An Iterative Scheme to Estimate the Values of Elastic Constants

(iii) An adequate number of velocity measurements are made to extract information about the elastic property of the solid as a function of pressure at more than two temperatures.

At P = 1 and within the experimental range of temperature, all the quantities in the above set of 12 relations are known; no iteration is required to estimate the values of the elastic constants of a solid as a function of temperature at one atmosphere.

At the next higher pressure all the quantities in the above set of relations are known except those involving $\lambda(l, m, n, P, T)$. The iterative procedure developed here yields a self-consistent estimate of the elastic constants of a solid and also the pressure and temperature derivatives of the linear thermal expansion and of the specific heat of the solid at a pressure P and temperature T. To initiate the procedure, we set

$$\left(\frac{\partial \chi^{T}(l, m, n, P, T)}{\partial T}\right)_{P} = \left(\frac{\partial \chi^{T}(l, m, n, P_{1}, T)}{\partial T}\right)_{P_{1}}$$
(13)

and

$$\left(\frac{\partial\beta(l, m, n, P, T)}{\partial T}\right)_{P} = \left(\frac{\partial\beta(l, m, n, P_{1}, T)}{\partial T}\right)_{P_{1}},$$
(14)

where P_1 is the preceding value of pressure. These enable us to compute $\beta(l, m, n, P, T)$ and $C_P(P, T)$. Next we set

$$\lambda(l, m, n, P, T) = \lambda(l, m, n, P_1, T), \qquad (15)$$

enabling us to compute $\rho(P, T)$ from the relation

$$\frac{1}{\varrho(P,T)} \left(\frac{\partial \varrho(P,T)}{\partial P} \right)_T = \chi^T(P,T) = \chi^T(1,0,0,P,T) + \chi^T(0,1,0,P,T) + \chi^T(0,0,1,P,T) .$$
(16)

Equation (16) is obtained by expressing $\chi^T(P, T)$ in terms of the three principal isothermal linear compressibilities through equation (6). L(l, m, n, P, T) is computed with the help of both equation (15) and the definition of $\lambda(l, m, n, P, T)$ given in the section dealing with notation. These with the known values of $\tau(l, m, n, J, P, T)$ enable us to estimate $C_{pq}^{S}(P, T)$ from equations (2). The use of relations (1), (4), (11), and (12) together with the assumptions (13) and (14)provide estimates of the values of $S_{pq}^T(P, T)$. From these estimates of $S_{pq}^T(P, T)$ we obtain $\chi^{T}(l, m, n, P, T)$, which by relation (10) yields a new estimate of $\lambda(l, m, n, P, T)$. If the new values of $\lambda(l, m, n, P, T)$ in the three principal directions agree with their respective values assumed at the beginning of the iteration, the estimated values of the elastic constants are correct and consistent with the assumptions represented by relations (13) and (14). If these values of $\lambda(l, m, n, P, T)$ do not agree with the previously assumed values iteration is repeated with these new values of $\lambda(l, m, n, P, T)$ as starting values and all the related quantities are recalculated. This process repeats until two consecutive estimates of $\lambda(l, m, n, P, T)$ in the three respective principal directions are equal in magnitude at the pressure P and a temperature T. The complete procedure is carried out at the pressure P and at all the temperatures at which the travel-time measurements were made. When all the elastic constants of

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Table 1 A flow chart of the iterative scheme to estimate the values of the elastic constants of a solid as a function of pressure and temperature. $A(l, m, n, P, T) = [\partial \chi^{T}(l, m, n, P, T)/\partial T]_{P}$ and $B(l, m, n, P, T) = [\partial \beta(l, m, n, P, T)/\partial T]_{P}$ Increase pressure (P) -Temperature (T) · next temperature In the three principal directions Set A(l, m, n, P, T) = A'(l, m, n, P, T) Set $A(l, m, n, P, T) = A(l, m, n, P_1, T)$ and $B(l, m, n, P, T) = B(l, m, n, P_1, T)$ Set B(l, m, n, P, T) == B'(l, m, n, P, T) $\beta(l, m, n, P, T)$ $\beta(P, T)$ In the three principal directions Set $\lambda(l, m, n, P, T) = \lambda(l, m, n, P_1, T)$ Set $\lambda(l, m, n, P, T)$ $=\lambda'(l, m, n, P, T)$ $\varrho(P, T)$ $C_P(P, T)$ Jth velocity mode at P and Tnext velocity mode L(l, m, n, J, P, T)V(l, m, n, J, P, T)When all velocity modes are calculated at P and T $C^{S} p q(P, T)$ $S^S p q(P, T)$ $\chi^{S}(l, m, n, P, T)$ $\Delta(l, m, n, P, T)$ $\chi^T(l, m, n, P, T)$ $\lambda'(l, m, n, P, T)$ If $\lambda'(l, m, n, P, T) \neq \lambda(l, m, n, P, T) \downarrow$ If $\lambda(l, m, n, P, T) = \lambda'(l, m, n, P, T)$ in each of the three principal directions When all $\varkappa^{T}(l, m, n, P, T)$ and L(l, m, n, P, T) are calculated at P A'(l, m, n, P, T)B'(l, m, n, P, T)If $B'(l, m, n, P, T) \neq B(l, m, n, P, T)$ or if $A'(l, m, n, P, T) \neq A(l, m, n, P, T)$ If A(l, m, n, P, T) = A'(l, m, n, P, T)

If A(l, m, n, P, T) = A'(l, m, n, P, T)and B(l, m, n, P, T) = B'(l, m, n, P, T)in each of the three principal directions

End