PHYSICAL REVIEW B VOLUME 1, NUMBER 4 15 FEBRUARY 1970

Role of the Initial Temperature in the Equations of State of an Elastic Dielectric*

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(Received 1 August 1969)

Partial differential equations are derived which describe the initial-temperature dependence of the equations of state of an elastic dielectric. These equations are applied to the case in which the equations of state can be represented by polynomials of degree 2 in the independent field variables—the displacement gradient and the electric displacement field. The special case of material symmetry *m3m* is introduced and applied to NaCl. It is found that for this crystal the initial temperature and the temperature of the system play equally significant roles in the equations of state.

I. INTRODUCTION

In this paper, we discuss the role of the temperature of the reference or initial state—the so-called initial temperature—in the equations of state of materials.[1] We shall be concerned only with the static elastic, dielectric, and thermal properties and we shall restrict the discussion to the case in which these properties are described by the following fields—the displacement gradient, the electric displacement field, the electric field, the absolute temperature, the entropy density, and an energy density.

The first part of the paper, Secs. II–IV, deals with the partial differential equations which describe the initial-temperature dependence of the equations of state. These equations are applied, in Secs. V–VII, to the case in which the equations of state can be represented by polynomials of order 2 in the independent field variables, namely the components of the displacement gradient and the electric displacement field. In Sec. VIII, we discuss the special case of a polynomial representation with material symmetry *m3m*. Section IX contains a discussion of the implications of the initial-temperature dependence of the coefficients describing a polynomial representation. In the final section, Sec. X, we apply the results of Sec. VIII to the special case of NaCl and show that the initial temperature and the temperature of the system play equally significantly roles in the equation of state.

II. DEFORMATION

The deformation and displacement of an elastic dielectric are completely described by two fields: (a) the set of position coordinates $X_i (i=1, 2, 3)$ specifying the positions of the volume elements making up the body in some initial or reference state and (b) the analogous set of position coordinates $x_i (i=1, 2, 3)$ describing their positions in the final configuration of interest. We shall suppose that x_i, X_i are measured in the same rectangular coordinate system. Set

$$x_i = X_i + u_i , \tag{1}$$

where u_i are the components of the displacement vector. If we regard the u_i as functions of the X_i, then

$$\left(\frac{\partial x_i}{\partial X_j}\right) = \delta_{ij} + \left(\frac{\partial u_i}{\partial X_j}\right), \tag{2}$$

where δ_{ij} is the Kronecker delta. $(\partial x_i/\partial X_j)$ and $(\partial u_i/\partial X_j)$ are, respectively, the deformation and displacement gradients. We shall use the latter quantity to describe the deformation. Let us introduce a second initial state described by the set of coordinates X_i' and define the corresponding displacement vector as above;

$$x_i = X_i' + u_i' . \tag{3}$$

Since Eqs. (1) and (3) refer to the same volume element,

$$X_i + u_i \equiv X_i' + u_i' \tag{4}$$

and, hence,

$$\left(\frac{\partial u_i}{\partial X_j}\right) = \left[\delta_{ik} + \left(\frac{\partial u_i'}{\partial X_k'}\right)\right]\left(\frac{\partial X_k'}{\partial X_j}\right) - \delta_{ij} , \tag{5}$$

where the Einstein summation convention is used here and in all later expressions. We set $(\partial u_i/\partial X_j) = u_{ij}$, $(\partial u_i'/\partial X_j') = u_{ij}'$, and replace (5) with

$$u_{ij} = (\delta_{ik} + u_{ik}')\left(\frac{\partial X_k'}{\partial X_j}\right) - \delta_{ij} . \tag{6}$$

Consider now a set of zero-stress states of the dielectric, obtained by heating the sample and at the same time keeping it free of applied surface tractions and electric displacement fields. Provided rigid translations and/or rotations of the sample are excluded, this set of states is uniquely determined by (a) the choice of zero-stress state prior to the heating and (b) the thermoelastic properties peculiar to the sample. Within the set, each state is uniquely specified by its temperature θ. In what follows, we shall only use initial states which are zero-stress states[1a] and we shall only consider changes of initial states involving two zero-stress states belonging to the same set in the sense described above. (Thus, we specifically exclude trivial changes of initial state achieved by rigid translations and/or rotations of the

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* Supported in part by the National Research Council of Canada.

[1] R. A. Toupin, J. Rat. Mech. Anal. 5, 849 (1956).

[1a] For a general discussion of the initial-configuration dependence of the equation of state, see W. Noll, Arch. Rat. Mech. Anal. 27, 1 (1967).

sample). Let us choose a zero-stress state as the initial state and let its temperature be denoted by θ_i. We shall assume that the properties of the dielectric are such that the displacement gradients describing the deformations of the remaining zero-stress states of this set are uniform, i.e., $(\partial^2 u_i/\partial X_j \partial X_k)\equiv 0$ for all i, j, k, and X_j. Thus, if we denote the displacement gradient of a zero-stress state by γ_{ij}, we can then write the position coordinates in these states in the form, Eq. (1),

$$x_i=(\delta_{ij}+\gamma_{ij})X_j.$$

γ_{ij} is the thermal expansion tensor. It is a function of the zero-stress state of interest and the initial state, i.e., $\gamma_{ij}=\gamma_{ij}(\theta,\theta_i)$. In particular, since $x_i=X_i$ when $\theta=\theta_i$,

$$\gamma_{ij}(\theta_i,\theta_i)=0, \quad \text{for all } i,\ j. \tag{7}$$

Similarly, for some other choice of initial state with temperature θ_i', we have

$$x_i=[\delta_{ij}+\gamma_{ij}'(\theta,\theta_i')]X_j', \tag{8a}$$

with

$$\gamma_{ij}'(\theta_i',\theta_i')=0.$$

Equation (6) holds for all states; when applied to zero-stress states, we find

$$\gamma_{ij}(\theta,\theta_i)=[\delta_{ik}+\gamma_{ik}'(\theta,\theta_i')]\left(\frac{\partial X_k'}{\partial X_j}\right)-\delta_{ij}.$$

In particular, by (7),

$$\gamma_{ij}(\theta_i',\theta_i)+\delta_{ij}=\left(\frac{\partial X_i'}{\partial X_j}\right). \tag{8b}$$

Eliminating $(\partial X_k'/\partial X_j)$ from (6) by means of (8a), we get

$$u_{ij}=u_{ik}'[\gamma_{kj}(\theta_i',\theta_i)+\delta_{kj}]+\gamma_{ij}(\theta_i',\theta_i). \tag{9}$$

Equation (9) describes the transformation law for a change in initial state. The inverse transformation is

$$u_{ij}'=[u_{ik}-\gamma_{ik}(\theta_i',\theta_i)]\Delta_{kj}(\theta_i',\theta_i), \tag{10}$$

where Δ_{ij} is the inverse tensor to $\delta_{ij}+\gamma_{ij}$, i.e.,

$$[\delta_{ik}+\gamma_{ik}(\theta_i',\theta_i)]\Delta_{kj}(\theta_i',\theta_i)=\delta_{ij}. \tag{11}$$

III. EQUATION OF STATE

It is a characteristic of theories[1–4] of the elastic dielectric that the stress vector $\mathbf{t}^0$ describing the surface tractions satisfies a boundary condition of the form

$$t_i^0=\tau_{ji}n_j, \tag{12}$$

where τ_{ij} is some tensor function of the field components chosen to describe the response of the dielectric and the n_i are the direction cosines of the outward normal at the point of interest at the surface.

