(using equation 74), the result is

$$\left(\frac{\partial \gamma_i}{\partial s_k}\right)_\theta = \gamma_i Q_k + D^\theta_{ik} + \gamma_j \left(\frac{\partial c^\theta_{ik}}{\partial T_j}\right)_\theta, \tag{87}$$

where

$$Q_k = \delta_k - \left(\frac{\partial \ln C_s}{\partial s_k}\right)_\theta, \tag{88}$$

$$D^\theta_{ik} = -\frac{V}{C_s}\left(\frac{\partial c^\theta_{ik}}{\partial \theta}\right)_T. \tag{89}$$

The following identity was also used in deriving (87):

$$\left(\frac{\partial}{\partial \theta}\right)_s = \left(\frac{\partial}{\partial \theta}\right)_T - \lambda_i \left(\frac{\partial}{\partial T_i}\right)_\theta. \tag{90}$$

Relations between the derivatives of the isothermal and isentropic elastic moduli can be derived as follows. Define

$$\mu_{ij} = c^\sigma_{ij} - c^\theta_{ij} = \theta\lambda_i\lambda_j/\rho C_s = \theta\rho C_s \gamma_i\gamma_j. \tag{91}$$

Differentiating (91) and using (87),

$$\left(\frac{\partial \mu_{ij}}{\partial T_k}\right)_\theta = S^\theta_{nk}(R_{ijn} - \mu_{ij}Q_n), \tag{92}$$

where

$$S^\theta_{ij} = \left(\frac{\partial s_i}{\partial T_j}\right)_\theta = (\mathbf{c}^\theta)^{-1}_{ij}, \tag{93}$$

i.e. S^θ_{ij} are the isothermal elastic compliances, and

$$R_{ijk} = \theta\rho C_s \left[\frac{\partial(\gamma_i\gamma_j)}{\partial s_k}\right]_\theta \tag{94}$$

$$= 2\mu_{ij}Q_k + \theta\rho\lambda_i D^\theta_{jk} + \theta\rho\lambda_j D^\theta_{ik} + \mu_{li}c^\theta_{jk,l} + \mu_{lj}c^\theta_{ik,l}, \tag{95}$$

where a comma preceeding a subscript denotes differentiation with respect to the corresponding stress component.

Similarly, differentiating (91) with respect to θ, and using (90),

$$\left(\frac{\partial \mu_{ij}}{\partial \ln \theta}\right)_T = \mu_{ij}\left[1 + \left(\frac{\partial \ln C_s}{\partial \ln \theta}\right)_s\right] + \theta\rho C_s \left[\frac{\partial(\gamma_i\gamma_j)}{\partial \ln \theta}\right]_s + \theta\lambda_k \left(\frac{\partial \mu_{ij}}{\partial T_k}\right)_\theta. \tag{96}$$

The relations developed so far in this section, i.e. equations (81), (83), (87), (92) and (96), are completely general in that they refer to a material of arbitrary symmetry under an arbitrary stress. They will now be specialized to the case of a material of cubic symmetry under a hydrostatic stress. As was pointed out in Section 2, only one strain parameter is required in this case, so that the application of these relations is simplified. Of course, the resulting relations can also be further specialized to the case of an isotropic material.

Under cubic symmetry, the thermal expansion tensor becomes

$$\alpha_i = \frac{1}{3}\alpha\delta_i, \quad \alpha = \alpha_i\delta_i = \left(\frac{\partial \ln V}{\partial \theta}\right)_T. \tag{97}$$

Thus,

$$\lambda_i = \frac{\alpha}{3}c^\theta_{ij}\delta_j = \frac{\alpha}{3}(c^\theta_{11} + 2c^\theta_{12})\delta_i = \alpha K_\theta \delta_i = \lambda\delta_i, \tag{98}$$

where K_θ is the isothermal bulk modulus, and

$$\gamma_i = \frac{\alpha K_\theta}{\rho C_s}\delta_i = \gamma\delta_i, \tag{99}$$

$$\mu_{ij} = \alpha\gamma\theta K_\theta \delta_i\delta_j = \mu\delta_i\delta_j. \tag{100}$$

Note, in particular, that $\mu_{11} = \mu_{12}$ and $\mu_{44} = 0$.

Under hydrostatic stress, $T_i = -P\delta_i$, where P is the pressure, and the strain of a material of cubic symmetry can be specified by the specific volume V. Thus

$$Q_i = \left[1 - \left(\frac{\partial \ln C_V}{\partial \ln V}\right)_\theta\right]\delta_i = Q\delta_i, \tag{101}$$

$$D^\theta_{ij} = -\frac{\gamma}{\alpha K_\theta}\left(\frac{\partial c^\theta_{ij}}{\partial \theta}\right)_P = \gamma\delta^\theta_{ij}, \tag{102}$$

where δ^θ_{ij} is the generalized isothermal analogue of the Anderson–Grüneisen parameter [17, 18]. With these results, equation (87) becomes

$$\left(\frac{\partial \gamma_i}{\partial s_j}\right)_\theta = \gamma\left[Q\delta_i\delta_j + \delta^\theta_{ij} - \left(\frac{\partial c^\theta_{ij}}{\partial P}\right)_\theta\right]. \tag{103}$$

There are three independent derivatives of γ_i in this case, just as there are three independent components each of c^θ_{ij} and δ^θ_{ij}. Note that Q does not contribute to $(\partial\gamma_4/\partial s_4)$. It may also be noted that this derivative is non-zero, even though under cubic symmetry γ_4 is zero. This is because the strain s_4 destroys cubic symmetry, thus allowing γ_4 to vary from zero as s_4 varies from zero. From (103)

$$\left(\frac{\partial \gamma}{\partial \ln V}\right)_\theta = \gamma\left[Q + \delta^\theta - \left(\frac{\partial K_\theta}{\partial P}\right)_\theta\right], \tag{104}$$

where $\delta^\theta = (\delta^\theta_{11} + 2\delta^\theta_{12})/3$; (104) was given by Basset *et al.* [19].

