

Finite-strain thermoelasticity based on multiplicative decomposition of deformation gradient

L. Vujošević * V. A. Lubarda †

Abstract

The constitutive formulation of the finite-strain thermoelasticity is revisited within the thermodynamic framework and the multiplicative decomposition of the deformation gradient into its elastic and thermal parts. An appealing structure of the Helmholtz free energy is proposed. The corresponding stress response and the entropy expressions are derived. The results are specified in the case of quadratic dependence of the elastic strain energy on the finite elastic strain. The specific and latent heats are discussed, and the comparison with the results of the classical thermoelasticity are given.

1 Introduction

The constitutive theory of finite-strain thermoelasticity is a classical and well developed topic of the non-linear continuum mechanics (e.g., Truesdell and Noll [1], Nowacki [2]). The formulation of the general theory is given in the thermodynamic framework by introducing the Helmholtz free energy as a function of the finite strain and temperature, and by exploring the conservation of energy and the second law of thermodynamics. This yields the constitutive expressions for the stress

*University of Montenegro, 81000 Podgorica, Yugoslavia

†CANU, 81000 Podgorica and UCSD, La Jolla, USA (e-mail: vlubarda@ucsd.edu)

and entropy, and the condition for the positive-definiteness of the heat conductivity tensor. Only two configurations of the material sample are considered in this approach at an arbitrary instant of deformation: the initial unstressed configuration at the uniform reference temperature, and the deformed configuration characterized by the non-uniform stress and temperature fields. There is an alternative but less employed approach to develop the thermoelastic constitutive theory, which is based on three configurations of the material sample. In addition to initial and deformed configurations, the third configuration is introduced by a conceptual isothermal destressing of the current configuration to zero stress. The total deformation gradient is then decomposed into the product of purely elastic and thermal parts. The resulting decomposition is then used to build the constitutive analysis. This approach was first introduced in the non-linear continuum mechanics by Stojanović and his associates [3–6], who considered both non-polar and polar materials. An inherent incompatibility of the intermediate configuration and its consequences on the development of the theory were examined in their work in detail. Further results were reported in a series of papers by Mićunović [7]. However, in contrast to an analogous decomposition of the elastoplastic deformation gradient into its elastic and plastic parts, introduced in the phenomenological finite-strain plasticity by Lee [8], which gained much attention in both single crystal and polycrystalline studies (e.g., Havner [9], Lubarda [10]), the decomposition of the thermoelastic deformation gradient was far less explored. An exception is a recent contribution by Imam and Johnson [11], who, apparently unaware of the original work by Stojanović *et al.*, used the decomposition to study the constitutive structure of the finite-deformation thermoelasticity. The objective of the present paper is to further elaborate on this topic, and to compare the results obtained by using two different approaches. In Section 2 we give a summary of the classical thermoelasticity, adding some new points in the consideration of the latent heats at finite strain and the derivation of the constitutive equations. Particular accent is given to the quadratic dependence of the free energy on the finite Lagrangian strain. The thermodynamic theory of thermoelasticity based on the multiplicative decomposition of deformation gradient is presented in Section 3. The results are explicitly given for elastically and thermally isotropic materials, with an indicated extension to

transversely isotropic and orthotropic materials. A physically appealing representation of the free energy is introduced and employed to derive the stress response and the entropy expression. The exact results are obtained in the case of the quadratic dependence of the elastic strain energy on the finite elastic strain. The relationships between the specific and latent heats at constant elastic and total strain are discussed, as well as the general connection between the two constitutive formulations. The concluding remarks are given in Section 4.

2 Classical theory of finite-strain thermoelasticity

In the classical thermodynamic formulation of the finite-strain thermoelasticity two configurations of the material sample are considered: the initial unstressed configuration \mathcal{B}_0 at the uniform reference temperature θ_0 , and the deformed configuration \mathcal{B} at the state of Cauchy stress $\boldsymbol{\sigma}$ and the temperature field θ (Fig. 1). The deformation gradient from \mathcal{B}_0 to \mathcal{B} is \mathbf{F} , and the corresponding Lagrangian strain is $\mathbf{E} = (\mathbf{F}^T \cdot \mathbf{F} - \mathbf{I})/2$. The second-order unit tensor is denoted by \mathbf{I} , and the superposed T denotes the transpose. If \mathbf{q} is the rate of heat flow by conduction in the deformed configuration, and $\mathbf{q}_0 = (\det \mathbf{F}) \mathbf{F}^{-1} \cdot \mathbf{q}$ is the corresponding nominal vector in the initial configuration, the principle of energy conservation gives

$$\dot{u} = \frac{1}{\rho_0} \left(\mathbf{T} : \dot{\mathbf{E}} - \nabla_0 \cdot \mathbf{q}_0 \right). \quad (1)$$

The specific internal energy (per unit mass) is u , the symmetric Piola–Kirchhoff stress \mathbf{T} is the work-conjugate to \mathbf{E} (such that $\mathbf{T} : \dot{\mathbf{E}} = \boldsymbol{\tau} : \mathbf{D}$, where $\boldsymbol{\tau} = (\det \mathbf{F}) \boldsymbol{\sigma}$ is the Kirchhoff stress and \mathbf{D} is the rate of deformation tensor – the symmetric part of the velocity gradient $\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1}$), the superposed dot stands for the material time derivative, the column $:$ denotes the trace product, and ∇_0 is the gradient operator with respect to initial coordinates ($\nabla_0 = \mathbf{F}^T \cdot \nabla$). The mass densities in the initial and deformed configurations are denoted by ρ_0 and ρ , respectively. Since there are no dissipative microstructural changes caused by thermoelastic deformation and the associated entropy production, the rate of the