We shall assume that the independent field variables are the displacement gradients u_{ij}, the electric displacement field components D_i, and the temperature θ; we then write

$$\tau_{ij}=\tau_{ij}(u_{ij},D_i,\theta,\theta_i), \tag{13}$$

$$E_i=E_i(u_{ij},D,\theta,\theta_i), \tag{14}$$

$$\sigma'=\sigma'(u_{ij},D_i,\theta,\theta_i), \tag{15}$$

where E_i and σ' are the electric field components and the entropy density (per unit mass), respectively. We shall regard Eqs. (13)–(15) as equations of state. It is clear from the following remarks why the initial temperature θ_i must appear as an explicit argument in the functions τ_{ij}, E_i, and σ'; the *values* of the displacement gradients are functions of θ_i whereas the *values* of τ_{ij}, E_i, and σ' in any given state cannot depend on θ_i; therefore, the functions in (13)–(15) must contain an explicit θ_i dependence sufficient to cancel the implicit θ_i dependence introduced by the u_{ij}. This argument provides the basis of the analysis given below.

The equation of state (13) has some unusual aspects: (i) The field τ_{ij} is defined only on the surface of the dielectric; (ii) the function τ_{ij} is in general a function of the n_i, the direction cosines of the normal to the surface at a point in question; (iii) there are nine τ_{ij}'s and nine u_{ij}'s, but in the region of a state with $D_i=0 (i=1,2,3)$ we cannot, in general, invert Eq. (13) to obtain a unique equation of state for the u_{ij}.

The last two points are best illustrated by considering a particular form for the τ_{ij}. From Refs. 4 and 5,

$$\tau_{ij}=\rho\left(\frac{\partial F}{\partial u_{ik}}\right)(\delta_{jk}+u_{jk})$$
$$-\left[\frac{D_k{}^A D_k{}^A}{2\epsilon_0}+\tfrac{1}{2}(E_k{}^V+E_k{}^A)(D_k{}^V-D_k{}^A)\right]\delta_{ij}, \tag{16}$$

where ρ is the mass density, F the free energy density, and ϵ_0 the permittivity of free space. The superscripts V and A refer to the field values in the dielectric and vacuum, respectively. The quantity in square brackets, and, hence, τ_{ij}, is a function of the n_i because $D_i{}^A$ and $E_i{}^A$ are related to $D_i{}^V$ and $E_i{}^V$ by the boundary conditions $n_i(D_i{}^V-D_i{}^A)=0$ and $e_{ijk}(E_j{}^V-E_j{}^A)n_k=0$, where e_{ijh} is the Levi-Civita density.

To prove (iii), consider the case in which $D_i{}^V=0$ $(i=1,2,3)$; then, since F is a function of the u_{ij} only through the six Lagrangian strain components[1] $\eta_{ij}=\frac{1}{2}(u_{ij}+u_{ji}+u_{ki}u_{kj})$,

$$\left(\frac{\partial F}{\partial u_{ik}}\right)(\delta_{jk}+u_{jk})=\tfrac{1}{2}\left(\frac{\partial F}{\partial \eta_{kl}}\right)[(\delta_{ik}+u_{ik})(\delta_{jl}+u_{jl})$$
$$+(\delta_{il}+u_{il})(\delta_{jk}+u_{jk})]. \tag{17}$$

Hence,

$$\tau_{ij}|_{D_i{}^V=0}=\tau_{ji}|_{D_i{}^V=0}, \tag{18}$$

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[2] R. A. Toupin, Int. J. Eng. Sci. 1. 101 (1963); see also Ref. 1.
[3] A. C. Eringen, Int. J. Eng. Sci. 1, 127 (1963).
[4] J. Grindlay, Phys. Rev. 149, 637 (1966).

[5] J. Grindlay and A. R. Redlack (unpublished).

i.e., the functions τ_{ij} are symmetric. Set

$$\tau_{ij}-\tau_{ij}(u_{ij},D_i^V,\theta,\theta_i)=f_{ij}.$$

From (18), the Jacobian

$$\frac{\partial(f_{11},f_{22},f_{33},f_{12},f_{13},f_{21},f_{23},f_{31},f_{32})}{\partial(u_{11},u_{22},u_{33},u_{12},u_{13},u_{21},u_{23},u_{31},u_{33})}$$

vanishes when $D_i^V=0$ $(i=1, 2, 3)$; therefore, in the region of any state with $D_i^V=0$ $(i=1, 2, 3)$, there is no unique inversion[6] of Eq. (13) for the u_{ij}'s in terms of the τ_{ij}'s. This result is particularly relevant in the theory of the elastic dielectric because it is customary to represent the functions τ_{ij} by a truncated power series in u_{ij} and D_i^V about the values $u_{ij}=0$, $D_i^V=0$, and, hence, from the comments made above, we see that we cannot invert this series to obtain the u_{ij}'s in terms of the τ_{ij}'s.[7]

It has been remarked above that the value of τ_{ij} cannot be a function of the choice of initial state, i.e., of θ_i. Thus, if we choose to describe the deformation of some state relative to two different initial states θ_i, and θ_i', we must have

$$\tau_{ij}(u_{kl},D_k,\theta,\theta_i)\equiv\tau_{ij}'(u_{kl}',D_k,\theta,\theta_i'), \qquad (19)$$

where u_{kl} and u_{kl}' are related by Eq. (9) and τ_{ij}' is the function appropriate to the equation of state for which the displacement gradients are measured relative to the primed initial state. Substituting for u_{kl} from (9), we write (19) in the form

$$\tau_{ij}\{\gamma_{kl}(\theta_i',\theta_i)+u_{km}'[\delta_{ml}+\gamma_{ml}(\theta_i',\theta_i)],\ D_k,\ \theta,\ \theta_i\}$$
$$\equiv\tau_{ij}'(u_{kl}',D_k,\theta,\theta_i'). \qquad (20)$$

Let us differentiate both sides of this identity with respect to θ_i, holding θ_i', θ, D_k, and u_{kl}' constant; hence,

$$\left(\frac{\partial\tau_{ij}}{\partial u_{kl}}\right)_{D,\theta,\theta_i}\left(\frac{\partial\gamma_{kl}}{\partial\theta_i}(\theta_i',\theta_i)+u_{km}'\frac{\partial\gamma_{ml}}{\partial\theta_i}(\theta_i',\theta_i)\right)$$
$$+\left(\frac{\partial\tau_{ij}}{\partial\theta_i}\right)_{u,D,\theta}=0. \qquad (21)$$

Substituting for u_{km}' from (10),

$$\left(\frac{\partial\tau_{ij}}{\partial u_{kl}}\right)_{D,\theta,\theta_i}\left[\Delta_{nm}(\theta_i',\theta_i)\frac{\partial\gamma_{ml}}{\partial\theta_i}(\theta_i',\theta_i)\right]$$
$$\times(\delta_{kn}+u_{kn})+\left(\frac{\partial\tau_{ij}}{\partial\theta_i}\right)_{u,D,\theta}=0. \qquad (22)$$

Equation (22) holds for all values of D_k, u_{kn}, θ, θ_i, and θ_i'. The variable θ_i' occurs only within the square bracket and, hence, this combination of quantities is independent of θ_i'.

