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DECOMPOSITION OF DEFORMATION AND REPRESENTATION OF THE FREE ENERGY FUNCTION FOR ISOTROPIC THERMOELASTIC SOLIDS

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Abstract—The constitutive equation for stress in a hyperelastic body undergoing nonisothermal deformation is derivable from a free energy function. This paper presents a postulate for decomposition of thermomechanical deformation, the properties of which are analogous to those associated with the Duhamel–Neumann postulate for linear thermoelasticity. That is, the deformation gradient is expressed as the product of a free thermal expansion gradient and an "effective" mechanical deformation gradient. This results in the decomposition of the free energy function into an isothermal, "effective" strain energy function and a function depending only on temperature. Some examples of biaxial extension and temperature change of an incompressible thin sheet are included.

1. INTRODUCTION

For a hyperelastic body undergoing nonisothermal deformation stress and entropy constitutive equations are derivable from a free energy function[1], which reduces to a strain energy function under isothermal deformation. For a linear thermoelastic material, the separate effects produced by temperature change and mechanical actions are taken to be additive in the sense of the Duhamel–Neumann postulate[2] for addition of thermal and mechanical strains. The implications of this postulate for nonisothermal deformations result in a free energy function which can be expressed as the sum of quadratic terms depending on "effective" mechanical strain and quadratic terms involving temperature change. This in turn provides a straightforward parameterization and identification problem for the classs of linear thermoelastic materials. Equivalent work for nonlinear elastic materials is considerably more limited, however, concentrated for the most part on experimental characterization of the strain energy function[3] or on purely analytical studies in which the strain energy or free energy function is expressed as a power series in terms of temperature change and a measure of deformation[4].

This paper presents a postulate for decomposition of thermomechanical deformation in hyperelastic solids, the implications of which are analogous to those associated with the Duhamel–Neumann postulate for linear elastic solids. That is, by expressing (local) nonisothermal deformation as the product of free thermal expansion and a stress-producing, isothermal mechanical deformation, it is possible to decompose the free energy function into an isothermal, "effective" strain energy function and a function depending only on temperature.

Following some preliminaries in Section 2, in which a thermal deformation gradient tensor is defined, the decomposition postulate is introduced in Section 3. This is followed in Section 4 by a discussion of representation of the free energy function in the light of the postulate. Section 5 specializes the work to mechanically incompressible materials and in Section 6 are contained several examples generalizing previous results for extension of incompressible thin sheets to incorporate the effect of simultaneous temperature change. In Section 7, the results of previous sections are specialized for small deformation and temperature change, leading to well-known results.

2. PRELIMINARIES

We recall first that the motion of a body B, referred to a global reference configuration β_0, may be written†

$$\mathbf{x} = \boldsymbol{\chi}(\mathbf{X}, t) \tag{1}$$

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†Vectors or tensors are denoted by bold-face type.

where $\mathbf{x}$ denotes the position vector at time t of a particle whose position vector in the reference configuration is denoted by $\mathbf{X}$. Anticipating applications in the next Section, we note that although choice of a reference configuration is arbitrary, a stress-free state of the body is often most convenient. A global configuration β_0 is mapped into an instantaneous configuration β under the deformation defined by (1); a local neighborhood N_0 of a particle is deformed into a neighborhood N in β. The mapping connecting the latter neighborhoods is characterized by the deformation gradient of the motion, denoted

$$\mathbf{F} = \frac{\partial \chi}{\partial \mathbf{X}}. \tag{2}$$

Associated with the deformation gradient tensor $\mathbf{F}$ we introduce for subsequent use the determinant

$$J = \det \mathbf{F}, \tag{3}$$

the symmetric deformation tensor

$$\mathbf{C} = \mathbf{F}^T\mathbf{F} \tag{4}$$

and the principal invariants of $\mathbf{C}$

$$\begin{aligned} I_1 &= tr\mathbf{C} \\ I_2 &= \tfrac{1}{2}[(tr\mathbf{C})^2 - tr\mathbf{C}^2] \\ I_3 &= \det \mathbf{C}. \end{aligned} \tag{5}$$

