

Hypertemperature in thermoelastic solids

Samuel Forest *, Michel Amestoy

Mines Paris, ParisTech, Centre des Matériaux / CNRS UMR 7633, BP 87, 91003 Evry cedex, France

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Abstract

The classical thermomechanics of solids is extended to incorporate a non-trivial dependence of the internal energy density function on the gradient of entropy. A generalized heat equation is derived for rigid heat conductors. The theory is shown to differ from existing models including gradient of temperature effects in the free energy. *To cite this article: S. Forest, M. Amestoy, C. R. Mecanique 336 (2008).*

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Résumé

Hypertempérature en thermomécanique des solides élastiques. Une extension de la thermomécanique classique des milieux continus est proposée afin d'incorporer des effets de gradient d'entropie dans la fonction densité d'énergie interne. On en déduit une équation de la chaleur généralisée pour les conducteurs rigides. La théorie proposée s'avère distincte d'une formulation basée sur l'introduction du gradient de température dans la densité d'énergie libre du milieu. *Pour citer cet article : S. Forest, M. Amestoy, C. R. Mecanique 336 (2008).*

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1. Introduction

In the theory of thermoelastic solids as settled in the works [1,2], it is well known that the free energy density ψ is a function $\hat{\psi}(\mathbf{F}, T)$ of the deformation gradient \mathbf{F} and temperature only and cannot depend on the temperature gradient. The state laws derived in this context are:

$$\eta = -\frac{\partial \hat{\psi}}{\partial T}, \quad \frac{\partial \hat{\psi}}{\partial \nabla T} = 0 \quad (1)$$

* Corresponding author.

E-mail address: samuel.forest@ensmp.fr (S. Forest).

Table 1
Set of variables involved in the description of mass transport and heat propagation

theory	thermodynamical force	phenomenological equations	flux vector	variable in balance equation
mass diffusion	chemical potential gradient $-\nabla\left(\frac{\mu}{T}\right)$	generalized Fick's law	mass flux \underline{J}	change in mass concentration \dot{c}
heat conduction	temperature gradient $-\nabla\left(\frac{1}{T}\right)$	Fourier's law	heat flux \underline{q}	change in entropy $\dot{\eta}$

where η is the entropy density variable. However, in the presence of varying temperature fields at the microstructure level, temperature gradient effects on the thermomechanical response of the material are expected due to the micro-heterogeneous nature of materials. Motivations for the introduction of such temperature gradient effects stem from higher order terms in the kinetic theory of gas [3,4] and from homogenization theory based on multiscale asymptotic expansions [5,6].

This justifies the need for the development of a phenomenological theory of temperature gradient effects in thermoelastic solids, as proposed in [7–10]. In these references, the Helmholtz free energy density ψ is a function $\hat{\psi}(\underline{F}, T, \nabla T)$ of the deformation gradient, temperature and temperature gradient at the material point. In [9], the classical relation between the internal energy and the free energy is modified to include the partial derivative of the free energy with respect to the temperature gradient. In contrast, in [7,6,10], the existence of additional scalar and vector generalized stresses a_T and \underline{b}_T was postulated, leading to the following generalized state laws:

$$\rho\eta = -\rho\frac{\partial\hat{\psi}}{\partial T} + a_T, \quad \underline{b}_T = \rho\frac{\partial\hat{\psi}}{\partial\nabla T} \quad (2)$$

where ρ is the mass density. The procedure adopted in these works relies on the introduction of an additional balance equation complementing the balance of linear momentum equation, as proposed in [11] for gradient of damage and in [12] for diffusion and phase field theories, where the additional balance equation is called balance of microforces.