We set

$$\Delta_{km}(\theta_i',\theta_i)\frac{\partial\gamma_{ml}}{\partial\theta_i}(\theta_i',\theta_i)=A_{kl}(\theta_i), \qquad (23)$$

where A_{kl} is a tensor function with a single temperature argument. Using the properties of Δ_{km}, Eq. (11), we solve for $(\partial\gamma_{ml}/\partial\theta_i)$:

$$\frac{\partial\gamma_{ij}}{\partial\theta_i}(\theta_i',\theta_i)=A_{ij}(\theta_i)+\gamma_{ik}(\theta_i',\theta_i)A_{kj}(\theta_i). \qquad (24)$$

It is clear that the prime and the subscript in the first temperature argument in γ_{ij} is redundant in (24), as these equations hold for all θ_i', i.e., all temperatures. With the introduction of the tensor A_{ij}, Eq. (22) takes the form

$$\left(\frac{\partial\tau_{ij}}{\partial u_{kl}}\right)_{D,\theta,\theta_i}A_{nl}(\theta_i)(\delta_{kn}+u_{kn})+\left(\frac{\partial\tau_{ij}}{\partial\theta_i}\right)_{D,\theta,u}=0. \qquad (25)$$

Similar considerations for E_i and σ' yield

$$\left(\frac{\partial E_i}{\partial u_{kl}}\right)_{D,\theta,\theta_i}A_{nl}(\theta_i)(\delta_{kn}+u_{kn})+\left(\frac{\partial E_i}{\partial\theta_i}\right)_{D,\theta,u}=0, \qquad (26)$$

$$\left(\frac{\partial\sigma'}{\partial u_{kl}}\right)_{D,\theta,\theta_i}A_{nl}(\theta_i)(\delta_{kn}+u_{kn})+\left(\frac{\partial\sigma'}{\partial\theta_i}\right)_{D,\theta,u}=0. \qquad (27)$$

Equations (25)–(27) are partial-differential equations describing the θ_i dependence of the functions τ_{ij}, E, and σ'.

IV. THERMAL EXPANSION

In this section, we discuss Eq. (24) and its solution. Let $f_{ij}(\theta_i)$ be a second-rank tensor which is a solution to the equation

$$\frac{df_{ij}}{d\theta_i}=-A_{ik}(\theta_i)f_{kj}(\theta_i). \qquad (28)$$

Set

$$\gamma_{ij}(\theta,\theta_i)=\mu_{ik}(\theta,\theta_i)f_{kj}^{-1}(\theta_i), \qquad (29)$$

where

$$f_{ij}(\theta_i)f_{jk}^{-1}(\theta_i)=\delta_{ik}. \qquad (30)$$

Then, from (28) and (29),

$$\frac{\partial\gamma_{ij}}{\partial\theta_i}(\theta,\theta_i)=\left(\frac{\partial\mu_{ik}}{\partial\theta_i}(\theta,\theta_i)\right)f_{kj}^{-1}(\theta_i)$$
$$+\mu_{ik}(\theta,\theta_i)f_{kl}^{-1}(\theta_i)A_{lj}(\theta_i). \qquad (31)$$

Substituting for γ_{ij} and its derivative from (29) and

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[6] See, for example, G..A. Gibson, *Advanced Calculus* (MacMillan and Co. Ltd., London, 1948), Chap. 5.

[7] The occurrence of a symmetric τ_{ij} does not reduce the number of independent boundary conditions because the τ_{ij} appear as linear combinations in these conditions [see Eq. (12)].

(31) in (24), we obtain

$$\frac{\partial\mu_{ij}}{\partial\theta_i}(\theta,\theta_i)=A_{il}(\theta_i)f_{lj}(\theta_i)\,,$$

or

$$\gamma_{ij}(\theta,\theta_i)=\left(\int_{\theta}^{\theta_i} A_{il}(\theta_i)f_{lk}(\theta_i)d\theta_i\right)f_{kj}^{-1}(\theta_i)\,, \quad (32)$$

since $\gamma_{ij}(\theta_i,\theta_i)=0$. The integrand in (32) is $-df_{ik}/d\theta_i$ and, hence,

$$\gamma_{ij}(\theta,\theta_i)=f_{ik}^{-1}(\theta_i)f_{kj}(\theta)-\delta_{ij}. \quad (33)$$

Thus, the demands placed by Eq. (24) on the thermal expansion γ_{ij} are satisfied if and only if γ_{ij} can be expressed in terms of a function of a single argument as shown in (33).

V. POLYNOMIAL REPRESENTATION

To explore the demands of Eqs. (25), (26), and (27), we represent the functions τ_{ij}, E_i, and σ' by the following polynomials:

$$\tau_{ij}(u_{kl},D_k,\theta,\theta_i)=\tau_{ij}{}^0+c_{ijkl}u_{kl}-h_{ijk}D_k+C_{ijklmn}u_{kl}u_{mn} +2b_{ijklm}u_{kl}D_m+q_{ijkl}D_kD_l\,, \quad (34)$$

$$E_i(u_{kl},D_k,\theta,\theta_i)=E_i{}^0-\tilde{h}_{kli}u_{kl}+\beta_{ij}D_j+\tilde{b}_{klmni}u_{kl}u_{mn} +2\tilde{q}_{klij}u_{kl}D_j+\eta_{ijk}D_jD_k\,, \quad (35)$$

$$\sigma'(u_{kl},D_k,\theta,\theta_i)=\sigma_0{}'-\hat{\tau}_{ij}{}^0u_{ij}-\hat{E}_i{}^0D_i-\tfrac{1}{2}\hat{c}_{ijkl}u_{ij}u_{kl} +\hat{h}_{ijk}u_{ij}D_k-\tfrac{1}{2}\hat{\beta}_{ij}D_iD_j. \quad (36)$$

$\tau_{ij}{}^0$ is the thermal stress, c_{ijkl} the elastic stiffness h_{ijk}, $\hat{h}_{ijk}$ the piezoelectric coefficients, C_{ijklmn} the nonlinear elastic coefficient, q_{ijkl} and $\tilde{q}_{ijkl}$ the electrostrictive coefficients, $E_i{}^0$ the thermal electric field, β_{ij} the dielectric permeability, and $\sigma_0{}'$ the entropy density in zero-displacement gradient and zero-electric displacement. The remaining coefficients have not, to our knowledge, been named. The θ and θ_i dependence of the functions τ_{ij}, E_i, and σ' is contained in these coefficients. As Eqs. (34)–(36) stand, the only relations between the coefficients are

$$C_{ijklmn}=C_{ijmnkl}\,, \quad (37)$$

$$q_{ijkl}=q_{ijlk}\,, \quad (38)$$

$$\tilde{b}_{klmni}=\tilde{b}_{mnkli}\,, \quad (39)$$

$$\hat{c}_{ijkl}=\hat{c}_{klij}\,, \quad (40)$$

$$\hat{\beta}_{ij}=\hat{\beta}_{ji}. \quad (41)$$

With the introduction of an energy density, further identities occur and these (see below) suggest the introduction of the factor 2 and the use of the tilde and circumflex notation in Eqs. (34)–(36).

