

THE LINEAR THEORY OF THERMOELASTICITY FROM THE VIEWPOINT OF RATIONAL THERMOMECHANICS

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Submitted January 5, 2005; accepted August 11, 2005

Keywords: Linear thermoelasticity, Thermal expansion tensor, Heat conductivity tensor, Specific heats, Isothermal and adiabatic elasticity tensors

Linear thermoelasticity is summarized for materials scientists and engineers from the viewpoint of exact theory (rational thermomechanics). It is developed in referential formulation, using the first Piola-Kirchhoff stress tensor, the referential heat flux, the free energy and the entropy as the material responses for which constitutive equations are given. The deformation gradient, the temperature and the referential temperature gradient are used as independent variables (simple thermoelastic materials). Linear approximations of the series expansions about a natural reference state and thermal equilibrium are invoked to define the elasticity tensor, the stress-temperature tensor, the thermal expansion tensor, the latent heat tensors, the heat conductivity tensor and the specific heats for anisotropic solids. Constitutive equations and linear thermoelastic properties of isotropic solids and fluids are derived as special cases.

INTRODUCTION

Thermoelastic properties are of primary interest in materials science and engineering. Examples are the coefficient of thermal expansion, the heat conductivity and the specific heats. Although experimental papers dealing with these properties are ubiquitous, a more detailed view into the literature reveals that the concept of thermoelastic properties itself and its underlying theoretical framework, linear thermoelasticity, is often not fully understood by materials scientists and engineers. The reason is that the exact treatments of the subject are mostly of a mathematical complexity that makes them unaccessible for a large part of the audience in the materials science and engineering community. On the other hand, many of the apparently general statements on thermoelasticity in basic materials science and engineering textbooks are incomplete or even wrong. There seems to be no up-to-date treatment available that would represent a reasonable compromise between these two extremes. It is the purpose of this paper to fill this gap.

Three objectives were used as guidelines here: First, this treatment should be as brief and concise as possible but should contain in a unified framework all purely thermoelastic properties arising in the linear theory. Second, the number of variables introduced should be kept to a minimum but sufficient to allow for materials of arbitrary symmetry. And third, a pragmatic com-

promise was sought between correctness of the statements and the attempt to explain the physical meaning of these statements in terms familiar to readers without requiring special knowledge in mathematics.

The present paper has grown out of a lecture given by the author for upper-level undergraduates within the Mechanics of Materials course at the ICT Prague since 1997 and exploits a certain feedback experienced through the years from the audience of students. It is based on a number of textbooks, monographs, and original papers of other authors, too many to be cited here, most of them rooted in the tradition of the Truesdell-Noll school of rational thermomechanics. Some of the most important of them, which have been directly used for or consulted during the preparation of this paper, are [1-9]. Among all the texts dealing with thermoelasticity, however, one deserves special mention: Šilhavý's book of 1997 [1]. This book, brilliantly condensing an enormous wealth of results in rational thermomechanics (by far exceeding the scope of thermoelasticity) and written in a concise mathematical style, may be considered as the most outstanding work in the field since Truesdell and Noll's handbook article of 1965 [2]. Although the present paper is meant to serve as an easy-to-grasp and self-contained introduction into the large literature on thermoelasticity in general, it has been tried, wherever possible, to be in accord with Šilhavý's authoritative treatment [1]. Thus, the interested materials scientist and engineer, after having read the present shortcut, will

be in a position to go one step further and to delve into the mathematical details of the theory by studying [1]. For these interested readers' better orientation page numbers have been added to reference [1] wherever cited in the text.

PRELIMINARIES

Mechanics in general deals with motion, while thermomechanics deals with motion and temperature. Continuum mechanics deals with the motion of material bodies, consisting of so-called material particles. The most fundamental function describing motion of material bodies in continuum mechanics is the so-called deformation function (transplacement) χ . This vector function χ uniquely determines the actual position \mathbf{x} of a material particle (in the sense of continuum mechanics) at time t , which has been at a referential position \mathbf{X} (in an arbitrarily chosen reference frame) at an arbitrarily chosen reference time:

$$\mathbf{x} = \chi(\mathbf{X}, t) . \quad (1)$$

For fixed \mathbf{X} (i.e. selecting a certain material particle) χ determines a trajectory, for fixed t (i.e. imaging the whole body at a certain moment) χ determines a configuration (placement). The referential gradient (i.e. the derivative with respect to the referential position) of the deformation function is a second-order tensor, the so-called deformation gradient (transplacement gradient)

$$\mathbf{F} \equiv \text{Grad } \mathbf{x} = \frac{\partial \chi(\mathbf{X}, t)}{\partial \mathbf{X}} . \quad (2)$$

The function χ contains complete information about the motion of a material body (translation, rotation, and change of volume and shape), while the deformation gradient \mathbf{F} is a local measure of motion and contains information only on rotation and change of volume and shape. Materials that can be modelled by using the deformation gradient (2) only (i.e. without invoking deformation gradients of higher order) are called simple materials [2] (materials with local response, i.e. materials for which the principle of local action [2] can be adopted). Obviously, most real materials of engineering interest can be modelled within this class. Note e.g. that a major part of the literature on elasticity (linear as well as non-linear) deals exclusively with simple materials, of course without explicitly emphasizing this fact.