Note that the transformation connecting the local configurations N_0 and N expressed by (2) is equivalent to the mapping of differentials:

$$d\mathbf{x} = \mathbf{F}\, d\mathbf{X}. \tag{6}$$

The deformation defined by (1) is said to be isothermal if the temperature θ at every particle of the body remains constant with respect to time and non-isothermal otherwise. In the latter instance, experience indicates that bodies undergo expansion (or contraction) because of temperature changes. Due to thermal expansion, a neighborhood N_0 in β_0 is mapped into a new configuration N_0^θ. If the mechanical constraints on N_0 applied by the remaining portion of the body are temporarily removed, i.e. N_0 is isolated from the body, N_0 can deform freely and, therefore, the local configuration N_0^θ, like N_0, is also a stress-free state. In other terms, such "free" thermal expansion produces no stress in the body. However, it is clear that dislocations (separation and overlapping) between adjacent thermally expanded neighborhoods N_0^θ will occur. If such dislocations can be eliminated by subjecting each local configuration to rigid-body motion alone, the existence of a global stress-free state is possible. Otherwise, the body undergoes thermal stress even in the absence of mechanical forces or constraints on the body.

The fact that local stress-free configurations may not be actually attainable in a body is not important in the discussion. Rather, we need only consider N_0^θ as an imagined local reference configuration from which "effective" stress-producing deformation is measured. Denoting differentials in N_0 and N_0^θ by $d\mathbf{X}$ and $d\mathbf{X}^\theta$, respectively, the local mapping can be expressed by

$$d\mathbf{X}^\theta = \mathbf{F}^\theta\, d\mathbf{X} \tag{7}$$

where $\mathbf{F}^\theta$ is called the thermal deformation gradient tensor. For thermally isotropic materials, $\mathbf{F}^\theta$ can be written†

$$\mathbf{F}^\theta = \gamma(\theta)\mathbf{I} \tag{8}$$

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†The extension to thermally anisotropic materials presents no formal difficulty.

where $\mathbf{I}$ is the identity tensor and $\gamma(\theta)$ is a scalar-valued function of temperature, reflecting intrinsic thermal expansion characteristics of the material of the body. Looking ahead to specialization of the results to linear thermoelasticity, we propose the following definition for $\gamma(\theta)$:

$$\gamma(\theta) = \exp\left[\int_{\theta_0}^{\theta} \alpha(s)\,\mathrm{d}s\right] \tag{9}$$

where $\alpha(\theta)$ is the usual (temperature-dependent) coefficient of linear thermal expansion and θ, θ_0 denote temperatures in $N_0{}^{\theta}$, N_0, respectively. In particular, if α is independent of temperature, (9) reduces to

$$\gamma(T) = \exp(\alpha T) \tag{10}$$

where

$$T \equiv \theta - \theta_0.$$

Further, if $\alpha T \ll 1$ (infinitesimal thermal strain)

$$\gamma(T) \cong 1 + \alpha T. \tag{11}$$

Volume change associated with free thermal expansion from N_0 to $N_0{}^{\theta}$ can be calculated from

$$J^{\theta} \equiv \det \mathbf{F}^{\theta} = \gamma^3. \tag{12}$$

We note here in passing that the isotropy group of a material in the reference state associated with N_0 is unaffected by free thermal expansion, in particular, a material mechanically isotropic in the reference state remains isotropic after free thermal expansion. This result follows directly from Noll's theorem[1].

3. DECOMPOSITION OF THERMOMECHANICAL DEFORMATION

We turn now to the original problem of decomposition of thermomechanical deformation. It remains only to connect the local transformations defined by (6) and (7). We proceed by defining a tensor $\bar{\mathbf{F}}$, the "effective" deformation gradient associated with the isothermal mapping $N_0{}^{\theta}$ to N:

$$\mathrm{d}\mathbf{x} = \bar{\mathbf{F}}\,\mathrm{d}\mathbf{X}^{\theta}. \tag{13}$$

Comparing (6), (7) and (13) gives

$$\mathbf{F} = \bar{\mathbf{F}}\mathbf{F}^{\theta} \tag{14}$$

or, using (8), for thermally isotropic materials,

$$\bar{\mathbf{F}} = \mathbf{F}(\mathbf{F}^{\theta})^{-1} = \mathbf{F}\gamma^{-1}.$$

The significance of (14) is that the local deformation defined by (1) and (2) is decomposed into two successive mappings, the first a free thermal expansion characterized by (7) and (8) and the second an "effective" stress-producing isothermal deformation defined by (13). Equation (14) provides a generalization of the Duhamel–Neumann postulate of addition of thermal and mechanical strains employed in linear thermoelasticity. Note also that a similar decomposition concept has been used by Lee and Liu [5], among others, in treating isothermal finite elastoplastic deformation.