Inserting these polynomial representations into the partial-differential equations (25)–(27) and treating u_{ij} and D_i as independent variables, we obtain the following differential equations:

$$\left(\frac{\partial\tau_{ij}{}^0}{\partial\theta_i}\right)_\theta+c_{ijkl}A_{kl}(\theta_i)=0\,, \quad (42)$$

$$\left(\frac{\partial c_{ijk}}{\partial\theta_i}\right)_\theta+c_{ijkn}A_{ln}(\theta_i)+2C_{ijmnkl}A_{mn}(\theta_i)=0\,, \quad (43)$$

$$\left(\frac{\partial h_{ijm}}{\partial\theta_i}\right)_\theta-2b_{ijklm}A_{kl}(\theta_i)=0\,, \quad (44)$$

$$\left(\frac{\partial E_i{}^0}{\partial\theta_i}\right)_\theta-\tilde{h}_{kli}A_{kl}(\theta_i)=0\,, \quad (45)$$

$$\left(\frac{\partial\tilde{h}_{kni}}{\partial\theta_i}\right)_\theta+\tilde{h}_{kli}A_{nl}(\theta_i)-2b_{mlkni}A_{ml}(\theta_i)=0\,, \quad (46)$$

$$\left(\frac{\partial\beta_{ij}}{\partial\theta_i}\right)_\theta+2\tilde{q}_{klij}A_{kl}(\theta_i)=0\,, \quad (47)$$

$$\left(\frac{\partial\sigma_0{}'}{\partial\theta_i}\right)_\theta-\hat{\tau}_{kl}{}^0A_{kl}(\theta_i)=0\,, \quad (48)$$

$$\left(\frac{\partial\hat{\tau}_{ij}{}^0}{\partial\theta_i}\right)_\theta+\hat{\tau}_{il}{}^0A_{jl}(\theta_i)+\hat{c}_{klij}A_{kl}(\theta_i)=0\,, \quad (49)$$

$$\left(\frac{\partial\hat{E}_i{}^0}{\partial\theta_i}\right)_\theta-\tilde{h}_{kli}A_{kl}(\theta_i)=0. \quad (50)$$

These results are exact, in the sense that the introduction of higher-order terms in the representations given in Eqs. (34)–(36) would not affect the form of Eqs. (42)–(47). The equations for the θ_i derivatives of C_{ijklmn}, q_{ijkl}, $\tilde{q}_{ijkl}$, b_{ijklm}, $\tilde{b}_{ijklm}$, η_{ijk}, $\hat{c}_{ijkl}$, $\hat{h}_{ijk}$, and $\hat{\beta}_{ij}$ contain the coefficients of the set of next-higher-order terms. Equations (42)–(50) describe the demands imposed by (25), (26), and (27) on the representations in (34), (35), and (36).

We note that the thermal expansion γ_{ij} at a point on the surface of the material satisfies the equations $\tau_{ij}n_i=0$ with $D_j=0$ ($j=1, 2, 3$). For the polynomial representation (34), we then have

$$0=(\tau_{ij}{}^0+c_{ijkl}\gamma_{kl}+C_{ijklmn}\gamma_{kl}\gamma_{mn})n_i\,, \quad j=1,2,3. \quad (51)$$

For systems which possess homogeneous zero-stress states, this set of equations determine the γ_{ij}.

VI. ENERGY DENSITY

The introduction of an energy density leads to relations between the coefficients describing the equations of state Eqs. (34)–(36). We shall restrict the discussion to the case of the relations satisfied by the coefficients $\tau_{ij}{}^0$, c_{ijkl}, h_{ijk}, $E_i{}^0$, $\tilde{h}_{ijk}$, β_{ij}, $\hat{\tau}_{ij}{}^0$, $\hat{E}_i{}^0$, $\hat{h}_{ijk}$, $\hat{c}_{ijk}$, and $\hat{\beta}_{ij}$. Consider a free-energy density $F(u_{ij},D_i,\theta,\theta_i)$. The equations of state take the form

$$\tau_{ij}=\rho\left(\frac{\partial F}{\partial u_{ik}}\right)_{D,\theta}(\delta_{jk}+u_{jk}), \tag{52}$$

$$E_i=\rho\left(\frac{\partial F}{\partial D_i}\right)_{\theta,u} \tag{53}$$

$$\sigma'=-\left(\frac{\partial F}{\partial \theta}\right)_{u,D}. \tag{54}$$

In writing (52), we have arbitrarily neglected[8] the Maxwell stress (the square bracket in Eq. (16)); this is a valid procedure in some circumstances.[9] The free-energy density $F(u_{ij},D_i,\theta,\theta_i)$ is invariant in form and value with respect to arbitrary changes in axes; hence, $F=F(\eta_{ij},\Pi_i,a,\theta_i,\theta)$, where $\eta_{ij}=\frac{1}{2}(u_{ij}+u_{ji}+u_{li}u_{lj})$, $\Pi_i=(\delta_{ij}+u_{ij})D_j$, and $a=D_iD_i$.[1] In a polynomial representation of F, the argument a is redundant. We set

$$\rho_0F(\eta_{ij},\Pi_i,\theta,\theta_i)=\rho_0F_0+H_{kl}{}^0\eta_{kl}+H_k{}^1\Pi_k +\tfrac{1}{2}H_{klmn}{}^2\eta_{kl}\eta_{mn}+H_{klm}{}^3\eta_{kl}\Pi_m+\tfrac{1}{2}H_{kl}{}^4\Pi_k\Pi_l, \tag{55}$$

where ρ_0 is the mass density in the initial state and $F_0=F(0,0,\theta,\theta_i)$. The H_{klmn}'s have the following properties:

$$H_{kl}{}^0=H_{lk}{}^0, \tag{56}$$

$$H_{klmn}{}^2=H_{mnkl}{}^2=H_{klnm}{}^2=H_{lkmn}{}^2, \tag{57}$$

$$H_{klm}{}^3=H_{lkm}{}^3, \tag{58}$$

$$H_{kl}{}^4=H_{lk}{}^4. \tag{59}$$

Inserting this representation for F into (52)–(54) and comparing it with (34)–(36), we find that

