tive relations which are implicitly frame-indifferent[5]. For this purpose, the tensors E and $\boldsymbol{\eta}$ (below) will be used as examples of the infinity of possible frame-indifferent strain tensors;

$$E_{ij} = \frac{1}{2}(f_{ij} + f_{ji} - f_{ik}f_{jk}), \tag{11}$$

$$\eta_{ij} = \frac{1}{2}(e_{ij} + e_{ji} + e_{ki}e_{kj}). \tag{12}$$

E is the invariant analogue of the conventional "Eulerian" strain tensor, $\boldsymbol{\epsilon}$, and $\boldsymbol{\eta}$ is the conventional "Lagrangian" strain tensor[4, 5]. It is convenient to define the deformation gradients **G** and **F** as

$$G_{ij} = \frac{\partial a_i}{\partial x_j} = \delta_{ij} - f_{ij}, \tag{13}$$

$$F_{ij} = \frac{\partial x_i}{\partial a_j} = \delta_{ij} + e_{ij} = (G^{-1})_{ij}, \tag{14}$$

and to note the relations

$$\frac{\partial}{\partial u_{kl}} = G_{pk}\frac{\partial}{\partial f_{pl}} = F_{lp}\frac{\partial}{\partial e_{kp}}. \tag{15}$$

Expressions for **T** and **c** in terms of **E** and $\boldsymbol{\eta}$ can now be derived using (11)–(15):

$$T_{ij} = \rho G_{mi}\frac{\partial A}{\partial E_{mn}}G_{nj}, \tag{16}$$

$$c_{ijkl} = \rho G_{mi}G_{pk}\frac{\partial^2 A}{\partial E_{mn}\partial E_{pq}}G_{nj}G_{ql} - P\Delta_{ij}^{kl}, \tag{17}$$

where

$$\Delta_{ij}^{kl} = -\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}, \tag{18}$$

and

$$T_{ij} = \rho F_{im}\frac{\partial A}{\partial \eta_{mn}}F_{jn}, \tag{19}$$

$$c_{ijkl} = \rho F_{im}F_{kp}\frac{\partial^2 A}{\partial \eta_{mn}\partial \eta_{pq}}F_{jn}F_{lq} - P\delta_{ij}^{kl} \tag{20}$$

where

$$\delta_{ij}^{kl} = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}. \tag{21}$$

The application of these expressions requires that the free energy, A, be specified as a function of strain, the usual approach in finite strain theory being to expand A as a Taylor series in some suitable strain measure, such as **E** or $\boldsymbol{\eta}$. In practice, these expansions will be truncated, and different truncation errors will be associated with expansions in terms of different strain measures. Thus the descriptions in terms of different strain tensors, equivalent up to this point, will no longer yield identical results. The development is simplified at this stage by specializing to the case where the material has cubic symmetry. In this case the response to hydrostatic stress is isotropic strain, so that the strain tensors reduce to scalar multiples of the unit tensor. These scalar strains are[1, 3, 4]

$$E = \frac{1}{2}[1 - (\rho/\rho_0)^{2/3}], \tag{22}$$

$$\eta = \frac{1}{2}[(\rho/\rho_0)^{-2/3} - 1]. \tag{23}$$

Thus, expanding A in terms of E, (16) and (17) take the form

$$P = -\frac{1}{3}\rho_0(1-2E)^{5/2}(c_0 + c_1E + c_2E^2 + c_3E^3 + \cdots), \tag{24}$$

$$c_{ijkl} = \rho_0(1-2E)^{7/2}(r_{ijkl}^0 + r_{ijkl}^1E + \frac{1}{2}r_{ijkl}^2E^2 + \cdots) - P\Delta_{ij}^{kl}. \tag{25}$$

The expression (24) for P has been given previously[1]. The parameters r_{ijkl}^n can be related to the c_{ijkl} and their pressure derivatives, evaluated in the natural state (where $E = 0$), by differentiating (25) and evaluating at $E = 0$:

$$r_{ijkl}^0 = V_0(c_{ijkl} + P_0\Delta_{ij}^{kl}), \tag{26}$$

$$r_{ijkl}^1 = -3V_0K_0(c'_{ijkl} + \Delta_{ij}^{kl}) + 7r_{ijkl}^0, \tag{27}$$

$$r_{ijkl}^2 = 9V_0K_0^2c''_{ijkl} - 3K_0'(r_{ijkl}^1 - 7r_{ijkl}^0) + 16r_{ijkl}^1 - 49r_{ijkl}^0, \tag{28}$$

where a prime denotes a pressure derivative, $V = 1/\rho$ is the specific volume, $K = -V(\partial P/\partial V)$ is the bulk modulus and subscript "0" denotes evaluation at $E = 0$ (implicit in c'_{ijkl} and c''_{ijkl}). The analogous expressions derived from (19) and (20) are:

$$P = -\frac{1}{3}\rho_0(1+2\eta)^{-1/2}(b_0 + b_1\eta + b_2\eta^2 + b_3\eta^3 + \cdots), \tag{29}$$

$$c_{ijkl} = \rho_0(1+2\eta)^{1/2}\left(t_{ijkl}^0 + t_{ijkl}^1\eta + \frac{1}{2}t_{ijkl}^2\eta^2 + \cdots\right) - P\delta_{ij}^{kl}, \tag{30}$$

$$t_{ijkl}^0 = V_0(c_{ijkl} + P_0\delta_{ij}^{kl}), \tag{31}$$

$$t_{ijkl}^1 = -3V_0K_0(c'_{ijkl} + \delta_{ij}^{kl}) - t_{ijkl}^0, \tag{32}$$

$$t_{ijkl}^2 = 9V_0K_0^2c''_{ijkl} - 3K_0'(t_{ijkl}^0 + t_{ijkl}^1) - 4t_{ijkl}^1 - t_{ijkl}^0. \tag{33}$$