In the theory of linear elasticity it is useful to introduce another vector function, the so-called displacement, via the definition

$$\mathbf{u}(\mathbf{X}, t) \equiv \chi(\mathbf{X}, t) - \mathbf{X} . \quad (3)$$

Using equation (3), the deformation gradient can be written as

$$\mathbf{F} = \text{Grad } \mathbf{x} = \frac{\partial \chi(\mathbf{X}, t)}{\partial \mathbf{X}} = \frac{\partial [\mathbf{X} + \mathbf{u}(\mathbf{X}, t)]}{\partial \mathbf{X}} = \mathbf{1} + \text{Grad } \mathbf{u} , \quad (4)$$

where $\text{Grad } \mathbf{u}$ is the displacement gradient and $\mathbf{1}$ the second-order unit tensor. For practical purposes it is often useful to apply only the change-of-volume-and-shape (i.e. strain) part of the deformation gradient \mathbf{F} . This is possible after eliminating the rotational part of \mathbf{F} via Cauchy's polar decomposition theorem, cf. e.g. [2,10]. The most popular strain measure, frequently applied in theories of nonlinear elasticity, is the Green-Lagrange strain tensor

$$\mathbf{G} \equiv \frac{1}{2} (\text{Grad } \mathbf{u} + \text{Grad } \mathbf{u}^T + \text{Grad } \mathbf{u}^T \text{Grad } \mathbf{u}) , \quad (5)$$

which is a symmetric second-order tensor (in contrast to \mathbf{F} , which is not symmetric in general), appropriate to describe finite (i.e. arbitrarily large) strains. In the theory of linear elasticity the so-called small strain tensor

$$\mathbf{E} \equiv \frac{1}{2} (\text{Grad } \mathbf{u} + \text{Grad } \mathbf{u}^T) . \quad (6)$$

is often used, cf. [10]. In addition to the vector field (1), continuum thermomechanics introduces an additional scalar field, the temperature

$$T = T(\mathbf{X}, t) \quad (7)$$

and its (referential) gradient

$$\text{Grad } T = \frac{\partial T(\mathbf{X}, t)}{\partial \mathbf{X}} . \quad (8)$$

Nonlinear thermoelasticity
in referential description

The material response of a simple thermoelastic material is assumed to depend on (more precisely, to be a function of) the deformation gradient (transplacement gradient) \mathbf{F} , the temperature T and its (referential) gradient $\text{Grad } T$. Invoking Truesdell's equipresence rule [2,3], there is no *a priori* reason to exclude a certain independent variable from any member of the set of constitutive equations. These are therefore as follows:

$$\mathbf{P} = \mathbf{P}(\mathbf{F}, T, \text{Grad } T) , \quad (9)$$

$$\mathbf{h} = \mathbf{h}(\mathbf{F}, T, \text{Grad } T) , \quad (10)$$

$$f = f(\mathbf{F}, T, \text{Grad } T) , \quad (11)$$

$$s = s(\mathbf{F}, T, \text{Grad } T) . \quad (12)$$

In these expressions \mathbf{P} is the first Piola-Kirchhoff stress tensor, \mathbf{h} the referential heat flux vector, $f \equiv u - Ts$ (with specific internal energy u) the specific free energy

(Helmholtz energy) and s the specific entropy. The first Piola-Kirchhoff stress tensor \mathbf{P} is related to the Cauchy stress tensor \mathbf{T} , cf. [10], by

$$\mathbf{P} = |J| \mathbf{T} \mathbf{F}^{-T}. \quad (13)$$

Similarly, the referential heat flux vector \mathbf{h} is related to the spatial (actual) heat flux vector \mathbf{q} via the relation

$$\mathbf{h} = |J| \mathbf{F}^{-1} \mathbf{q}. \quad (14)$$

In these expressions $\mathbf{F}^{-T} = (\mathbf{F}^{-1})^T = (\mathbf{F}^T)^{-1}$ is the transpose of the inverse deformation gradient (or the inverse of the transposed deformation gradient) and J the Jacobian determinant $J \equiv \det \mathbf{F} \neq 0$ (non-singular).

Note that the first Piola-Kirchhoff stress tensor \mathbf{P} is not symmetric, in contrast to the second Piola-Kirchhoff stress tensor \mathbf{S} , cf. [10], which is

$$\mathbf{S} = |J| \mathbf{F}^{-1} \mathbf{T} \mathbf{F}^{-T}. \quad (15)$$

In referential description, where all variables are referential fields, i.e. functions of time t and the referential position \mathbf{X} , the balance laws of rational thermo-mechanics (continuum mechanics and thermodynamics) are as follows (for simplicity only the local or differential forms of the balances, i.e. those valid for uniform bodies, are given here; in the case of non-uniform bodies, of course, global or integral forms have to be used):

1. *Mass balance:*

$$\dot{\rho}_0 = 0, \quad (16)$$

where $\rho_0 = \rho |J|$ is the referential density and ρ the actual density of the material.