Since temperature and entropy are dual quantities in the classical theory of thermoelastic solids, it is equally legitimate to raise the question of entropy gradient effects in thermoelasticity. In the present work, we investigate a non-trivial dependence of the internal energy function $\epsilon = \hat{\epsilon}(\underline{F}, \eta, \nabla\eta)$ on deformation gradient, entropy and entropy gradient, which can arise in the presence of an additional balance equation accounting for microstructure effects. In classical thermoelasticity, the role of entropy and temperature can be interchanged, by means of the usual Legendre transform of the relevant potential function. In contrast, in gradient theories, the choice of the primal variable is crucial. Because of the spatial derivation, it is obvious that two theories involving $\nabla\eta$ or ∇T cannot be equivalent. Reasons for preferring the enhancement of the set of state variables to the entropy gradient rather temperature gradient, are based on the analogy between heat transfer and mass transport theories, shown in Table 1. Gradients of the potential variables induce fluxes entering the mass or energy balance equations. In diffusion theory, the gradient of the chemical potential μ induces a mass flux \underline{J} which in turn implies a change in concentration \dot{c} . In the generalized diffusion theory of [12], this change in concentration \dot{c} is associated with microforces the power of which is represented by a linear functional in \dot{c} (but not in $\dot{\mu}$). In the thermal problem, the gradient of temperature induces a heat flux \underline{q} which, in turn, leads to an evolution $\dot{\eta}$ in the balance of energy equation. The proposed gradient of entropy theory will assume the existence of microforces described by a power functional in $\dot{\eta}$, and fulfilling their own balance of momentum equation. Accordingly, a strong analogy will be found between the proposed gradient of entropy theory and the generalized diffusion model of Cahn–Hilliard [13,12].

Incentives from the literature for introducing entropy gradient effects are far less numerous than for temperature gradients. One may mention Ref. [14] which deals with interface layers in mixtures of fluids.

The gradient of entropy theory is explored in Section 2. In the case of heat conduction in rigid bodies, a generalized heat equation is derived in Section 3. The gradient of entropy theory is compared to the gradient of temperature model in Section 4.

Throughout this work, a , \underline{a} , $\underline{\underline{A}}$ denote zeroth, first and second order tensors. The nabla operator ∇ refers to partial derivation with respect to current spatial coordinates.

2. Gradient of entropy theory

In continuum thermomechanics after [1], a thermodynamic process is characterized by the evolution of the following field quantities defined on the body:

- the deformation $\underline{\mathbf{x}} = \Phi(\underline{\mathbf{X}}, t)$ gives the current position of material point $\underline{\mathbf{X}} \in \Omega_0$, Ω_0 being a reference configuration of the body; the corresponding Eulerian velocity field is denoted by $\underline{\mathbf{v}}(\underline{\mathbf{x}}, t)$; the current mass density is $\rho(\underline{\mathbf{x}}, t)$; the deformation gradient and the velocity gradient are:

$$\underline{\mathbf{F}} = \frac{\partial \Phi}{\partial \underline{\mathbf{X}}}, \quad \underline{\mathbf{L}} = \dot{\underline{\mathbf{F}}} \cdot \underline{\mathbf{F}}^{-1} = \nabla \underline{\mathbf{v}} \quad (3)$$

- the traction vector $\underline{\mathbf{t}}(\underline{\mathbf{x}}, t)$ at a surface point of the boundary of any subdomain of the body; the body force per unit mass $\underline{\mathbf{f}}(\underline{\mathbf{x}}, t)$;
- the (symmetric) Cauchy stress tensor $\underline{\underline{\sigma}}(\underline{\mathbf{x}}, t)$;
- the specific internal energy $\epsilon(\underline{\mathbf{x}}, t)$, the specific entropy $\eta(\underline{\mathbf{x}}, t)$ and local temperature $T(\underline{\mathbf{x}}, t)$;
- the heat flux vector $\underline{\mathbf{q}}(\underline{\mathbf{x}}, t)$, the heat supply $r(\underline{\mathbf{x}}, t)$ per unit mass and time.

A fundamental distinction is made between universal balance laws and material-dependent constitutive equations.

2.1. Balance equations

The balance of linear momentum for a continuous body is written in the form of the principle of virtual power [15]. The sum of the virtual power of internal, external and acceleration forces acting on any material subdomain $\mathcal{D} \subset \Omega$ in any virtual vector field $\underline{\mathbf{v}}^*$ vanishes at each instant t of the evolution:

$$\mathcal{P}^{(i)}(\underline{\mathbf{v}}^*) + \mathcal{P}^{(e)}(\underline{\mathbf{v}}^*) = \mathcal{P}^{(a)}(\underline{\mathbf{v}}^*), \quad \forall \mathcal{D} \subset \Omega, \quad \forall \underline{\mathbf{v}}^* \quad (4)$$