$$\tau_{ij}{}^0=H_{ij}{}^0, \tag{60}$$

$$c_{ijkl}=(H_{ijkl}{}^2-H_{ij}{}^0\delta_{kl}+H_{lj}{}^0\delta_{ik}+H_{il}{}^0\delta_{jk}), \tag{61}$$

$$-h_{ijk}=H_{ijk}{}^3+H_j{}^1\delta_{ik}, \tag{62}$$

$$E_i{}^0=H_i{}^1, \tag{63}$$

$$-\tilde{h}_{ijk}=H_{ijk}{}^3+H_j{}^1\delta_{ik}-H_k{}^1\delta_{ij}, \tag{64}$$

$$\beta_{ij}=H_{ij}{}^4, \tag{65}$$

$$\sigma_0'=-(\partial F_0/\partial\theta)_{\theta_i}, \tag{66}$$

$$\hat{\tau}_{ij}{}^0=(\partial H_{ij}{}^0/\partial\theta)_{\theta_i}/\rho_0, \tag{67}$$

$$\hat{E}_i{}^0=(\partial H_i{}^0/\partial\theta)_{\theta_i}/\rho_0, \tag{68}$$

$$\hat{h}_{ijk}=-(\partial H_{ijk}{}^2/\partial\theta)_{\theta_i}/\rho_0, \tag{69}$$

$$\hat{c}_{ijkl}=[(\partial H_{ijkl}{}^2/\partial\theta)_{\theta_i}+(\partial H_{jl}{}^0/\partial\theta)_{\theta_i}\delta_{ik}]/\rho_0, \tag{70}$$

$$\hat{\beta}_{ij}=(\partial H_{ij}{}^4/\partial\theta)_{\theta_i}/\rho_0. \tag{71}$$

From (60), (65), (67), (69), (71), and the properties of the $H_{ijkm}{}^{\alpha}$'s, Eqs. (56)–(59), we deduce that

$$\tau_{ij}{}^0=\tau_{ji}{}^0,\quad \beta_{ij}=\beta_{ji}, \tag{72}$$

$$\hat{\tau}_{ij}{}^0=\hat{\tau}_{ji}{}^0,\quad \hat{h}_{ijk}=\hat{h}_{jik}, \tag{73}$$

$$\hat{\beta}_{ij}=\hat{\beta}_{ji}. \tag{74}$$

These conditions on the coefficients appearing in (34)–(36) are a direct result of the introduction of an energy density. It is clear from Eqs. (60)–(71) that the θ_i dependence of τ_{ij}, h_{ijk}, etc. may be deduced from the θ_i dependence of the $H_{ijk}{}^{\alpha}$'s and conversely.

VII. MATERIAL SYMMETRY *m*3*m*

In this section, we apply the results obtained above to the special case of material symmetry *m*3*m*. For this symmetry, the tensor invariants of odd rank vanish identically and those of even rank are invariant under the coordinate transformations $x_1\rightarrow x_2$, $x_2\rightarrow -x_1$, $x_3\rightarrow x_3$ and $x_1\rightarrow x_2$, $x_2\rightarrow x_3$, $x_3\rightarrow x_1$[10]; hence,

$$\text{(i)}\quad \tau_{11}{}^0=\tau_{22}{}^0=\tau_{33}{}^0 \tag{75}$$

and the remaining elements vanish (similarly, for $H_{ij}{}^0$, β_{ij}, $\tau_{ij}{}^0$ and β_{ij}).

$$\text{(ii)}\quad \begin{aligned}&\tilde{q}_{1111}=\tilde{q}_{2222}=\tilde{q}_{3333}\\ &\tilde{q}_{1122}=\tilde{q}_{2211}=\tilde{q}_{2233}=\tilde{q}_{3322}=\tilde{q}_{3311}=\tilde{q}_{1133}\\ &\tilde{q}_{1212}=\tilde{q}_{2121}=\tilde{q}_{3131}=\tilde{q}_{1313}=\tilde{q}_{2323}=\tilde{q}_{3232}\\ &\tilde{q}_{1212}=\tilde{q}_{2112}=\tilde{q}_{3113}=\tilde{q}_{1331}=\tilde{q}_{2332}=\tilde{q}_{3223}\end{aligned} \tag{76}$$

and the remaining elements vanish (similarly for c_{ijkl}).

$$\text{(iii)}\quad \begin{aligned}&q_{1111}=q_{2222}=q_{3333}\\ &q_{1122}=q_{2211}=q_{2233}=q_{3322}=q_{3311}=q_{1133}\\ &q_{1212}=q_{2121}=q_{3131}=q_{1313}=q_{2323}=q_{3232}\\ &=q_{1221}=q_{2112}=q_{3113}=q_{1331}=q_{2332}=q_{3223}\end{aligned} \tag{77}$$

and the remaining elements vanish (similarly, for $H_{ijk}{}^2$ and $\tilde{c}_{ijk}$).

We shall assume that the thermal expansion tensor γ_{ij} is an invariant of the symmetry group *m*3*m*[11]; hence, we set

$$\gamma_{ij}=\gamma\delta_{ij},$$

where

$$\gamma=[f(\theta)/f(\theta_i)-1], \tag{78}$$

Eq. (33), is a root of

$$0=\tau_{11}{}^0+(c_{1111}+2c_{1122})\gamma+(C_{111111}+4C_{111122}+2C_{112233}+2C_{112222})\gamma^2, \tag{79}$$

[see Eq. (51)].

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[8] The extension of the calculation to the case of nonvanishing Maxwell stresses is straightforward, in principle, but tedious to carry out explicitly.

[9] J. Grindlay, in *Proceedings of the International Meeting on Ferroelectricity*, edited by V. Dvorak (Czechoslovakian Institute of Physics, Prague, 1966), p. 433.

[10] R. R. Birss, in *Reports on Progress in Physics*, edited by A. C. Strickland (Institute of Physics and Physical Society, London, 1963), Vol. XXVI, p. 307.

[11] The γ_{ij} of a material in a given zero-stress state is the thermodynamically stable root of Eq. (51). Thus, it is possible for γ_{ij} to display a lower symmetry than the material symmetry of the coefficients $\tau_{ij}{}^0$, c_{ijkl}, and C_{ijklmn}.

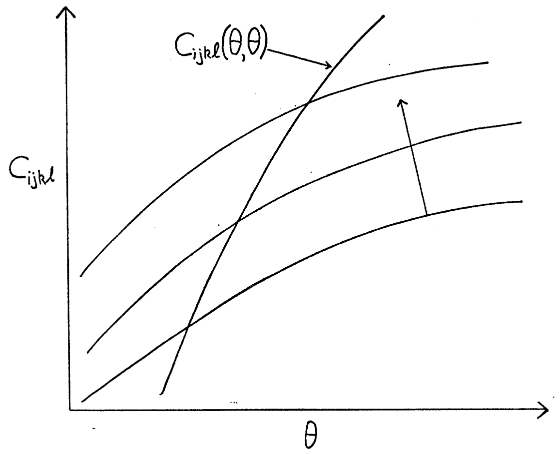

FIG. 1. Sketch of the family of curves $c_{ijkl}(\theta,\theta_i)$ versus θ with parameter θ_i.