Equations equivalent to (32) and (33) have been given by Birch[15] and Barsch and Chang[13]. It may be noted that the r_{ijkl}^n and t_{ijkl}^n can also be related to partial contractions of the third and fourth order elastic constants[13]. For the case of cubic symmetry considered here, the parameters c_n of (24) are related to the parameters r^n_{ijkl} of (25) by

$$c_1 = 3(r^0_{1111} + 2r^0_{1122}), \quad (34)$$

$$c_2 = \frac{3}{2}(r^1_{1111} + 2r^1_{1122}), \quad (35)$$

$$c_3 = \frac{1}{2}(r^2_{1111} + 2r^2_{1122}). \quad (36)$$

Analogous relations hold between the b_n of (29) and the t^n_{ijkl} of (30). Again, for cubic symmetry,

$$\Delta^{11}_{11} = -3, \quad \Delta^{22}_{11} = -1, \quad \Delta^{23}_{23} = -1, \quad (37)$$

$$\delta^{11}_{11} = 1, \quad \delta^{22}_{11} = -1, \quad \delta^{23}_{23} = 1. \quad (38)$$

Note that the pressure terms in (25) and (30) need not be taken to the same order as the expressions (24) and (29). For instance, if the original expansion of A in terms of E was to the fourth order, terms up to the third order in E would be kept in (24), but only terms up to second order in E need be kept in (25), since the c_{ijkl} involve second derivatives of A, whereas the pressure involves the first derivative. This truncation procedure differs from that of Thomsen[4], who retained the cubic term in the pressure term in his fourth-order expression for c_{ijkl}. This cubic term is incomplete.

3. THERMAL EFFECTS IN THE QUASI-HARMONIC APPROXIMATION

An approximate description of thermal effects can be included in the preceding finite strain equations by expanding the theory of lattice dynamics, in the quasi-harmonic approximation, into the domain of finite strain. This extension in the present case is a straightforward generalization of the treatment given in Paper I. The Helmholtz free energy of a lattice, A, is the sum of the static lattice potential, $\bar{\phi}$, and the vibrational energy, A_s. In the quasi-harmonic approximation, $A_s = A_q$, where A_q, the quasi-harmonic vibrational energy, depends on strain only through the lattice eigenfrequencies, ω_ν [1, 2]. The strain dependence of A_q can thus be made explicit by expanding the (squared) eigenfrequencies in terms of strain. For instance, in terms of $\mathbf{E}$, the generalization of equation (26) of Paper I is

$$\omega_\nu{}^2 = (\omega_\nu{}^2)_0\left(1 + g^\nu_{ij}E_{ij} + \frac{1}{2}h^\nu_{ijkl}E_{ij}E_{kl} + \cdots\right), \quad (39)$$

where g^ν_{ij} and h^ν_{ijkl}, etc. are parameters. With the parameters thus defined, the corresponding expansion of A_q is

$$A_q(\mathbf{E}, T) = A_q{}^0(T) + \frac{1}{2}g_{ij}U_q{}^0E_{ij} + \frac{1}{8}[(2h_{ijkl} - g_{ij}g_{kl})U_q{}^0 - g_{ij}g_{kl}TC_q{}^0]E_{ij}E_{kl} + \cdots, \quad (40)$$

where

$$U_q = A_q - T\left(\frac{\partial A_q}{\partial T}\right)_{\mathbf{E}} \quad (41)$$

is the vibrational contribution to the internal energy in the quasi-harmonic approximation, and

$$C_q = \left(\frac{\partial U_q}{\partial T}\right)_{\mathbf{E}} \quad (42)$$

is the specific heat at constant strain in the quasi-harmonic approximation. As in Paper I, the extended Grüneisen approximation has been invoked by assuming that the g^ν_{ij} and h^ν_{ijkl} are independent of ν (or can be replaced by averages over ν [1]), so that the index ν has been dropped in (40). Comparing the expansion (40) with (17) and its expanded form, (25), and recalling that $A = \bar{\phi} + A_q$, the temperature dependence of the parameters r^n_{ijkl} can be derived. Thus,

$$r^0_{ijkl} = \bar{\phi}^0_{ijkl} + \frac{1}{4}(2h_{ijkl} - g_{ij}g_{kl})U_q{}^0 - \frac{1}{4}g_{ij}g_{kl}TC_q{}^0, \quad (43)$$

where the $\bar{\phi}^0_{ijkl}$ are second derivatives of $\bar{\phi}$ with respect to $\mathbf{E}$. By the argument given at length in Paper I, the expansion of A_q need be carried only to two orders less than the expansion of ϕ. Thus, for a fourth-order expansion of $\bar{\phi}$, for instance, it is sufficient to include the thermal terms only up to c_1 and r^0_{ijkl} in (24) and (25).

Equations analogous to these in terms of $\boldsymbol{\eta}$ can be derived in a similar manner. Thus, writing

$$\omega_\nu{}^2 = (\omega_\nu{}^2)_0\left(1 + g^{\nu'}_{ij}\eta_{ij} + \frac{1}{2}h^{\nu'}_{ijkl}\eta_{ij}\eta_{kl} + \cdots\right), \quad (44)$$

one obtains

$$t^0_{ijkl} = \bar{\phi}^0_{ijkl} + \frac{1}{4}(2h'_{ijkl} - g'_{ij}g'_{kl})U^0_q - \frac{1}{4}g'_{ij}g'_{kl}TC^0_q. \quad (45)$$

The parameters g_{ij} and h_{ijkl} can be related to a generalized Grüneisen parameter and its strain derivatives. A generalized Grüneisen parameter can be defined thermodynamically as