Associated with the effective deformation gradient tensor $\bar{\mathbf{F}}$ defined in (14) we note the results (all follow easily from previous definitions):

$$\begin{aligned}\bar{J} &\equiv \det \bar{\mathbf{F}} = J/\gamma^3\\ \bar{\mathbf{C}} &\equiv \bar{\mathbf{F}}^T\bar{\mathbf{F}} = \mathbf{C}/\gamma^2\\ \bar{I}_1 &\equiv tr\bar{\mathbf{C}} = I_1/\gamma^2\\ \bar{I}_2 &= \tfrac{1}{2}[(tr\bar{\mathbf{C}})^2 - tr\bar{\mathbf{C}}^2] = I_2/\gamma^4\\ \bar{I}_3 &\equiv \det \bar{\mathbf{C}} = I_3/\gamma^6.\end{aligned} \tag{15}$$

The results up to this point are independent of any particular assumptions of material mechanical constitution, apart from thermal isotropy. In the next section, we will indicate their utility in clarifying the problem of identifying the free energy function for a thermoelastic solid.

4. THE FREE ENERGY FUNCTION

Constitutive equations for a hyperelastic material are derivable from a free energy function $\psi(\mathbf{C}, \theta)$ as follows[1]:

$$\begin{aligned}\mathbf{T} &= 2\rho\mathbf{F}\frac{\partial\psi}{\partial\mathbf{C}}\mathbf{F}^T\\ \eta &= -\frac{\partial\psi}{\partial\theta}\end{aligned} \tag{16}$$

where $\mathbf{T}$ denotes the Cauchy stress tensor, η the specific entropy and ρ the mass density of the material body referred to its current configuration. Under isothermal deformation, the free energy function may be replaced by a strain energy function $W(\mathbf{C}, \theta)$ in which case $(16)_1$ is replaced by

$$\mathbf{T} = 2\rho\mathbf{F}\frac{\partial W}{\partial\mathbf{C}}\mathbf{F}^T. \tag{17}$$

In this instance, the argument θ of the strain energy function $W(\mathbf{C}, \theta)$ merely indicates the (constant) temperature at which isothermal deformation takes place.

We have shown in Section 3 that a nonisothermal deformation can be decomposed locally as the product of a free thermal expansion and an effective isothermal deformation. Since the former is stress-free, the value of the stress tensor depends explicitly on the *effective* deformation gradient. Keeping in mind again the fact that free thermal expansion does not affect the isotropy group of the material, (17) must be expressible in the alternative form

$$\mathbf{T} = 2\bar{\rho}\,\bar{\mathbf{F}}\frac{\partial W}{\partial\bar{\mathbf{C}}}(\bar{\mathbf{C}}, \theta)\bar{\mathbf{F}}^T. \tag{18}$$

Introducing the notation

$$\bar{W}(\mathbf{C}, \theta) \equiv W(\bar{\mathbf{C}}, \theta), \tag{19}$$

and using (14) and $(15)_2$ in (18) leads to the stress constitutive equation

$$\mathbf{T} = 2\rho\mathbf{F}\frac{\partial\bar{W}}{\partial\mathbf{C}}(\mathbf{C}, \theta)\mathbf{F}^T \tag{20}$$

which replaces (18). Comparing (20) and $(16)_1$, we see that $\partial\psi/\partial\mathbf{C} = \partial\bar{W}/\partial\mathbf{C}$, whence

$$\begin{aligned}\psi(\mathbf{C}, \theta) &= \bar{W}(\mathbf{C}, \theta) + h(\theta)\\ &= W(\bar{\mathbf{C}}, \theta) + h(\theta)\end{aligned} \tag{21}$$