For *m3m*, Eqs. (42)–(50) take the form

$$\left(\frac{\partial\tau_{11}{}^0}{\partial\theta_i}\right)_\theta+A_{11}(\theta_i)(c_{1111}+2c_{1122})=0, \tag{80}$$

$$\left(\frac{\partial c_{1111}}{\partial\theta_i}\right)_\theta+A_{11}(\theta_i)[c_{1111}+2(C_{111111}+2C_{111122})]=0, \tag{81}$$

$$\left(\frac{\partial c_{1122}}{\partial\theta_i}\right)_\theta+A_{11}(\theta_i)[c_{1122}+2(C_{111122}+C_{112222}+C_{112233})]=0, \tag{82}$$

$$\left(\frac{\partial c_{1212}}{\partial\theta_i}\right)_\theta+A_{11}(\theta_i)[c_{1212}+2(C_{121112}+C_{212111}+C_{211233})]=0, \tag{83}$$

$$\left(\frac{\partial\beta_{11}}{\partial\theta_i}\right)_\theta+2A_{11}(\theta_i)(\tilde{q}_{1111}+2\tilde{q}_{2211})=0, \tag{84}$$

$$\left(\frac{\partial\sigma_0{}'}{\partial\theta_i}\right)_\theta-\tau_{11}{}^0A_{11}(\theta_i)=0, \tag{85}$$

$$\left(\frac{\partial\hat{\tau}_{11}{}^0}{\partial\theta_i}\right)+A_{11}(\theta_i)(\hat{\tau}_{11}{}^0+\hat{c}_{1111}+2\hat{c}_{1122})=0, \tag{86}$$

with

$$A_{11}=-(df/d\theta_i)/f, \tag{87}$$

and

$$(\partial\gamma/\partial\theta_i)_\theta=A_{11}(\theta_i)(1+\gamma). \tag{88}$$

The symmetry properties of the C_{ijklmn} are discussed in Appendix A.

We now solve Eqs. (80)–(82) to obtain the explicit θ and θ_i dependence of $\tau_{11}{}^0$. Set

$$c=(c_{1111}+2c_{1122}),$$
$$C=(C_{111111}+4C_{111122}+2C_{112233}+2C_{112222}). \tag{89}$$

Then, Eqs. (79) and (80) and the sum of (81) plus twice (82) read

$$0=\tau_{11}{}^0+c\gamma+C\gamma^2, \tag{90}$$

$$\left(\frac{\partial\tau_{11}{}^0}{\partial\theta_i}\right)_\theta+A_{11}c=0, \tag{91}$$

$$\left(\frac{\partial c}{\partial\theta_i}\right)_\theta+A_{11}[c+2C]=0. \tag{92}$$

Equations (90), (91), and (92) have solutions of the form

$$\tau_{11}{}^0(\theta,\theta_i)=[f(\theta_i)-f(\theta)]k(\theta)\times\{h(\theta)+\tfrac{1}{2}[f(\theta_i)-f(\theta)]\}, \tag{93}$$

$$c(\theta,\theta_i)=k(\theta)f(\theta_i)\{h(\theta)+[f(\theta_i)-f(\theta)]\}, \tag{94}$$

$$C(\theta,\theta_i)=k(\theta)f^2(\theta_i)/2 \tag{95}$$

(see Appendix B). $k(\theta)$ and $h(\theta)$ are arbitrary functions. Inserting the expression for $\tau_{11}{}^0$ from (93) in (85) and integrating with respect to θ_i, we get

$$\sigma_0{}'(\theta,\theta_i)=k(\theta)\{[h(\theta)-\tfrac{1}{2}f^2(\theta)]\ln f(\theta_i)+f(\theta_i)[f(\theta)-h(\theta)]+f^2(\theta_i)\}+g(\theta), \tag{96}$$

where $g(\theta)$ is an arbitrary function of θ. Equations (78) and (93)–(96) show how the θ and θ_i dependence of γ, $\tau_{11}{}^0$, c, C, and $\sigma_0{}'$ may be expressed in terms of four single variable functions f, h, k, and g. These are the only conclusions of this kind that we have been able to draw from Eqs. (80)–(86).

With the introduction of the free-energy density representation, (55), $\tau_{11}{}^0$, c_{1111}, c_{1122}, c_{1212}, β_{11}, $\hat{\tau}_{11}{}^0$, and $\hat{\beta}_{11}$ satisfy the following equations [see Eqs. (60)–(71)]:

$$\tau_{11}{}^0=H_{11}{}^0,\quad \hat{\tau}_{11}{}^0=(\partial H_{11}{}^0/\partial\theta)_{\theta_i}/\rho_0, \tag{97}$$

$$\beta_{11}=H_{11}{}^4,\quad \hat{\beta}_{11}=(\partial H_{11}{}^4/\partial\theta)_{\theta_i}/\rho_0, \tag{98}$$

$$\begin{gathered}c_{1111}=H_{1111}{}^2+H_{11}{}^0,\\ \hat{c}_{1111}=[(\partial H_{1111}{}^2/\partial\theta)_{\theta_i}+(\partial H_{11}{}^0/\partial\theta)_{\theta_i}]/\rho_0,\end{gathered} \tag{99}$$

$$c_{1122}=H_{1122}{}^2-H_{11}{}^0,\quad \hat{c}_{1122}=(\partial H_{1122}{}^2/\partial\theta)_{\theta_i}/\rho_0, \tag{100}$$

$$\begin{gathered}c_{1212}=H_{1212}{}^2+H_{11}{}^0,\\ \hat{c}_{1212}=[(\partial H_{1212}{}^2/\partial\theta)_{\theta_i}+(\partial H_{11}{}^0/\partial\theta)_{\theta_i}]/\rho_0.\end{gathered} \tag{101}$$

Using these identities, we now show that Eq. (86) can be derived from (80). This appears to be the only effect the introduction of F has on Eqs. (60)–(71). Inserting $\hat{\tau}_{11}{}^0$, $\hat{c}_{1111}$, and $\hat{c}_{1122}$ from (97), (98), and (99) into Eq. (86), we have

$$\frac{1}{\rho_0}\frac{\partial}{\partial\theta}\left[\left(\frac{\partial H_{11}{}^0}{\partial\theta_i}\right)_\theta+A_{11}(\theta_i)[2H_{11}{}^0+H_{1111}{}^2+2H_{1122}{}^2]-\frac{H_{11}{}^0}{\rho_0}\left(\frac{\partial\rho_0}{\partial\theta_i}\right)\right]=0. \tag{102}$$

Now,

$$\left(\frac{\partial\rho_0}{\partial\theta_i}\right)=3\rho_0A_{11}, \tag{103}$$

(see Ref. 12) and, hence, Eq. (102) can be written in the form

$$\frac{1}{\rho_0}\frac{\partial}{\partial\theta}\left[\left(\frac{\partial H_{11}{}^0}{\partial\theta_i}\right)_\theta+A_{11}(\theta_i)\times[-H_{11}{}^0+H_{1111}{}^2+2H_{1122}{}^2]\right]=0. \quad (104)$$

On inserting $\tau_{11}{}^0$, c_{1111}, and c_{1122} from Eqs. (97), (99), and (100) into the left side of Eq. (80), we obtain precisely the quantity in square brackets in Eq. (104); hence, Eq. (86) is equivalent to Eq. (80).

