+ \beta(0, 1, 0, P, T) m^2 + \beta(0, 0, 1, P, T) n^2 \}, \quad (7)$$

$$\beta(P, T) = \beta(1, 0, 0, P, T) + \beta(0, 1, 0, P, T) + \beta(0, 0, 1, P, T). \quad (8)$$

From the definition of isothermal linear compressibility, we have

$$\begin{aligned} \chi^T(l, m, n, P, T) &= - \frac{1}{L(l, m, n, P, T)} \left(\frac{\partial L(l, m, n, P, T)}{\partial P} \right)_T \\ &= \frac{1}{\lambda(l, m, n, P, T)} \left(\frac{\partial \lambda(l, m, n, P, T)}{\partial P} \right)_T. \end{aligned} \quad (9)$$

Since the suffix J has no significance in the above relation, it has been omitted from $L(l, m, n, J, P, T)$. By integrating equation (9) with respect to pressure, we obtain

$$\lambda(l, m, n, P, T) = \lambda(l, m, n, P_1, T) \exp \{ (P - P_1) \chi^T(l, m, n, P, T) \}, \quad (10)$$

by taking into account definition (9) which implies that $\chi^T(l, m, n, P, T)$ remains constant in the range of integration P to P_1 . Again the temperature derivative of linear compressibility is related to the pressure derivative of the linear thermal expansion of a material by

$$\left(\frac{\partial \chi^T(l, m, n, P, T)}{\partial T} \right)_P = - \left(\frac{\partial \beta(l, m, n, P, T)}{\partial P} \right)_T \quad (11)$$

and the pressure derivative of specific heat may be written as

$$\left(\frac{\partial C_P(P, T)}{\partial P} \right)_T = - \frac{T}{\varrho(P, T)} \left\{ \beta^2(P, T) + \left(\frac{\partial \beta(P, T)}{\partial T} \right)_P \right\}. \quad (12)$$

Use of the above set of relations enables one to estimate the values of the elastic constants of a solid at high pressure without *a priori* knowledge of the compressibility of the substance.

4. General Iterative Scheme

In general the iterative scheme proposed here attempts to obtain self-consistent estimates of $\lambda(l, m, n, P, T)$ in the three principal directions, i.e. $\lambda(1, 0, 0, P, T)$, $\lambda(0, 1, 0, P, T)$, and $\lambda(0, 0, 1, P, T)$ at pressure P and temperature T . The scheme presented below assumes the following:

(i) The temperature dependence of the linear expansion coefficients are known at one atmosphere.

(ii) The value of specific heat is known as a function of temperature at one atmosphere.