where at this point $h(\theta)$ is an arbitrary function of temperature. From (21) it is seen that the free energy function for nonisothermal deformation of an elastic material is expressible as the sum of a strain energy function W (whose arguments are "effective" deformation $\bar{\mathbf{C}}$ and reference temperature θ) and a function h depending only on temperature, the latter having no direct effect on stress. Accordingly, the stress tensor associated with nonisothermal deformation can be calculated from the isothermal strain energy function W, in which the argument $\mathbf{C}$ is replaced by $\bar{\mathbf{C}}$. Implications of this result for material characterization are significant: isothermal experiments conducted over a range of constant reference temperatures are sufficient to identify constitutive material parameters, e.g. the two constants defining a Mooney–Rivlin material. Further illustrations of the result appearing in (21) are given in Sections 6 and 7.

Up to this point we have tacitly assumed that the temperature is a specified function (of position and time). However, for a coupled theory of thermoelasticity, deformation and temperature fields cannot be calculated independently, i.e. they are connected through the energy balance equation. Therefore, from an experimental standpoint identification of the function $h(\theta)$ appearing in (21) is difficult to separate from identification of a constitutive equation for the heat flux vector, the structure of which is discussed in [1], Section 96. Although this leads to a much broader problem than can be discussed here, it may be useful to relate the function $h(\theta)$ to the definition of specific heat at constant deformation, a concept that is useful both in uncoupled, nonlinear thermomechanics and in linear thermomechanics with or without coupling. Accordingly, we set

$$C_F(\mathbf{C},\theta) \equiv \theta \frac{\partial \eta}{\partial \theta}. \tag{22}$$

Using the constitutive equation for entropy $(16)_2$ together with (21) in (22) gives

$$h''(\theta) = -\left[\frac{C_F(\mathbf{C},\theta)}{\theta} + \frac{\partial^2 \bar{W}}{\partial \theta^2}(\mathbf{C},\theta)\right]. \tag{23}$$

Initial conditions associated with (23) are conveniently chosen as

$$\begin{aligned} h'(\theta_0) &= 0 \\ h(\theta_0) &= 0. \end{aligned} \tag{24}$$

Note that when the structure of the isothermal strain energy function W (hence $\bar{W}$) is known, the function $h(\theta)$ can be identified with the specific heat at constant deformation through (23) and (24). In the special cases where C_F is constant (see Section 7) or a function only of temperature, (23) and (24) lead directly to determination of $h(\theta)$.

5. MECHANICALLY INCOMPRESSIBLE MATERIALS

A material is mechanically incompressible if it undergoes only isochoric motions under isothermal conditions. Using the decomposition (14) for non-isothermal deformation it follows that the "effective" mechanical component must be isochoric, i.e.

$$\bar{J} = 1$$

or from (14)

$$J = J^\theta. \tag{25}$$

For thermally isotropic material (25) reduces to

$$J = \gamma^3. \tag{26}$$

The stress constitutive equation $(16)_1$ for a mechanically incompressible elastic solid has the modified form [1]

$$\mathbf{T} = -p\mathbf{I} + 2\rho\mathbf{F}\frac{\partial \psi}{\partial \mathbf{C}}\mathbf{F}^T \tag{27}$$

where p is a scalar pressure which must be found from the context of a particular application of (27). Similarly, (20) must be replaced by

$$\mathbf{T} = -p\mathbf{I} + 2\rho\mathbf{F}\frac{\partial \bar{W}}{\partial \mathbf{C}}\mathbf{F}^T. \tag{28}$$

If an incompressible elastic solid is also isotropic with respect to the reference configuration, the strain energy function can be written in the special form

$$W = W(I_1, I_2, \theta). \tag{29}$$

Utilizing the definitions contained in (15) and (19), together with (29), permits us to write (28) in the more explicit form

$$\mathbf{T} = -p\mathbf{I} + \frac{2\rho_0}{\gamma^7}\mathbf{F}\left[\gamma^2\frac{\partial W}{\partial \bar{I}_1}\mathbf{I} + \frac{\partial W}{\partial \bar{I}_2}(I_1\mathbf{I} - \mathbf{C})\right]\mathbf{F}^T \tag{30}$$

where ρ_0 denotes density of the material referred to the reference configuration β_0 at temperature θ_0.