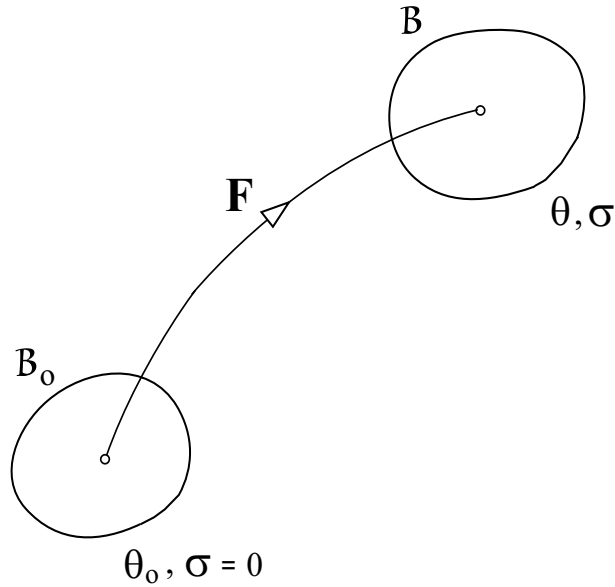


Figure 1: The initial unstressed configuration \mathcal{B}_0 at the uniform reference temperature θ_0 , and the deformed configuration \mathcal{B} at the temperature θ and the stress state $\boldsymbol{\sigma}$. The deformation gradient from the initial to deformed configuration is \mathbf{F} .

specific entropy η is due to heat flow only, so that

$$\theta \dot{\eta} = -\frac{1}{\rho_0} \nabla_0 \cdot \mathbf{q}_0 = -\frac{1}{\rho} \nabla \cdot \mathbf{q}. \quad (2)$$

Since the heat spontaneously flows in the direction of the negative temperature gradient, it is required that

$$\frac{1}{\rho_0} \mathbf{q}_0 \cdot \nabla_0 \theta = \frac{1}{\rho} \mathbf{q} \cdot \nabla \theta < 0. \quad (3)$$

The Helmholtz free energy per unit mass is $\psi = u - \theta \eta$. By differentiation and incorporation of Eqs. (1) and (2), its rate can be expressed as

$$\dot{\psi} = \frac{1}{\rho_0} \mathbf{T} : \dot{\mathbf{E}} - \eta \dot{\theta}. \quad (4)$$

This shows that the function $\psi = \psi(\mathbf{E}, \theta)$ is a thermodynamic potential for determining the stress \mathbf{T} and the entropy η . Indeed,

$$\dot{\psi} = \frac{\partial \psi}{\partial \mathbf{E}} : \dot{\mathbf{E}} + \frac{\partial \psi}{\partial \theta} \dot{\theta}, \tag{5}$$

and the comparison with Eq. (4) establishes the constitutive relations (e.g., Truesdell and Noll [1])

$$\mathbf{T} = \rho_0 \frac{\partial \psi}{\partial \mathbf{E}}, \tag{6}$$

$$\eta = -\frac{\partial \psi}{\partial \theta}. \tag{7}$$

2.1 Coupled heat equation

Suppose that the heat flow is governed by a generalized Fourier law of heat conduction

$$\mathbf{q} = -\mathbf{k}(\theta) \cdot \nabla \theta, \quad \mathbf{q}_0 = -\mathbf{k}_0(\mathbf{F}, \theta) \cdot \nabla_0 \theta, \tag{8}$$

where the symmetric tensors of conductivities \mathbf{k} and \mathbf{k}_0 are related by

$$\mathbf{k}_0(\mathbf{F}, \theta) = (\det \mathbf{F}) \mathbf{F}^{-1} \cdot \mathbf{k}(\theta) \cdot \mathbf{F}^{-T}. \tag{9}$$

In view of the requirement (3), the tensors \mathbf{k} and \mathbf{k}_0 are both positive-definite. The substitution of Eq. (8) into Eq. (2) gives

$$\theta \dot{\eta} = \frac{1}{\rho_0} \left[\mathbf{k}_0 : (\nabla_0 \otimes \nabla_0) \theta + \frac{\partial \mathbf{k}_0}{\partial \theta} : (\nabla_0 \theta \otimes \nabla_0 \theta) \right], \tag{10}$$

and

$$\theta \dot{\eta} = \frac{1}{\rho} \left[\mathbf{k} : (\nabla \otimes \nabla) \theta + \frac{d\mathbf{k}}{d\theta} : (\nabla \theta \otimes \nabla \theta) \right], \tag{11}$$

where \otimes stands for the outer tensor product. Usually \mathbf{k} is assumed to be temperature-independent, and the second term on the right-hand side can be omitted. On the other hand, from Eq. (7) one has

$$\theta \dot{\eta} = -\theta \left(\frac{\partial^2 \psi}{\partial \mathbf{E} \partial \theta} : \dot{\mathbf{E}} + \frac{\partial^2 \psi}{\partial \theta^2} \dot{\theta} \right). \tag{12}$$

Introducing the second-order tensor of the latent heat $\boldsymbol{\ell}_E$ and the specific heat c_E , both at constant strain, by

$$\boldsymbol{\ell}_E = -\frac{1}{\rho_0} \theta \frac{\partial \mathbf{T}}{\partial \theta} = -\theta \frac{\partial^2 \psi}{\partial \mathbf{E} \partial \theta}, \quad (13)$$

$$c_E = \theta \frac{\partial \eta}{\partial \theta} = -\theta \frac{\partial^2 \psi}{\partial \theta^2}, \quad (14)$$

we can rewrite Eq. (12) as

$$\theta \dot{\eta} = \boldsymbol{\ell}_E : \dot{\mathbf{E}} + c_E \dot{\theta}. \quad (15)$$

The coupled heat equation is obtained by combining Eqs. (10) and (15). This yields

$$\frac{1}{\rho_0} \left[\mathbf{K}_0 : (\nabla_0 \otimes \nabla_0) \theta + \frac{\partial \mathbf{K}_0}{\partial \theta} : (\nabla_0 \theta \otimes \nabla_0 \theta) \right] = \boldsymbol{\ell}_E : \dot{\mathbf{E}} + c_E \dot{\theta}. \quad (16)$$

Recalling that $\dot{\mathbf{E}} = \mathbf{F}^T \cdot \mathbf{D} \cdot \mathbf{F}$, an alternative representation is

$$\frac{1}{\rho} \left[\mathbf{k} : (\nabla \otimes \nabla) \theta + \frac{d\mathbf{k}}{d\theta} : (\nabla \theta \otimes \nabla \theta) \right] = (\mathbf{F} \cdot \boldsymbol{\ell}_E \cdot \mathbf{F}^T) : \mathbf{D} + c_E \dot{\theta}. \quad (17)$$