VIII. DISCUSSION

In this section, we describe some of the implications of the θ_i dependence of the equation of state. The discussion will be restricted to the case of the elastic stiffness c_{ijkl}.

We have seen in the previous sections that, in general, the elastic stiffness must be regarded as a function of two variables, θ, the temperature of the state of interest and θ_i, the temperature of the initial state. In Fig. 1, we have depicted a family of curves c_{ijkl}-versus-θ, with parameter θ_i. Experimentally, we would expect to get one curve of this family from a set of static measurements in which stresses are applied isothermally and the resultant changes in lengths and/or angles (relative to some initial state) are recorded. In contrast, in a dynamic measurement of c_{ijkl}, the sample is induced to vibrate about the stress free state at the temperature of interest and this measurement, therefore, yields—after the transformation from adiabatic to isothermal constraint is carried out—$c_{ijkl}(\theta,\theta)$. This function is clearly not a member of the family $c_{ijkl}(\theta,\theta_i)$ sketched in Fig. 1. We must, therefore, conclude that static and dynamic measurements give different θ functions for c_{ijkl}. In particular, the slopes of the curves $\theta_i\equiv$ const and $\theta_i\equiv\theta$ are $(\partial c_{1111}/\partial\theta)_{\theta_i}$ and $(dc_{1111}/d\theta)=[(\partial c_{1111}/\partial\theta)_{\theta_i}+(\partial c_{1111}/\partial\theta_i)_\theta]$, respectively. It is shown in Sec. IX that, in the case of NaCl, the difference between these quantities is significant.

IX. NUMERICS

From (83) and (84),

$$\frac{1}{c_{1111}}\left(\frac{\partial c_{1111}}{\partial\theta_i}\right)_\theta=-A_{11}\left(1+\frac{2(C_{111111}+2C_{111122})}{c_{1111}}\right), \quad (105)$$

$$\frac{1}{\beta_{11}}\left(\frac{\partial\beta_{11}}{\partial\theta_i}\right)_\theta=-\frac{2A_{11}}{\beta_{11}}[\tilde{q}_{1111}+2\tilde{q}_{1122}]. \quad (106)$$

We expand $f(\theta)$ in powers of $(\theta-\theta_i)$ and use the approximation

$$f(\theta)\cong f(\theta_i)[1-\alpha(\theta-\theta_i)]; \quad (107)$$

hence, from (87) and (88),

$$A_{11}=-\alpha, \quad (108)$$

$$\gamma(\theta,\theta_i)=\alpha(\theta-\theta_i). \quad (109)$$

Thus, α is the coefficient of linear expansion. In the case of NaCl, the parameters appearing on the right of (105) and (106) have the following values:

$$A=-4\times10^{-5}\ {}^\circ\mathrm{K}^{-1}, \quad (\mathrm{RT, Ref.\ 13})$$
$$\beta_{11}=0.17/\epsilon_0, \quad (\mathrm{RT, Ref.\ 14}),$$
$$\tilde{q}_{1111}=-2/\epsilon_0{}^*, \quad (0^\circ\mathrm{K, Ref.\ 15}),$$
$$\tilde{q}_{1122}=0.26/\epsilon_0{}^*, \quad (0^\circ\mathrm{K, Ref.\ 15}),$$
$$c_{1111}=4.9\times10^{11}\ \mathrm{dyn/cm}^2, \quad (\mathrm{RT, Ref.\ 16})$$
$$C_{111111}=-5.8\times10^{11}\ \mathrm{dyn/cm}^{2*}, \quad (\mathrm{RT, Ref.\ 17})$$
$$C_{111122}=-5.8\times10^{10}\ \mathrm{dyn/cm}^{2*}, \quad (\mathrm{RT, Ref.\ 17}).$$

RT stands for room temperature. The asterisk indicates theoretical values. With these data and Eqs. (105) and (106), we can calculate $(\partial c_{1111}/\partial\theta_i)/c_{1111}$ and estimate the value of $(\partial\beta_{11}/\partial\theta_i)/\beta_{11}$ at room temperature; hence,

$$\frac{1}{c_{1111}}\left(\frac{\partial c_{1111}}{\partial\theta_i}\right)_\theta=-4.8\times10^{-4}\,{}^\circ\mathrm{K}^{-1}, \quad (110)$$

$$\frac{1}{\beta_{11}}\left(\frac{\partial\beta_{11}}{\partial\theta_i}\right)_\theta=-7\times10^{-4}\,{}^\circ\mathrm{K}^{-1}. \quad (111)$$

Overton and Swim (Ref. 18) and Robinson and Hallett (Ref. 14) report the following room-temperature values (Ref. 19):

$$\frac{1}{c_{1111}}\left(\frac{dc_{1111}}{d\theta}\right)^{\mathrm{ad}}=8\times10^{-4}\,{}^\circ\mathrm{K}^{-1},$$

$$\frac{1}{\beta_{11}}\left(\frac{d\beta_{11}}{d\theta}\right)=-(5.9\times10^{-4})\,{}^\circ\mathrm{K}^{-1}. \quad (112)$$

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[12] The value of the mass density cannot be a function of the choice of initial state and, hence, Eq. (25):

$$(\partial\rho/\partial u_{kl})A_{nl}(\theta_i)(\delta_{kn}+u_{kn})+(\partial\rho/\partial\theta_i)=0.$$

Now, $\rho=\rho_0[1-u_{ii}+0(u_{ij}u_{kl})]$, where ρ_0 is the mass density in the initial state described by θ_i and, hence,

$$-\rho_0A_{ii}(\theta_i)+(\partial\rho_0/\partial\theta_i)=0.$$

When $A_{ii}=A_{11}\delta_{ij}$, we obtain (103).

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[14] M. C. Robinson and A. C. Hollis-Hallett, Can. J. Phys. **44**, 2211 (1966).

[15] J. Grindlay and H. C. Wong, Can. J. Phys. **47**, 1563 (1969).

[16] J. K. Galt, Phys. Rev. **73**, 1460 (1948).

[17] P. B. Ghate, Phys. Rev. **139**, A1666 (1965).

[18] W. C. Overton and R. T. Swim, Phys. Rev. **84**, 758 (1951).

[19] Robinson and Hallett measured the permeability at constant (zero) stress, i.e., $(\partial E_i/\partial D_i)_{\tau,\theta}$. Standard arguments for *m3m* symmetry yield

$$(\partial E_i/\partial D_i)_{\tau,\theta}=\beta+(\tilde{q}_{1111}+2\tilde{q}_{1122})\gamma.$$

See, for example, J. Grindlay, *An Introduction to the Phenomenological Theory of Ferroelectricity* (Pergamon Press, Ltd., Oxford, 1970). With the constraint $\theta\equiv\theta_i$, $\gamma\equiv0$ and, hence, $(\partial E_i/\partial D_i)_{\tau,\theta}=\beta$.