6. EXAMPLE: UNIFORM BIAXIAL EXTENSION AND TEMPERATURE CHANGE OF AN INCOMPRESSIBLE, ISOTROPIC THIN SHEET

Consider a thin sheet subjected to homogeneous deformation with extension ratios λ_i in the direction of rectangular cartesian coordinate axes X_i; the deformation is produced by uniform edge tractions with the lateral faces of the sheet ($X_3 = \pm h_0$) free of applied tractions. A uniform temperature change is maintained relative to a stress-free reference state. Accordingly, the thermomechanical state of the sheet is expressible in terms of the principal extension ratios λ_i and the temperature θ, from which γ can be calculated from (9).

From the incompressibility condition (26),

$$\lambda_3 = \frac{\gamma^3}{\lambda_1\lambda_2}$$

and from (5)

$$I_1 = \lambda_1^2 + \lambda_2^2 + \frac{\gamma^6}{\lambda_1^2\lambda_2^2}.$$

Using these results and setting $T_{33} = 0$ in (30) gives

$$p = \frac{2\rho_0}{\lambda_1^2\lambda_2^2}\left[\gamma\frac{\partial W}{\partial \bar{I}_1} + \frac{(\lambda_1^2 + \lambda_2^2)}{\gamma}\frac{\partial W}{\partial \bar{I}_2}\right] \tag{31}$$

and therefore from (30) we have further

$$\begin{aligned} T_{11} &= \frac{2\rho_0(\lambda_1^4\lambda_2^2 - \gamma^6)}{\lambda_1^2\gamma^5}\left[\frac{1}{\lambda_2^2}\frac{\partial W}{\partial \bar{I}_1} + \frac{1}{\gamma^2}\frac{\partial W}{\partial \bar{I}_2}\right] \\ T_{22} &= \frac{2\rho_0(\lambda_1^2\lambda_2^4 - \gamma^6)}{\lambda_2^2\gamma^5}\left[\frac{1}{\lambda_1^2}\frac{\partial W}{\partial \bar{I}_1} + \frac{1}{\gamma^2}\frac{\partial W}{\partial \bar{I}_2}\right]. \end{aligned} \tag{32}$$

These results may be further specialized to give several cases of interest:
(a) Isothermal, equal biaxial extension

$\lambda_1 = \lambda_2 = \lambda$ and $\gamma = 1$, from which (32) gives

$$T_{11} = T_{22} = 2\rho_0\left(\lambda^2 - \frac{1}{\lambda^4}\right)\left(\frac{\partial W}{\partial \bar{I}_1} + \lambda^2\frac{\partial W}{\partial \bar{I}_2}\right). \tag{33}$$

Equation (33) is the same as that appearing on page 302 of [3].
(b) Equal biaxial extension with temperature change

$$\lambda_1 = \lambda_2 = \lambda,\ \gamma = \exp\left[\int_{\theta_0}^{\theta} \alpha(s)\,\mathrm{d}s\right] \text{prescribed.}$$

From (32)

$$T_{11} = T_{22} = 2\rho_0\left(\frac{\lambda^2}{\gamma^7} - \frac{1}{\lambda^4\gamma}\right)\left(\gamma^2\frac{\partial W}{\partial \bar{I}_1} + \lambda^2\frac{\partial W}{\partial \bar{I}_2}\right). \tag{34}$$

(c) In-plane constraint with temperature change

$$\lambda_1 = \lambda_2 = 1,\ \gamma \text{ as in (2) above.}$$

From (32)

$$T_{11} = T_{22} = 2\rho_0\left(\frac{1-\gamma^6}{\gamma^7}\right)\left(\gamma^2\frac{\partial W}{\partial \bar{I}_1} + \frac{\partial W}{\partial \bar{I}_2}\right) \tag{35}$$

If the sheet is assumed to be a Neo-Hookean material,

$$W = \mu(\bar{I}_1 - 3)$$

where μ is a material property. Substituting into (35) and using (11), neglecting terms in αT higher than first order,

$$T_{11} = T_{22} = -12\rho_0\mu\alpha T.$$

This result agrees with that of the linear theory of thermoelasticity if the term $2\rho_0\mu$ is identified with the shear modulus of the (incompressible) material.