Since the symmetric Piola–Kirchhoff stress tensor is related to the Cauchy stress by $\mathbf{F} \cdot \mathbf{T} \cdot \mathbf{F}^T = (\det \mathbf{F}) \boldsymbol{\sigma}$, the latent heat tensor in Eq. (17) can be expressed as

$$\mathbf{F} \cdot \boldsymbol{\ell}_E \cdot \mathbf{F}^T = -\frac{1}{\rho} \theta \frac{\partial \boldsymbol{\sigma}}{\partial \theta}. \quad (18)$$

2.2 Free energy representation

If it is assumed that the stress \mathbf{T} linearly depends on the finite strain \mathbf{E} , and if the specific and latent heats depend linearly on the temperature θ according to

$$c_E = c_E^0 + c(\theta - \theta_0), \quad \boldsymbol{\ell}_E = \frac{\theta}{\theta_0} \boldsymbol{\ell}_E^0, \quad (19)$$

where $c = \text{const.}$, while c_E^0 and ℓ_E^0 are the the specific and latent heats at $\theta = \theta_0$ and $\mathbf{E} = \mathbf{0}$, it readily follows that the free energy is

$$\begin{aligned} \psi = & \frac{1}{2\rho_0} \mathbf{\Lambda}_0 :: (\mathbf{E} \otimes \mathbf{E}) - (\ell_E^0 : \mathbf{E}) \frac{\theta - \theta_0}{\theta_0} \\ & + (c_E^0 - c\theta_0) \left(\theta - \theta_0 - \theta \ln \frac{\theta}{\theta_0} \right) - \frac{1}{2} c (\theta - \theta_0)^2. \end{aligned} \quad (20)$$

The fully symmetric fourth-order tensor $\mathbf{\Lambda}_0$ is the isothermal elastic moduli tensor (at the temperature $\theta = \theta_0$). The corresponding stress and entropy expressions are

$$\mathbf{T} = \mathbf{\Lambda}_0 : \mathbf{E} - \frac{\rho_0}{\theta_0} \ell_E^0 (\theta - \theta_0), \quad (21)$$

and

$$\eta = \frac{1}{\theta_0} \ell_E^0 : \mathbf{E} + (c_E^0 - c\theta_0) \ln \frac{\theta}{\theta_0} + c(\theta - \theta_0). \quad (22)$$

Introducing the second-order tensor of thermal expansion $\boldsymbol{\alpha}_0$ by

$$\mathbf{\Lambda}_0 : \boldsymbol{\alpha}_0 = \frac{\rho_0}{\theta_0} \ell_E^0, \quad (23)$$

equation (21) can be rewritten as

$$\mathbf{E} = \mathbf{\Lambda}_0^{-1} : \mathbf{T} + \boldsymbol{\alpha}_0 (\theta - \theta_0). \quad (24)$$

For the elastically and thermally isotropic material,

$$\mathbf{\Lambda}_0 = \lambda_0 \mathbf{I} \otimes \mathbf{I} + 2\mu_0 \mathbf{II}, \quad \boldsymbol{\alpha}_0 = \alpha_0 \mathbf{I}, \quad \frac{\rho_0}{\theta_0} \ell_E^0 = 3\alpha_0 \kappa_0 \mathbf{I}, \quad (25)$$

where \mathbf{II} is the symmetric fourth-order unit tensor with the rectangular components $(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})/2$ (δ_{ij} being the Kronecker delta), λ_0 and μ_0 are the Lamé constants, $\kappa_0 = \lambda_0 + 2\mu_0/3$ is the elastic bulk modulus, and α_0 is the coefficient of linear thermal expansion. The constitutive equations (21), (22), and (24) accordingly become

$$\mathbf{T} = \lambda_0 (\text{tr } \mathbf{E}) \mathbf{I} + 2\mu_0 \mathbf{E} - 3\alpha_0 (\theta - \theta_0) \kappa_0 \mathbf{I}, \quad (26)$$

$$\eta = \frac{3}{\rho_0} \alpha_0 \kappa_0 \text{tr } \mathbf{E} + (c_E^0 - c\theta_0) \ln \frac{\theta}{\theta_0} + c(\theta - \theta_0), \quad (27)$$

$$\mathbf{E} = \frac{1}{2\mu_0} \left[\mathbf{T} - \frac{\lambda_0}{3\kappa_0} (\text{tr } \mathbf{T}) \mathbf{I} \right] + \alpha_0 (\theta - \theta_0) \mathbf{I}. \quad (28)$$

The trace of \mathbf{E} is $\text{tr } \mathbf{E} = \mathbf{E} : \mathbf{I}$, and similarly for $\text{tr } \mathbf{T}$. With the isotropic tensor of heat conductivities

$$\mathbf{k} = k \mathbf{I}, \quad k = \text{const.}, \quad (29)$$

the heat equation (16) becomes

$$(\det \mathbf{F}) k \nabla^2 \theta = 3\alpha_0 \kappa_0 \theta \text{tr } \dot{\mathbf{E}} + \rho_0 [c_E^0 + c(\theta - \theta_0)] \dot{\theta}. \quad (30)$$

The Laplacian operator is $\nabla^2 = \nabla \cdot \nabla = \nabla_0 \cdot \mathbf{C}^{-1} \cdot \nabla_0$, and the right Cauchy–Green deformation tensor is $\mathbf{C} = \mathbf{F}^T \cdot \mathbf{F}$. If the approximation $\theta \approx \theta_0$ is made on the right-hand side, and if \mathbf{E} is taken to be the infinitesimal strain, Eq. (30) reduces to the well-known coupled heat equation of the isotropic linear thermoelasticity (e.g., Boley and Weiner [12], Parkus [13]).