Both measurements were carried out dynamically (i.e., $\theta \equiv \theta_i$); this fact is indicated by the use of the total derivative notation (see Sec. VIII). The superscript ad denotes the adiabatic value; it is superfluous in the case of the permeability but not in the case of the elastic stiffness c_{1111} of NaCl (see reference in footnote 19). Since the adiabatic correction for c_{1111} is small, we conclude from these results that, for NaCl at room temperature,

$$\left|\left(\frac{\partial c_{1111}}{\partial \theta_i}\right)_\theta\right| \sim \left|\left(\frac{\partial c_{1111}}{\partial \theta}\right)_{\theta_i}\right|,$$

and

$$\left|\left(\frac{\partial \beta_{11}}{\partial \theta_i}\right)_\theta\right| \sim \left|\left(\frac{\partial \beta_{11}}{\partial \theta}\right)_{\theta_i}\right|.$$

APPENDIX A

The nonlinear elastic coefficients C_{ijvwxy}, Eq. (29), can be written in terms of the $H_{ijk}{}^{\alpha}$'s, Eqs. (49) and (50); we find

$$\begin{aligned}C_{ijvwxy} = \tfrac{1}{2}[&H_{ij}{}^0(J_{vwxy}+J_{xyvw}) \\ &+H_{wy}{}^0\delta_{iv}\delta_{jx}+H_{wy}{}^0\delta_{ix}\delta_{jv}-\delta_{vw}(H_{yj}{}^0\delta_{ix}+H_{yi}{}^0\delta_{jx}) \\ &-\delta_{xy}(H_{wj}{}^0\delta_{iv}+H_{wi}{}^0\delta_{jv})+H_{ijwy}{}^2\delta_{vx}-H_{ijxy}{}^2\delta_{vw} \\ &-H_{ijvw}{}^2\delta_{xy}+H_{yjvw}{}^2\delta_{ix}+H_{wjxy}{}^2\delta_{iv} \\ &+H_{yivw}{}^2\delta_{jx}+H_{wixy}{}^2\delta_{jv}]+H_{ijvwxy}{}^5,\end{aligned} \tag{A1}$$

with

$$\begin{aligned}&J_{1111}=J_{2222}=J_{3333}=1, \\ &J_{1122}=J_{2211}=J_{1133}=J_{3311}=J_{2233}=J_{3322}=J_{1221}=J_{2112} \\ &\qquad =J_{1331}=J_{3113}=J_{2332}=J_{3223}=\tfrac{1}{2};\end{aligned}$$

the remaining J_{vwxy}'s vanish.

The coefficients C_{ijvwxy} have the property that

$$C_{ijvwxy}=C_{ijxyvw}=C_{jivwxy}. \tag{A2}$$

The first equality holds as a result of the definition of these coefficients, Eq. (29), and the second equality results from the introduction of an energy density together with the demands of rotational invariance [see discussion under (iii) in Sec. 1].

For material symmetry *m3m* the C_{ijvwxy} are invariant under the transformations $x_1 \to x_2$, $x_2 \to -x_1$, $x_3 \to x_3$ and $x_1 \to x_2$, $x_2 \to x_3$, $x_3 \to x_1$; hence,

$$\begin{aligned}C_{111111}&=H_{111111}{}^5+\tfrac{3}{2}H_{1111}{}^2, \\ C_{111122}&=H_{111122}{}^5+\tfrac{1}{2}(H_{1122}{}^2-H_{1111}{}^2-H_{11}{}^0) \\ C_{221111}&=H_{111122}{}^5-\tfrac{1}{2}H_{1122}{}^2+H_{11}{}^0, \\ C_{111212}&=H_{111212}{}^5+2H_{1212}{}^2+\tfrac{1}{2}H_{1122}{}^0+H_{11}{}^0, \\ C_{121112}&=H_{111212}{}^5+\tfrac{1}{2}(H_{1212}{}^2+H_{1122}{}^2-H_{11}{}^0), \\ C_{112112}&=H_{111212}{}^5+H_{1212}{}^2+\tfrac{1}{2}H_{11}{}^0, \\ C_{122111}=C_{212111}&=H_{111212}{}^5+\tfrac{1}{2}H_{1111}{}^2, \\ C_{212313}&=H_{121323}{}^5+H_{1212}{}^2+\tfrac{1}{2}H_{11}{}^0, \\ C_{123213}=C_{123231}&=H_{121323}{}^5+\tfrac{1}{2}H_{1212}{}^2, \\ C_{211233}=C_{121233}&=H_{121233}{}^5+\tfrac{1}{2}(H_{1122}{}^2-H_{1212}{}^2-H_{11}{}^0), \\ C_{331212}&=H_{121233}{}^5+\tfrac{1}{2}H_{1122}{}^2, \\ C_{332112}&=H_{121233}{}^5+\tfrac{1}{2}H_{11}{}^0, \\ C_{221212}&=H_{121222}{}^5+\tfrac{1}{2}H_{1111}{}^2, \\ C_{332211}&=H_{112233}{}^5-H_{1133}{}^2+\tfrac{1}{2}H_{11}{}^0.\end{aligned}$$

The remaining coefficients, which cannot be obtained from these results using the subscript interchanges quoted above, vanish identically.

APPENDIX B

To solve Eqs. (90)–(92), we first eliminate $\tau_{11}{}^0$, γ, and C between Eqs. (88) and (90)–(92) to get

$$c''+c'(3A_{11}-A_{11}'/A_{11})+2A_{11}{}^2c=0, \tag{B1}$$

where $c'=(\partial c/\partial \theta_i)_\theta$, etc. We set

$$c(\theta,\theta_i)=k(\theta)\exp-\int H(\theta,\theta_i)d\theta_i,$$

where $k(\theta)$ is some arbitrary function of θ. Then, $H(\theta,\theta_i)$ satisfies the Ricatti equation

$$H'=H^2-(3A_{11}-A_{11}'/A_{11})H+2A_{11}{}^2. \tag{B2}$$

A particular solution to this equation is $H=A_{11}$; hence,[20]

$$c(\theta,\theta_i)=k(\theta)f(\theta_i)\{h(\theta)+[f(\theta_i)-f(\theta)]\}. \tag{B3}$$

With this solution, we may then deduce expressions for $\tau_{11}{}^0$, C; hence,

$$\begin{aligned}\tau_{11}{}^0(\theta,\theta_i)=&[f(\theta_i)-f(\theta)]k(\theta) \\ &\times\{h(\theta)+\tfrac{1}{2}[f(\theta_i)-f(\theta)]\},\end{aligned} \tag{B4}$$

$$C(\theta,\theta_i)=k(\theta)f^2(\theta_i)/2. \tag{B5}$$

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[20] H. T. H. Piaggio, *Differential Equations* (G. Bell and Sons, London, 1952), Chap. XV.