7. LINEARIZATION

The previous example illustrates a special case of linearization. Under the restrictions of small deformation and temperature change, the results of previous sections lead to well-known results. In place of (4), the approximation

$$\mathbf{C} \simeq \mathbf{I} + 2\boldsymbol{\epsilon} \tag{36}$$

is adopted, where $\boldsymbol{\epsilon}$ is the infinitesimal strain tensor. Similarly, thermal expansion is characterized by (11),

$$\gamma \cong 1 + \alpha T.$$

The linearized form of the decomposition of thermomechanical deformation can be obtained from $(15)_2$, i.e. from

$$\bar{\mathbf{C}} = \frac{\mathbf{C}}{\gamma^2}.$$

Using the linearizations (11) and (36), neglecting terms of order two and higher in strains and defining an infinitesimal effective strain tensor $\bar{\boldsymbol{\epsilon}}$ such that $\bar{\mathbf{C}} \simeq \mathbf{I} + 2\bar{\boldsymbol{\epsilon}}$, there results

$$\bar{\boldsymbol{\epsilon}} = \boldsymbol{\epsilon} - \alpha T\mathbf{I}, \tag{37}$$

which is the Duhamel–Neumann postulate of linear thermomechanics. The isothermal strain energy function for a linear elastic solid can be written

$$W(\boldsymbol{\epsilon}) = \tfrac{1}{2}\boldsymbol{\epsilon} : \mathbf{E} : \boldsymbol{\epsilon} \tag{38}$$

where $\mathbf{E}$ is a rank four tensor whose components are elastic moduli, (apart from an immaterial constant reference density ρ_0).

From (19) we have

$$\bar{W}(\boldsymbol{\epsilon}) = W(\bar{\boldsymbol{\epsilon}}) = \tfrac{1}{2}(\boldsymbol{\epsilon} - \alpha T\mathbf{I}):\mathbf{E}:(\boldsymbol{\epsilon} - \alpha T\mathbf{I}). \tag{39}$$

Assuming that the specific heat C_F is constant, substitution of (39) in (23), subject to initial conditions (24) gives, after discarding higher order terms

$$h(T) = -\frac{1}{2}\left(\alpha^2 T^2 \mathbf{I}:\mathbf{E}:\mathbf{I} + \frac{C_F}{\theta_0} T^2\right) \tag{40}$$

and from (21)

$$\psi(\boldsymbol{\epsilon}, T) = \tfrac{1}{2}\boldsymbol{\epsilon}:\mathbf{E}:\boldsymbol{\epsilon} - B:\boldsymbol{\epsilon}T - \frac{1}{2}\frac{C_F}{\theta_0}T^2 \tag{41}$$

where

$$\rho_0\mathbf{B} \equiv \alpha\,\mathbf{I}:\rho_0\mathbf{E} \tag{42}$$

is the thermal stress tensor. Finally, linearized forms of constitutive equations (16)

$$\mathbf{T} = \rho_0 \frac{\partial\psi}{\partial\boldsymbol{\epsilon}}$$

$$\eta = -\frac{\partial\psi}{\partial T}$$

together with the quadratic function (41) yield the well-known results

$$\begin{aligned} \mathbf{T} &= \rho_0\mathbf{E}:\boldsymbol{\epsilon} - \rho_0\mathbf{B}T \\ \eta &= \mathbf{B}:\boldsymbol{\epsilon} + \frac{C_F}{\theta_0}T. \end{aligned} \tag{43}$$

8. CONCLUSION

This paper presents a method of decomposing nonisothermal deformation that generalizes the advantages afforded by the Duhamel-Neumann postulate of linear thermomechanics, namely, separation of thermal and mechanical contributions to the total deformation at a particle. Implications for analytical and experimental characterization of the free energy function, as well as for numerical computation of field problems are thereby made clear. Utilizing current isothermal models of nonlinear elastic materials found in the literature, one can construct solutions for boundary value problems in nonlinear thermoelasticity employing techniques such as the Finite Element Method.

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