It is noted that for $c \neq c_E^0/\theta_0$ in Eq. (20), the strain \mathbf{E} and the temperature θ cannot be expressed explicitly in terms of the stress \mathbf{T} and the entropy η . However, for $c = c_E^0/\theta_0$ (resulting in the quadratic dependence of ψ on θ), we obtain

$$\mathbf{E} = \left[\mathbf{\Lambda}_0^{-1} - \frac{1}{a_0} (\boldsymbol{\alpha}_0 \otimes \boldsymbol{\alpha}_0) \right] : \mathbf{T} + \frac{\rho_0}{a_0} \eta \boldsymbol{\alpha}_0, \quad (31)$$

$$\theta = \theta_0 + \frac{1}{a_0} (\rho_0 \eta - \boldsymbol{\alpha}_0 : \mathbf{T}). \quad (32)$$

The scalar parameter a_0 is defined by

$$a_0 = \frac{\rho_0 c_E^0}{\theta_0} + \boldsymbol{\alpha}_0 : \mathbf{\Lambda}_0 : \boldsymbol{\alpha}_0. \quad (33)$$

In the isotropic case these expressions simplify to

$$\mathbf{E} = \frac{1}{2\mu_0} \left[\mathbf{T} - \frac{\lambda_0}{3\kappa_0} (\text{tr } \mathbf{T}) \mathbf{I} \right] + \frac{\alpha_0}{a_0} (\rho_0 \eta - \alpha_0 \text{tr } \mathbf{T}) \mathbf{I}, \quad (34)$$

$$\theta = \theta_0 + \frac{1}{a_0} (\rho_0 \eta - \alpha_0 \text{tr } \mathbf{T}), \quad (35)$$

$$a_0 = \frac{\rho_0 c_E^0}{\theta_0} + 9\alpha_0^2 \kappa_0. \quad (36)$$

Finally, the comment is made regarding the temperature dependence of the elastic moduli. If ψ is taken to be a cubic function of the strain components and temperature, the resulting second-order elastic moduli are temperature-dependent, but not the third-order elastic moduli. Some aspects of this analysis can be found in [14]. Analogous statement holds for higher-order polynomial representations of the free energy function.

3 Thermoelastic analysis based on the multiplicative decomposition

An alternative approach to develop the constitutive theory of thermoelastic material response is based on the introduction of an intermediate configuration \mathcal{B}_θ , which is obtained from the current configuration \mathcal{B} by isothermal elastic unloading to zero stress (Fig. 2). The isothermal elastic deformation gradient from \mathcal{B}_θ to \mathcal{B} is denoted by \mathbf{F}_e , and the thermal deformation gradient from \mathcal{B}_0 to \mathcal{B}_θ by \mathbf{F}_θ . The total deformation gradient \mathbf{F} , which maps an infinitesimal material element $d\mathbf{X}$ from the initial configuration to $d\mathbf{x} = \mathbf{F} \cdot d\mathbf{X}$ in the current configuration, can then be decomposed as

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_\theta. \quad (37)$$

This decomposition was first introduced in (the non-polar and polar) finite-strain thermoelasticity by Stojanović *et al.* [3–6]. An analogous decomposition of the elastoplastic deformation gradient in its elastic and plastic parts was introduced by Lee [8]. Earlier contributions toward the introduction of the intermediate configuration in the constitutive analysis of different materials include Eckart [15] and Kröner [16]. For the inhomogeneous deformation and temperature fields only \mathbf{F} is a true deformation gradient, whose components are the partial derivatives $\partial \mathbf{x} / \partial \mathbf{X}$. In contrast, the mappings from \mathcal{B}_θ to \mathcal{B} and from \mathcal{B}_0 to \mathcal{B}_θ are not, in general, continuous one-to-one mappings, so that \mathbf{F}_e and \mathbf{F}_θ are not defined as the gradients of the respective mappings (which may not exist), but as the point functions (local deformation gradients). Various geometric and kinematic aspects of the incompatibility of the intermediate configuration are discussed in [17].

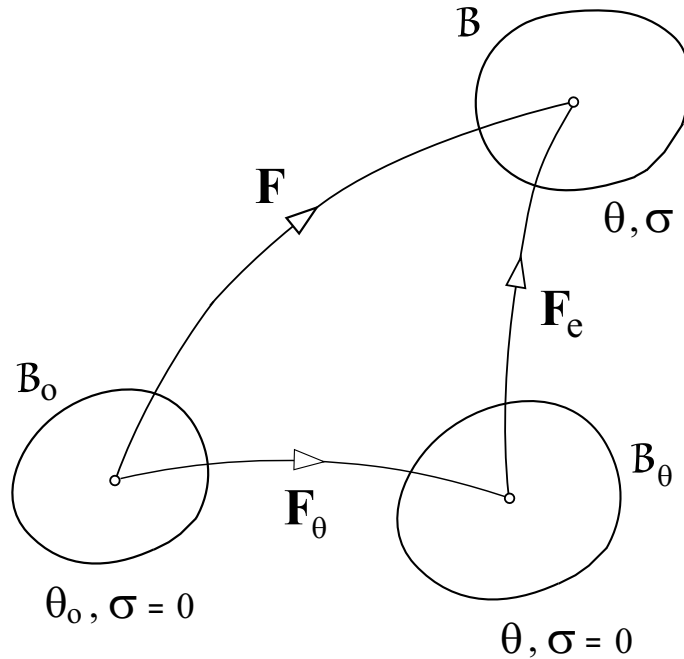


Figure 2: The intermediate configuration \mathcal{B}_θ at nonuniform temperature θ is obtained from the deformed configuration \mathcal{B} by isothermal destressing to zero stress. The deformation gradient from initial to deformed configuration \mathbf{F} is decomposed into elastic part \mathbf{F}_e and thermal part \mathbf{F}_θ , such that $\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_\theta$.