$$\mathcal{P}^{(i)}(\underline{\mathbf{v}}^*) = - \int_{\mathcal{D}} \underline{\underline{\sigma}} : \underline{\mathbf{L}}(\underline{\mathbf{v}}^*) \, dV \quad (5)$$

$$\mathcal{P}^{(e)}(\underline{\mathbf{v}}^*) = \int_{\mathcal{D}} \rho \underline{\mathbf{f}} \cdot \underline{\mathbf{v}}^* \, dV + \int_{\partial \mathcal{D}} \underline{\mathbf{t}} \cdot \underline{\mathbf{v}}^* \, dS, \quad \mathcal{P}^{(a)}(\underline{\mathbf{v}}^*) = \int_{\mathcal{D}} \rho \dot{\underline{\mathbf{v}}} \cdot \underline{\mathbf{v}}^* \, dV \quad (6)$$

The exploitation of the method of virtual power leads to the classical field equation $\text{div } \underline{\underline{\sigma}} + \rho \underline{\mathbf{f}} = \rho \dot{\underline{\mathbf{v}}}$ and the boundary condition $\underline{\mathbf{t}} = \underline{\underline{\sigma}} \cdot \underline{\mathbf{n}}$, $\underline{\mathbf{n}}$ being the unit outer normal vector. The mentioned symmetry of the Cauchy stress tensor already takes full account of the balance of moment of momentum, in the absence of volume couples.

In the present Note, we postulate that additional contributions to the power of internal and external forces exist, in the form:

$$\mathcal{P}_{\chi}^{(i)}(\dot{\eta}^*) = - \int_{\mathcal{D}} (a_{\eta} \dot{\eta}^* + \underline{\mathbf{b}}_{\eta} \cdot \nabla \dot{\eta}^*) \, dV, \quad \mathcal{P}_{\chi}^{(e)}(\dot{\eta}^*) = \int_{\mathcal{D}} (a_{\eta}^p \dot{\eta}^* + \underline{\mathbf{b}}_{\eta}^p \cdot \nabla \dot{\eta}^*) \, dV + \int_{\partial \mathcal{D}} a_{\eta}^c \dot{\eta}^* \, dS \quad (7)$$

in addition to the purely mechanical parts (5) and (6), where $\dot{\eta}^*$ is a field of virtual rate of change of entropy density. These power densities involve internal scalar and vector microstresses a_{η} , $\underline{\mathbf{b}}_{\eta}$, on the one hand, and prescribed external scalar and vector volume microforces a_{η}^p , $\underline{\mathbf{b}}_{\eta}^p$ and a surface microtraction a_{η}^c , on the other hand. Such additional contributions to mechanical power have been proposed for internal variables in [16,17,10], damage variables in [11], atomic concentration and order parameters in [12], and temperature itself in [7]. The index χ indicates the microheterogeneous origin and size-dependent nature of the phenomena to be accounted for.

The exploitation of the principle of virtual power with respect to the virtual field $\dot{\eta}^*$ results in the following independent variational equation:

$$\mathcal{P}_{\chi}^{(i)}(\dot{\eta}^*) + \mathcal{P}_{\chi}^{(e)}(\dot{\eta}^*) = 0, \quad \forall \mathcal{D} \subset \Omega, \quad \forall \dot{\eta}^* \quad (8)$$

provided that no microinertia effects are attached to variable η [18]. It is used to derive a balance equation associated with variable η in addition to the balance of momentum equation, and the associated boundary condition:

$$\operatorname{div}(\underline{\mathbf{b}}_\eta - \underline{\mathbf{b}}_\eta^p) - a_\eta + a_\eta^p = 0, \quad \forall \underline{\mathbf{x}} \in \mathcal{D}, \quad a_\eta^c = (\underline{\mathbf{b}}_\eta - \underline{\mathbf{b}}_\eta^p) \cdot \underline{\mathbf{n}}, \quad \forall \underline{\mathbf{x}} \in \partial \mathcal{D} \quad (9)$$

This balance equation is similar to Gurtin's microforce balance in [12], with a slight extension represented by the introduction of a possible prescribed volume microforce vector $\underline{\mathbf{b}}_\eta^p$.