To specialize equations (92) and (96), note first that

$$\left(\frac{\partial \mu_{ij}}{\partial P}\right)_\theta = -\left(\frac{\partial \mu_{ij}}{\partial T_k}\right)_\theta \delta_k$$

and that $S_{nk}\delta_k = \delta_n/3K_\theta$. Then

$$R_{ijk}\delta_k = R\delta_i\delta_j = 6\mu\left(\frac{\partial \ln \gamma}{\partial \ln V}\right)_\theta \delta_i\delta_j, \quad (105)$$

and

$$\left(\frac{\partial \mu_{ij}}{\partial P}\right)_\theta = \left(\frac{\partial \mu}{\partial P}\right)_\theta \delta_i\delta_j$$
$$= -(R - 3\mu Q)/3K_\theta\delta_i\delta_j$$
$$= -\frac{\mu}{K_\theta}\left[2\left(\frac{\partial \ln \gamma}{\partial \ln V}\right)_\theta - Q\right]\delta_i\delta_j. \quad (106)$$

The specialization of equation (96) is

$$\left(\frac{\partial \mu}{\partial \theta}\right)_P = \frac{\mu}{\theta}\left[1 + \left(\frac{\partial \ln C_V}{\partial \ln \theta}\right)_V + 2\left(\frac{\partial \ln \gamma}{\partial \ln \theta}\right)_V\right] - \lambda\left(\frac{\partial \mu}{\partial P}\right). \quad (107)$$

Relations equivalent to (106), (107) were given by Barsch[20].

Finally, note that equation (104) involves the derivatives of the isothermal elastic modulus, whereas it is usually the derivatives of the isentropic modulus which are measured experimentally. The conversion from the temperature derivative of one to the other involves $(\partial\mu/\partial\theta)_P$, which involves $(\partial\mu/\partial P)_\theta$, which in turn involves δ^θ. Equations (102), (104), (106) and (107) can be solved for $(\partial\mu/\partial P)_\theta$ in terms of just derivatives of isentropic quantities:

$$\left(\frac{\partial \mu}{\partial P}\right)_\theta = \frac{\mu}{K_\theta}\left\{2\left(\frac{\partial K_\sigma}{\partial P}\right)_\theta - Q + \frac{2}{\lambda}\left(\frac{\partial K_\sigma}{\partial \theta}\right)_P - 2\gamma\left[1 + \left(\frac{\partial \ln C_V}{\partial \ln \theta}\right)_V + 2\left(\frac{\partial \ln \gamma}{\partial \ln \theta}\right)_V\right]\right\}. \quad (108)$$

5. DISCUSSION

The comments made in Paper I, Section 4, concerning the independence of the approximations made in the thermal and finite strain parts of the theory, the Grüneisen approximation, the expansion of γ as a function of volume, the relationship of this work to that of Thomsen[3, 4] and the capabilities of this theory all apply here in the more general case. In particular, note that this theory predicts that the $c_{\alpha\beta}$ are non-linear in temperature at high temperature and constant pressure[4], and that the $(\partial^2 c_{\alpha\beta}/\partial P\,\partial T)$ are non-zero, in general. Thus, a non-zero value of one of these mixed derivatives does not necessarily mean that a higher order thermal theory is required. Tests of the adequacy of the quasi-harmonic theory will be discussed in a subsequent paper.

The more general theory given here contains the special theory of Paper I, which can be obtained through the relations (34–36), (56) and (57). It is thus a theory of great utility which is capable of describing the effects of shock-compression and isothermal compression as well as the elastic moduli and elastic velocities as functions of pressure and temperature. Applications demonstrating this utility will be given in a subsequent paper.

The primary parameters which enter these equations are the $r^n_{\alpha\beta}$ or $t^n_{\alpha\beta}$ of (25) and (30), the g_α and $h_{\alpha\beta}$ or $h'_{\alpha\beta}$ of (43) and (45), and the density in the reference state, ρ_0. These are related to a similar number of secondary parameters: to $c_{\alpha\beta}$, $c'_{\alpha\beta}$, etc. through (26–28) or (31–33), to the thermal expansion tensor, α_β, through (51) and (83), and to the temperature derivatives of the elastic moduli through (52) and (87–89). In the case of cubic symmetry and hydrostatic prestress, the volume coefficient of thermal expansion, α, enters through (99), and the temperature derivatives of the $c_{\alpha\beta}$ through (58–60), (64–66) and (101–103). The evaluation of these parameters follows a scheme analogous to that outlined in Paper I.

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