The decomposition (37) is not unique because arbitrary rigid-body rotation can be superposed to \mathcal{B}_θ preserving it unstressed. However, we shall be able to specify \mathbf{F}_θ , and thus the decomposition (37), uniquely in each considered case or type of the material anisotropy. For example, for transversely isotropic material with the axis of isotropy parallel to the unit vector \mathbf{n}_0 in the configuration \mathcal{B}_0 , we specify \mathbf{F}_θ by

$$\mathbf{F}_\theta = (\zeta - \vartheta)\mathbf{n}_0 \otimes \mathbf{n}_0 + \vartheta \mathbf{I}, \quad (38)$$

where $\zeta = \zeta(\theta)$ is the stretch ratio due to thermal expansion in the direction \mathbf{n}_0 , while $\vartheta = \vartheta(\theta)$ is the thermal stretch ratio in any direction within the plane of isotropy (orthogonal to \mathbf{n}_0). An extension of the

representation (38) to orthotropic materials is straightforward. In each case, the Lagrangian strain can be decomposed as

$$\mathbf{E} = \mathbf{E}_\theta^T \cdot \mathbf{E}_e \cdot \mathbf{F}_\theta + \mathbf{E}_\theta. \quad (39)$$

The elastic and thermal strain tensors are

$$\mathbf{E}_e = \frac{1}{2} (\mathbf{F}_e^T \cdot \mathbf{F}_e - \mathbf{I}), \quad \mathbf{E}_\theta = \frac{1}{2} (\mathbf{F}_\theta^T \cdot \mathbf{F}_\theta - \mathbf{I}). \quad (40)$$

Thus, the elastic strain and its rate can be expressed as

$$\mathbf{E}_e = \mathbf{F}_\theta^{-T} \cdot (\mathbf{E} - \mathbf{E}_\theta) \cdot \mathbf{F}_\theta^{-1}, \quad (41)$$

$$\dot{\mathbf{E}}_e = \mathbf{F}_\theta^{-T} \cdot \dot{\mathbf{E}} \cdot \mathbf{F}_\theta^{-1} - \mathbf{D}_\theta - \mathbf{E}_e \cdot \mathbf{L}_\theta - \mathbf{L}_\theta^T \cdot \mathbf{E}_e, \quad (42)$$

where $\mathbf{L}_\theta = \dot{\mathbf{F}}_\theta \cdot \mathbf{F}_\theta^{-1}$ and \mathbf{D}_θ is its symmetric part.

The analysis will be restricted in the sequel to isotropic materials, for which the thermal part of the deformation gradient is

$$\mathbf{F}_\theta = \vartheta(\theta) \mathbf{I}. \quad (43)$$

The scalar $\vartheta = \vartheta(\theta)$ is the thermal stretch ratio in an arbitrary direction. In this case

$$\mathbf{E}_e = \frac{1}{\vartheta^2} (\mathbf{E} - \mathbf{E}_\theta), \quad \mathbf{E}_\theta = \frac{1}{2} (\vartheta^2 - 1) \mathbf{I}. \quad (44)$$

Upon thermal expansion from the initial temperature θ_0 to the current temperature θ , an infinitesimal volume element dV_0 from the configuration \mathcal{B}_0 becomes $dV_\theta = (\det \mathbf{F}_\theta) dV_0$ in the configuration \mathcal{B}_θ , such that

$$\frac{d}{dt} (dV_\theta) = (\text{tr } \mathbf{L}_\theta) dV_\theta. \quad (45)$$

The time differentiation is designated by d/dt , and

$$\mathbf{L}_\theta = \frac{\dot{\vartheta}}{\vartheta} \mathbf{I} = \frac{1}{\vartheta} \frac{d\vartheta}{d\theta} \dot{\theta} \mathbf{I}. \quad (46)$$

The substitution of Eq. (46) into Eq. (45) gives

$$\frac{d}{dt} (dV_\theta) = \frac{3}{\vartheta} \frac{d\vartheta}{d\theta} dV_\theta \dot{\theta}. \quad (47)$$

The temperature-dependent coefficient of linear thermal expansion $\alpha = \alpha(\theta)$ is defined by (e.g., [18,19])

$$\frac{d}{dt} (dV_\theta) = 3\alpha(\theta) dV_\theta \dot{\theta}. \quad (48)$$

The coefficient of volumetric thermal expansion is equal to 3α . Comparing Eqs. (47) and (48) establishes the differential connection between the thermal stretch ratio and the coefficient of thermal expansion,

$$\alpha(\theta) = \frac{1}{\vartheta} \frac{d\vartheta}{d\theta}. \quad (49)$$

Upon integration this gives

$$\vartheta(\theta) = \exp \left[\int_{\theta_0}^{\theta} \alpha(\theta) d\theta \right]. \quad (50)$$

In view of Eqs. (42) and (49), the rate of elastic strain can now be written as

$$\dot{\mathbf{E}}_e = \frac{1}{\vartheta^2(\theta)} \left[\dot{\mathbf{E}} - \alpha(\theta) (\mathbf{I} + 2\mathbf{E}) \dot{\theta} \right]. \quad (51)$$

3.1 Free energy and constitutive expressions

The following representation of the Helmholtz free energy suggests itself in the framework of finite-strain thermoelasticity based on the multiplicative decomposition

$$\psi = \psi_e(\mathbf{E}_e, \theta) + \psi_\theta(\theta), \quad (52)$$

where ψ_e is an isotropic function of the elastic strain \mathbf{E}_e and temperature θ . This should be compared with the representation (20) of classical theory, in which ψ depends on the total strain \mathbf{E} and temperature θ . The time-rate of the free energy is

$$\dot{\psi} = \frac{\partial \psi_e}{\partial \mathbf{E}_e} : \dot{\mathbf{E}}_e + \frac{\partial \psi_e}{\partial \theta} \dot{\theta} + \frac{d\psi_\theta}{d\theta} \dot{\theta}. \quad (53)$$

Upon substitution of Eq. (51), there follows

$$\dot{\psi} = \frac{1}{\vartheta^2} \frac{\partial \psi_e}{\partial \mathbf{E}_e} : \dot{\mathbf{E}} - \left[\frac{\alpha}{\vartheta^2} \frac{\partial \psi_e}{\partial \mathbf{E}_e} : (\mathbf{I} + 2\mathbf{E}) - \frac{\partial \psi_e}{\partial \theta} - \frac{d\psi_\theta}{d\theta} \right] \dot{\theta}. \quad (54)$$

The comparison with Eq. (4) then yields the constitutive relations

$$\mathbf{T} = \frac{\rho_0}{\vartheta^2} \frac{\partial \psi_e}{\partial \mathbf{E}_e}, \quad (55)$$

$$\eta = \alpha \frac{\partial \psi_e}{\partial \mathbf{E}_e} : (\mathbf{I} + 2\mathbf{E}_e) - \frac{\partial \psi_e}{\partial \theta} - \frac{d\psi_\theta}{d\theta}. \quad (56)$$