It is essential that the power of external forces $(7)_2$ contributes to the global balance of energy:

$$\dot{\mathcal{E}} + \mathcal{P}^{(a)}(\underline{\mathbf{v}}) = \int_{\mathcal{D}} \rho \dot{\epsilon} \, dV + \mathcal{P}^{(a)}(\underline{\mathbf{v}}) = \mathcal{P}^{(e)}(\underline{\mathbf{v}}) + \mathcal{P}_\chi^{(e)}(\dot{\eta}) - \int_{\partial \mathcal{D}} \underline{\mathbf{q}} \cdot \underline{\mathbf{n}} \, dS + \int_{\mathcal{D}} \rho r \, dV \quad (10)$$

An alternative form is obtained after taking the generalized principle of virtual power into account:

$$\dot{\mathcal{E}} = -\mathcal{P}^{(i)}(\underline{\mathbf{v}}) - \mathcal{P}_\chi^{(i)}(\dot{\eta}) - \int_{\partial \mathcal{D}} \underline{\mathbf{q}} \cdot \underline{\mathbf{n}} \, dS + \int_{\mathcal{D}} \rho r \, dV \quad (11)$$

The local form of energy balance follows:

$$\rho \dot{\epsilon} = \underline{\boldsymbol{\sigma}} : \underline{\mathbf{L}} + a_\eta \dot{\eta} + \underline{\mathbf{b}}_\eta \cdot \nabla \dot{\eta} - \operatorname{div} \underline{\mathbf{q}} + \rho r \quad (12)$$

The entropy principle is assumed to keep its classical global form, for any material subdomain $\mathcal{D} \subset \Omega$:

$$\frac{d}{dt} \int_{\mathcal{D}} \rho \eta \, dV \geq - \int_{\partial \mathcal{D}} \frac{\underline{\mathbf{q}}}{T} \, dS + \int_{\mathcal{D}} \rho \frac{r}{T} \, dV \quad (13)$$

The additional contributions appear in the generalized Clausius–Duhem inequality:

$$\rho (T \dot{\eta} - \dot{\epsilon}) + \underline{\boldsymbol{\sigma}} : \underline{\mathbf{L}} + a_\eta \dot{\eta} + \underline{\mathbf{b}}_\eta \cdot \nabla \dot{\eta} - \frac{\underline{\mathbf{q}}}{T} \cdot \nabla T \geq 0 \quad (14)$$

2.2. Constitutive equations

The constitutive functions of such thermoelastic solids depend on the set of state variables $(\underline{\mathbf{F}}, \eta, \nabla \eta)$:

$$\epsilon = \hat{\epsilon}(\underline{\mathbf{F}}, \eta, \nabla \eta), \quad \underline{\boldsymbol{\sigma}} = \hat{\boldsymbol{\sigma}}(\underline{\mathbf{F}}, \eta, \nabla \eta), \quad T = \hat{T}(\underline{\mathbf{F}}, \eta, \nabla \eta), \quad \underline{\mathbf{q}} = \hat{\underline{\mathbf{q}}}(\underline{\mathbf{F}}, \eta, \nabla \eta) \quad (15)$$

complemented by two additional generalized stress functions:

$$a_\eta = \hat{a}_\eta(\underline{\mathbf{F}}, \eta, \nabla \eta), \quad \underline{\mathbf{b}}_\eta = \hat{\underline{\mathbf{b}}}_\eta(\underline{\mathbf{F}}, \eta, \nabla \eta) \quad (16)$$

After inserting these constitutive relationships, the Clausius–Duhem inequality (14) becomes:

$$\rho \left(T - \frac{\partial \hat{\epsilon}}{\partial \eta} + \frac{a_\eta}{\rho} \right) \dot{\eta} + \left(\underline{\boldsymbol{\sigma}} \cdot \underline{\mathbf{F}}^{-T} - \rho \frac{\partial \hat{\epsilon}}{\partial \underline{\mathbf{F}}} \right) : \underline{\dot{\mathbf{F}}} + \left(\underline{\mathbf{b}}_\eta - \rho \frac{\partial \hat{\epsilon}}{\partial \nabla \eta} \right) \cdot \nabla \dot{\eta} - \frac{\underline{\mathbf{q}}}{T} \cdot \nabla T \geq 0 \quad (17)$$