The identity is here noted,

$$\mathbf{I} + 2\mathbf{E} = \vartheta^2 (\mathbf{I} + 2\mathbf{E}_e). \quad (57)$$

Owing to the relationship $\rho_0 = (\det \mathbf{F}_\theta) \rho_\theta = \vartheta^3 \rho_\theta$ between the densities ρ_0 in the configuration \mathcal{B}_0 and ρ_θ in the configuration \mathcal{B}_θ , the stress response in Eq. (55) can be written as

$$\mathbf{T} = \vartheta \mathbf{T}_e, \quad \mathbf{T}_e = \rho_\theta \frac{\partial \psi_e}{\partial \mathbf{E}_e}. \quad (58)$$

The last expression also follows from the more general relationship

$$\mathbf{T} = (\det \mathbf{F}_\theta) \mathbf{F}_\theta^{-1} \cdot \mathbf{T}_e \cdot \mathbf{F}_\theta^{-T}. \quad (59)$$

3.2 Analysis of stress response

An appealing feature of the thermoelastic constitutive formulation based on the multiplicative decomposition is that the function $\psi_e(\mathbf{E}_e, \theta)$ can be taken as one of the well-known strain energy functions of the isothermal finite-strain elasticity (e.g., Ogden [20], Holzapfel [21]), except that the coefficients of the strain-dependent terms are now functions of the temperature. For example, suppose that ψ_e is a quadratic function of the strain components, such that

$$\rho_\theta \psi_e = \frac{1}{2} \lambda(\theta) (\text{tr } \mathbf{E}_e)^2 + \mu(\theta) \mathbf{E}_e : \mathbf{E}_e, \quad (60)$$

where $\lambda(\theta)$ and $\mu(\theta)$ are the temperature-dependent Lamé moduli. It follows that

$$\mathbf{T}_e = \lambda(\theta) (\text{tr } \mathbf{E}_e) \mathbf{I} + 2\mu(\theta) \mathbf{E}_e = \mathbf{\Lambda}_e(\theta) : \mathbf{E}_e. \quad (61)$$

The elastic moduli tensor is

$$\mathbf{\Lambda}_e(\theta) = \lambda(\theta) \mathbf{I} \otimes \mathbf{I} + 2\mu(\theta) \mathbf{II}. \quad (62)$$

Consequently, substituting Eqs. (51) and (61) into $\mathbf{T} = \vartheta \mathbf{T}_e$, the stress response becomes

$$\mathbf{T} = \frac{1}{\vartheta(\theta)} \left[\lambda(\theta)(\text{tr } \mathbf{E}) \mathbf{I} + 2\mu(\theta) \mathbf{E} \right] - \frac{3}{2} \left[\vartheta(\theta) - \frac{1}{\vartheta(\theta)} \right] \kappa(\theta) \mathbf{I}. \quad (63)$$

The temperature-dependent bulk modulus is $\kappa(\theta) = \lambda(\theta) + 2\mu(\theta)/3$. This is an exact expression for the thermoelastic stress response associated with the quadratic representation of ψ_e in terms of the finite elastic strain \mathbf{E}_e . If the Lamé moduli are taken to be temperature-independent, and if the approximation

$$\vartheta(\theta) \approx 1 + \alpha_0(\theta - \theta_0) \quad (64)$$

is adopted (α_0 being the coefficient of linear thermal expansion at $\theta = \theta_0$), Eq. (63) reduces to Eq. (26). When \mathbf{E} and \mathbf{T} are there interpreted as the infinitesimal strain and the Cauchy stress, the equation coincides with the well-known Duhamel–Neumann expression of isotropic linear thermoelasticity. Note also that the elastic strain energy ψ_e of Eq. (60) can be recast in terms of the total strain as

$$\begin{aligned} \rho_0 \psi_e = & \frac{1}{\vartheta} \left[\frac{1}{2} \lambda(\theta)(\text{tr } \mathbf{E})^2 + \mu(\theta) \mathbf{E} : \mathbf{E} \right] \\ & - \frac{3}{2} \kappa(\theta) \left(\vartheta - \frac{1}{\vartheta} \right) \left[\text{tr } \mathbf{E} - \frac{3}{4} (\vartheta^2 - 1) \right]. \end{aligned} \quad (65)$$

This confirms the result (63) through $\mathbf{T} = \rho_0 \partial \psi_e / \partial \mathbf{E}$.

3.3 Entropy expression

The entropy expression (56) can be recast by using the stress expression (55) as

$$\eta = \frac{1}{\rho_0} \alpha \mathbf{T} : (\mathbf{I} + 2\mathbf{E}) - \frac{\partial \psi_e}{\partial \theta} - \frac{d\psi_\theta}{d\theta}. \quad (66)$$

We proceed next with the evaluation of the term $\partial\psi_e/\partial\theta$. In the case of the quadratic strain energy representation (60), we have

$$\rho_0 \psi_e = \frac{1}{2} \vartheta^3 \mathbf{T}_e : \mathbf{E}_e. \quad (67)$$

Thus,

$$\rho_0 \left(\frac{\partial\psi_e}{\partial\theta} \right)_{\mathbf{E}_e} = \frac{3}{2} \vartheta^2 \frac{d\vartheta}{d\theta} \mathbf{T}_e : \mathbf{E}_e + \frac{1}{2} \vartheta^3 \left(\frac{\partial\mathbf{T}_e}{\partial\theta} \right)_{\mathbf{E}_e} : \mathbf{E}_e, \quad (68)$$

i.e.,

$$\rho_0 \left(\frac{\partial\psi_e}{\partial\theta} \right)_{\mathbf{E}_e} = \frac{3}{2} \alpha \left[\mathbf{T} : \mathbf{E} - \frac{1}{2} (\vartheta^2 - 1) \text{tr} \mathbf{T} \right] + \frac{1}{2} \vartheta^3 \left(\frac{\partial\mathbf{T}_e}{\partial\theta} \right)_{\mathbf{E}_e} : \mathbf{E}_e. \quad (69)$$

The temperature gradient of the stress tensor is

$$\left(\frac{\partial\mathbf{T}_e}{\partial\theta} \right)_{\mathbf{E}_e} = \frac{d\mathbf{\Lambda}_e}{d\theta} : \mathbf{E}_e. \quad (70)$$

Recalling the stress expression

$$\mathbf{T} = \frac{1}{\vartheta} \mathbf{\Lambda}_e : \left[\mathbf{E} - \frac{1}{2} (\vartheta^2 - 1) \mathbf{I} \right], \quad (71)$$

it can be readily verified that

$$\vartheta \left(\frac{\partial\mathbf{T}_e}{\partial\theta} \right)_{\mathbf{E}_e} = \left(\frac{\partial\mathbf{T}}{\partial\theta} \right)_{\mathbf{E}} + \alpha (\mathbf{T} + 3\vartheta \kappa \mathbf{I}). \quad (72)$$

Consequently,

$$\begin{aligned} \vartheta^3 \left(\frac{\partial\mathbf{T}_e}{\partial\theta} \right)_{\mathbf{E}_e} : \mathbf{E}_e &= \left(\frac{\partial\mathbf{T}}{\partial\theta} \right)_{\mathbf{E}} : \left[\mathbf{E} - \frac{1}{2} (\vartheta^2 - 1) \mathbf{I} \right] \\ &+ \alpha \left[\mathbf{T} : \mathbf{E} + \frac{1}{2} (1 + \vartheta^2) \text{tr} \mathbf{T} \right]. \end{aligned} \quad (73)$$

Inserting Eq. (73) into Eq. (69) gives

$$\begin{aligned} \rho_0 \left(\frac{\partial\psi_e}{\partial\theta} \right)_{\mathbf{E}_e} &= 2\alpha \mathbf{T} : \mathbf{E} + \frac{1}{2} \alpha (2 - \vartheta^2) \text{tr} \mathbf{T} \\ &+ \frac{1}{2} \left(\frac{\partial\mathbf{T}}{\partial\theta} \right)_{\mathbf{E}} : \left[\mathbf{E} - \frac{1}{2} (\vartheta^2 - 1) \mathbf{I} \right]. \end{aligned} \quad (74)$$

When this is substituted into Eq. (66), the entropy becomes

$$\eta = \frac{1}{2\rho_0} \vartheta^2 \alpha \operatorname{tr} \mathbf{T} - \frac{1}{2\rho_0} \left(\frac{\partial \mathbf{T}}{\partial \theta} \right)_{\mathbf{E}} : \left[\mathbf{E} - \frac{1}{2} (\vartheta^2 - 1) \mathbf{I} \right] - \frac{d\psi_\theta}{d\theta}. \quad (75)$$

Since

$$\vartheta \operatorname{tr} \mathbf{T} = 3 \kappa \left[\operatorname{tr} \mathbf{E} - \frac{3}{2} (\vartheta^2 - 1) \right], \quad (76)$$

equation (75) can be rearranged as

$$\eta = \frac{1}{2\rho_0} \left[3 \vartheta \alpha \kappa \mathbf{I} - \left(\frac{\partial \mathbf{T}}{\partial \theta} \right)_{\mathbf{E}} \right] : \left[\mathbf{E} - \frac{1}{2} (\vartheta^2 - 1) \mathbf{I} \right] - \frac{d\psi_\theta}{d\theta}. \quad (77)$$

Finally, recalling the expression for the latent heat (13), the entropy is

$$\eta = \frac{1}{2} \left(\frac{1}{\theta} \ell_E + \frac{3}{\rho_0} \vartheta \alpha \kappa \mathbf{I} \right) : \left[\mathbf{E} - \frac{1}{2} (\vartheta^2 - 1) \mathbf{I} \right] - \frac{d\psi_\theta}{d\theta}. \quad (78)$$

This is an exact expression for η within the approximation used for the strain energy, Eq. (60).

An alternative route to derive Eq. (78) is to express the elastic strain energy ψ_e as

$$\rho_0 \psi_e = \frac{1}{2} \mathbf{T} : \mathbf{E} - \frac{1}{4} (\vartheta^2 - 1) \operatorname{tr} \mathbf{T}. \quad (79)$$

The partial differentiation then gives

$$\left(\frac{\partial \psi_e}{\partial \theta} \right)_{\mathbf{E}} = -\frac{1}{2\theta} \ell_E : \mathbf{E} + \frac{1}{4\theta} (\vartheta^2 - 1) \operatorname{tr} \ell_E - \frac{1}{2\rho_0} \vartheta^2 \alpha \operatorname{tr} \mathbf{T}, \quad (80)$$

which recovers Eq. (78) via $\eta = -(\partial\psi/\partial\theta)_E$.

The latent heat ℓ_E can be calculated from Eq. (72) as

$$\ell_E = -\frac{1}{\rho_0} \theta \left(\frac{\partial \mathbf{T}}{\partial \theta} \right)_{\mathbf{E}} = -\frac{1}{\rho_0} \theta \left[\vartheta \left(\frac{\partial \mathbf{T}_e}{\partial \theta} \right)_{\mathbf{E}_e} - \alpha (\mathbf{T} + 3 \vartheta \kappa \mathbf{I}) \right]. \quad (81)$$

The substitution of Eq. (70) with Eq. (44) gives

$$\ell_E = \frac{1}{\rho_0} \theta \left\{ \alpha (\mathbf{T} + 3 \vartheta \kappa \mathbf{I}) - \frac{1}{\vartheta} \frac{d\mathbf{\Lambda}_e}{d\theta} : \left[\mathbf{E} - \frac{1}{2} (\vartheta^2 - 1) \mathbf{I} \right] \right\}. \quad (82)$$

If elastic moduli are independent of temperature, and the components of the stress \mathbf{T} are much smaller than the bulk modulus κ , above reduces to

$$\boldsymbol{\ell}_E = \frac{3}{\rho_0} \vartheta \alpha \theta \kappa \mathbf{I}, \quad (83)$$

while the entropy expression (78) becomes

$$\eta = \frac{3}{\rho_0} \vartheta \alpha \kappa \left[\text{tr} \mathbf{E} - \frac{3}{2} (\vartheta^2 - 1) \right] - \frac{d\psi_\theta}{d\theta}. \quad (84)$$