from which the state laws are derived, based on the Coleman–Noll arguments:¹

$$\underline{\boldsymbol{\sigma}} = \rho \frac{\partial \hat{\epsilon}}{\partial \underline{\mathbf{F}}} \cdot \underline{\mathbf{F}}^T, \quad T = \frac{\partial \hat{\epsilon}}{\partial \eta} - \frac{a_\eta}{\rho}, \quad \underline{\mathbf{b}}_\eta = \rho \frac{\partial \hat{\epsilon}}{\partial \nabla \eta} \quad (18)$$

Accordingly, the temperature is found to be equal to the partial derivative of the internal energy function with respect to entropy complemented by a contribution of the internal scalar microstress a_η . The internal microstress vector $\underline{\mathbf{b}}_\eta$ is nothing but the partial derivative of internal energy with respect to the entropy gradient. It is called the hypertemperature vector. The residual dissipation reduces to the thermal part:

$$-\frac{\underline{\mathbf{q}}}{T} \cdot \nabla T \geq 0 \quad (19)$$

¹ The Coleman–Noll procedure is not systematically used in the literature. For some authors that do not use it, the state laws (18) are simply postulated.

3. Impact on heat equation

First consequences of the additional or modified state laws established previously are investigated in the simplest case, namely that of the rigid heat conductor. After inserting the state laws (18) in the local energy balance (12), the following usual form of the heat equation is recovered:

$$\rho T \dot{\eta} = -\operatorname{div} \underline{\mathbf{q}} + \rho r \quad (20)$$

In the sequel, a specific constitutive function for internal energy is chosen for the illustration of the modifications brought in the governing equations of thermal conduction by the introduction of entropy gradient effects. A specific constitutive relation will also be needed for the heat flux vector in order to obtain an explicit partial differential equation for entropy. In the present theory, there is no need for departing from the classical Fourier law of heat conduction:

$$\underline{\mathbf{q}} = -\kappa \nabla T \quad (21)$$

written here for isotropic materials for simplicity. Indeed, the thermal dissipation inequality (19) is identically fulfilled when Fourier law (21) is adopted. So in the present theory, heat still flows from hot to cold and there is no up-hill heat diffusion.

The explicit heat equation associated with the gradient of entropy theory is now derived within the framework of small perturbations for isotropic materials. We take $r = 0$, $a_\eta^p = 0$ and $\underline{\mathbf{b}}_\eta^p = 0$ for the sake of brevity. Material homogeneity is also assumed for simplicity. The mass density ρ is constant and homogeneous.

The expression of the internal energy density function in a rigid heat conducting body is linearized around the reference entropy value η_0 . According to the gradient of entropy model, it contains quadratic terms in the entropy and entropy gradient:

$$\rho \hat{\epsilon}(\eta, \nabla \eta) = \rho \eta T_0 + \frac{\rho^2 (\eta - \eta_0)^2}{4\beta} + \frac{1}{2} A_\eta \nabla \eta \cdot \nabla \eta \quad (22)$$

where β and A_η are (strictly positive) material parameters. The expression of the generalized stresses are derived from the additional state and balance laws:

$$\underline{\mathbf{b}}_\eta = \rho \frac{\partial \hat{\epsilon}}{\partial \nabla \eta} = A_\eta \nabla \eta, \quad a_\eta = \operatorname{div} \underline{\mathbf{b}}_\eta = A_\eta \Delta \eta \quad (23)$$

where Δ is the Laplace operator. Compared to classical linearized thermal diffusion, the temperature function is modified as follows:

$$T = \frac{\partial \hat{\epsilon}}{\partial \eta} - \frac{a_\eta}{\rho} = T_0 + \frac{\rho(\eta - \eta_0)}{2\beta} - \frac{A_\eta}{\rho} \Delta \eta \quad (24)$$

Keeping the usual form (21) of Fourier heat conduction law, the heat equation can now be derived as

$$\rho T_0 \dot{\eta} = \kappa \Delta T = \kappa \left(\frac{\rho}{2\beta} \Delta \eta - \frac{A_\eta}{\rho} \Delta^2 \eta \right) \quad (25)$$