The function ψ_θ can be constructed to fit experimental data for the specific heat c_E . For example, if

$$\psi_\theta = -\frac{1}{2} \left(\frac{c_E^0}{\theta_0} + \frac{9}{\rho_0} \alpha_0^2 \kappa_0 \right) (\theta - \theta_0)^2, \quad (85)$$

equation (84) reduces to

$$\begin{aligned} \eta &= \frac{1}{\rho_0} \alpha_0 \text{tr} \mathbf{T} + \left(\frac{c_E^0}{\theta_0} + \frac{9}{\rho_0} \alpha_0^2 \kappa_0 \right) (\theta - \theta_0) \\ &= \frac{3}{\rho_0} \alpha_0 \kappa_0 \text{tr} \mathbf{E} + \frac{c_E^0}{\theta_0} (\theta - \theta_0), \end{aligned} \quad (86)$$

in agreement with Eq. (35).

3.4 Relationships between latent heats and related expressions

As recognized from the previous analysis, the specific entropy can be expressed as either of the two functions

$$\eta = \hat{\eta}(\mathbf{E}, \theta) = \bar{\eta}(\mathbf{E}_e, \theta). \quad (87)$$

Consequently,

$$\theta d\eta = \boldsymbol{\ell}_E : d\mathbf{E} + c_E d\theta = \boldsymbol{\ell}_{E_e} : d\mathbf{E}_e + c_{E_e} d\theta. \quad (88)$$

The two tensors of latent heats are here

$$\boldsymbol{\ell}_E = \theta \frac{\partial \hat{\eta}}{\partial \mathbf{E}}, \quad \boldsymbol{\ell}_{E_e} = \theta \frac{\partial \bar{\eta}}{\partial \mathbf{E}_e}, \quad (89)$$

while the two specific heats are

$$c_E = \theta \frac{\partial \hat{\eta}}{\partial \theta}, \quad c_{E_e} = \theta \frac{\partial \bar{\eta}}{\partial \theta}. \quad (90)$$

For example, the specific heat at constant elastic strain c_{E_e} represents the heat amount required to increase the temperature of the unit mass by $d\theta$ at the constant elastic strain ($d\mathbf{E}_e = \mathbf{0}$). The latent heat ℓ_{E_e} is the second-order tensor whose ij component represents the heat amount associated with a change of the corresponding strain component by dE_{ij}^e , at fixed temperature and fixed values of the remaining five elastic strain components. Similar interpretations hold for c_E and ℓ_E . It readily follows that

$$\ell_{E_e} = \vartheta^2 \ell_E, \quad (91)$$

$$c_{E_e} = c_E + \alpha \ell_E : (\mathbf{I} + 2\mathbf{E}). \quad (92)$$

It is noted that

$$\ell_E : (\mathbf{I} + 2\mathbf{E}) = \ell_{E_e} : (\mathbf{I} + 2\mathbf{E}_e). \quad (93)$$

Furthermore, one can show that

$$\left(\frac{\partial \bar{\eta}}{\partial \mathbf{E}_e} \right)_\theta = \frac{\alpha}{\rho_\theta} (3\kappa \mathbf{I} + 4\mathbf{T}_e) - \frac{\partial^2 \psi_e}{\partial \mathbf{E}_e \partial \theta}, \quad (94)$$

and

$$\left(\frac{\partial \mathbf{T}_e}{\partial \theta} \right)_{\mathbf{E}_e} = -3\alpha \mathbf{T}_e + \rho_\theta \frac{\partial^2 \psi_e}{\partial \mathbf{E}_e \partial \theta}. \quad (95)$$

Therefore, there is a relationship

$$\rho_\theta \ell_{E_e} = \alpha \theta (3\kappa \mathbf{I} + \mathbf{T}_e) - \theta \left(\frac{\partial \mathbf{T}_e}{\partial \theta} \right)_{\mathbf{E}_e}. \quad (96)$$

This should be compared with the classical expression

$$\rho_0 \ell_E = -\theta \left(\frac{\partial \mathbf{T}}{\partial \theta} \right)_{\mathbf{E}}. \quad (97)$$

The transition between the two expressions is straightforward by using Eq. (72).

4 Conclusion

Based on the multiplicative decomposition of thermoelastic deformation gradient into its elastic and thermal parts, we proposed the Helmholtz free energy representation according to Eq. (52). This yields the expression (58) for the stress response and the expression (56) for the entropy. In the case of the quadratic dependence of the elastic strain energy on finite elastic strain (60), the stress and entropy expressions are given by Eqs. (63) and (78). The corresponding latent heat at constant strain is given by Eq. (82). The latent and specific heats at constant elastic and total strain are related by Eqs. (91) and (92). The derived results appear to be attractive for the application because of their simplicity and the suitability for the direct incorporation of the experimental data regarding the temperature dependence of the elastic moduli, thermal expansion, and specific heats. An extension of the theory to anisotropic and composite materials with more involved representations of the elastic strain energy is also possible and worthwhile further research (see Mićunović [22]). A continuation of the study of thermoelastic polar materials within the framework of the multiplicative decomposition, initiated by Stojanović *et al.* [3–6], is another important objective, particularly in view of the recently revived interest in the non-local theories of elastic and inelastic material behavior (e.g., Aifantis [23], Bardenhagen and Triantafyllidis [24], Fleck and Hutchinson [25]).

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Termoelastičnost konačnih deformacija zasnovana na multiplikativnoj dekompoziciji deformacionog gradijenta

UDK 531.01, 536.76

Konstitutivna formulacija termoelastičnosti konačnih deformacija je revidirana unutar termodinamičkog pogleda i multiplikativne dekompozicije deformacionog gradijenta u njegov elastični and termički deo. Jedna sugestivna struktura Helmholtzove slobodne energije je zatim predložena. Odgovarajući izrazi za naponski dgovor i entropiju su izvedeni. Rezultati se ograničavaju na slučaj kvadratne zavisnosti slobodne energije od konačne elastične deformacije. Diskutuju se specifična i latentna toplota i daju uporedjenja sa klasičnom termoelastičnošću.