This enhanced heat equation has the structure of the Cahn–Hilliard equation in mass transport theory as derived in [13,12]. It involves a characteristic (positive) length l_η related to material parameters:

$$\rho T_0 \dot{\eta} = \frac{\rho \kappa}{2\beta} (\Delta \eta - l_\eta^2 \Delta^2 \eta), \quad \text{with } l_\eta^2 = \frac{2\beta A_\eta}{\rho^2} \quad (26)$$

The classical heat equation is retrieved for a vanishing intrinsic length scale $l_\eta = 0$, or equivalently $A_\eta = 0$, in the absence of prescribed external microforces. The additional contribution in (26) can account for size effects in heat conduction in microheterogeneous bodies.

4. Status of the gradient of temperature model

Eq. (24) relating temperature and entropy, still in the linear context, can be substituted into the expression of internal energy (22) in order to get the following form of the free energy density:

$$\begin{aligned} \rho \hat{\psi}(T, \nabla T, \Delta \eta) = & \epsilon - T\eta = -\rho(T - T_0)\eta_0 - \beta(T - T_0)^2 + \frac{2A_\eta \beta^2}{\rho^2} \nabla T \cdot \nabla T \\ & + \frac{4A_\eta^2 \beta^2}{\rho^3} \nabla T \cdot \nabla(\Delta \eta) + \frac{\beta A_\eta^2}{\rho^2} (\Delta \eta)^2 + \frac{2\beta^2 A_\eta^3}{\rho^4} \nabla(\Delta \eta) \cdot \nabla(\Delta \eta) \end{aligned} \quad (27)$$

The first line of the previous expression corresponds to the quadratic form expected in a linearized theory of rigid heat conductors incorporating the temperature gradient as a state variable:

$$\rho \hat{\psi}_T(T, \nabla T) = -\rho(T - T_0)\eta_0 - \frac{1}{2} \frac{\rho C_\varepsilon}{T_0} (T - T_0)^2 + \frac{1}{2} A_T \nabla T \cdot \nabla T \quad (28)$$

with $\beta = \rho C_\varepsilon / 2T_0$ as usual, C_ε being the specific heat capacity at constant strain, and adopting the identification relation $A_T T_0^2 = A_\eta C_\varepsilon^2$. This corresponds to the linearized gradient of temperature theory proposed in [6]. As expected, the second line of (27) shows that the gradient of entropy and gradient of temperature theories are not equivalent. They differ by terms involving powers larger than one of the material parameter A_η . Within the relevant framework for which the contribution of A_η in Eq. (22) is sufficiently small, it turns out that the terms involving powers of A_η larger than one in (27) can be neglected. Accordingly, the gradient of temperature model (28) can be regarded as an acceptable approximation of the reference gradient of entropy theory.

The generalized heat equation (25) derived in the gradient of entropy theory can be rewritten in the form:

$$\rho C_\varepsilon \dot{T} = \kappa \Delta T - \frac{A_\eta C_\varepsilon^2}{T_0} \Delta \dot{T} - \frac{A_\eta^2 C_\varepsilon^2}{\rho T_0} \Delta^2 \dot{\eta} \quad (29)$$

Within the already mentioned context of a sufficiently small contribution A_η , the last term proportional to A_η^2 can be neglected, so that the heat equation becomes:

$$\rho C_\varepsilon \dot{T} = \kappa \Delta T - T_0 A_T \Delta \dot{T} \quad (30)$$

This equation is nothing but the heat equation derived from a potential of the form (28). It deviates from the classical heat equation by an additional contribution which is proportional to the Laplacian of the temperature rate of change. It involves a characteristic (positive) time $\tau_T = T_0 A_T / \kappa$.

The derived equation (30) is identical to the first Cattaneo equation as reported in [4]. The derivation of this equation in [4] is based on a modification of Fourier's heat conduction law and does not require a dependence of the energy function on gradient of temperature nor gradient of entropy. In contrast, the classical structure of Fourier's law is preserved in the present approach. In the present work, the first Cattaneo equation can be regarded as an acceptable approximation of (29) derived from the gradient of entropy model.

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