2. *Linear momentum balance:*

$$\rho_0 \dot{\mathbf{v}} = \text{Div } \mathbf{P} + \rho_0 \mathbf{b}, \quad (17)$$

where Div is the referential divergence operator $\text{Div } \mathbf{P} \equiv \text{tr}(\text{Grad } \mathbf{P})$, where tr denotes the trace, a superimposed dot ($\dot{\mathbf{v}}$) a material (or substantial) time derivative, \mathbf{v} the velocity and \mathbf{b} the specific body force.

3. *Angular momentum balance:*

$$\mathbf{P} \mathbf{F}^T = \mathbf{F} \mathbf{P}^T. \quad (18)$$

Note that for the second Piola-Kirchhoff stress tensors the angular momentum balance reduces to the symmetry statement

$$\mathbf{S} = \mathbf{S}^T, \quad (19)$$

while the linear momentum balance adopts the more complicated form

$$\rho_0 \dot{\mathbf{v}} = \text{Div}(\mathbf{S} \mathbf{F}^T) + \rho_0 \mathbf{b}. \quad (20)$$

Because of its symmetry, the second Piola-Kirchhoff stress tensor is more adequate to develop constitutive theories of non-linear elasticity or thermoelasticity. Nevertheless, in cases where the *linear* theory is aimed at, the first Piola-Kirchhoff stress tensor is equally convenient. The advantage of the latter (being the natural variable complementary to $\dot{\mathbf{F}}$ in the energy balance, see below) is, that the application of the Coleman-Noll approach (see below) is more convenient.

4. *Energy balance:*

$$\rho_0 \dot{u} = \mathbf{P} \cdot \dot{\mathbf{F}} - \text{Div } \mathbf{h} + \rho_0 Q, \quad (21)$$

where u is the specific internal energy, Q the specific heat supply and the inner product $\mathbf{P} \cdot \dot{\mathbf{F}} = \text{tr}(\mathbf{P} \dot{\mathbf{F}})$ is a scalar quantity describing the dissipation of mechanical energy. In thermoelastic materials without viscosity, i.e. in the absence of memory effects, this latter part of dissipation is usually weak (it is present only in shock waves or moving phase boundaries, cf. [1], p. 152).

5. *Entropy inequality (Clausius-Duhem inequality):*

$$\rho_0 \dot{s} \geq -\text{Div} \frac{\mathbf{h}}{T} + \rho_0 \frac{Q}{T}, \quad (22)$$

where s is the specific entropy.

In the following we exploit a combination of the energy balance (first law of thermodynamics) and the entropy balance (second law of thermodynamics), the so-called dissipation inequality, cf. [1], p. 77:

$$\rho_0 (\dot{f} + s \dot{T}) - \mathbf{P} \cdot \dot{\mathbf{F}} + \frac{\mathbf{h}}{T} \cdot \text{Grad } T \leq 0. \quad (23)$$

According to Coleman and Noll's interpretation of the second law of thermodynamics [4] we now insert the material time derivative (i.e. a special case of what has been called "total differential" in traditional thermodynamics) of the free energy f ,

$$\dot{f} = \left(\frac{\partial f}{\partial \mathbf{F}} \right) \cdot \dot{\mathbf{F}} + \left(\frac{\partial f}{\partial T} \right) \cdot \dot{T} + \left(\frac{\partial f}{\partial \text{Grad } T} \right) \cdot \overbrace{\text{Grad } T}^{\dot{\text{Grad}} T}, \quad (24)$$

with $\overbrace{\text{Grad } T}^{\dot{\text{Grad}} T}$ being the material time derivative of the referential temperature gradient, into the dissipation inequality:

$$\rho_0 \left(s + \frac{\partial f}{\partial T} \right) \cdot \dot{T} - \left[\mathbf{P} - \rho_0 \left(\frac{\partial f}{\partial \mathbf{F}} \right) \right] \cdot \dot{\mathbf{F}} - \rho_0 \left(\frac{\partial f}{\partial \text{Grad } T} \right) \cdot \overbrace{\text{Grad } T}^{\dot{\text{Grad}} T} + \frac{\mathbf{h}}{T} \cdot \text{Grad } T \leq 0. \quad (25)$$

This inequality must be valid for arbitrary thermo-mechanical processes, i.e. for arbitrary values of all time rates, i.e. $\dot{\mathbf{F}}$, \dot{T} and $\dot{\text{Grad}} T$. This corresponds to the Coleman-Noll interpretation of the second law which states roughly that the constitutive equations must be

such that the entropy inequality (22) is satisfied in all thermomechanical processes or more precisely, in every smooth admissible process (it is evident that $A=B=C=0$ and $D \geq 0$ must hold if the inequality $Ax+By+Cz+D \geq 0$ is to hold for arbitrary values of x, y, z ; for a more precise formulation of this statement cf. [4]).

There are three direct consequences of this application of the dissipation inequality:

First result - *Thermostatic relations*:

$$\mathbf{P} = \rho_0 \left(\frac{\partial f}{\partial \mathbf{F}} \right), \quad s = -\frac{\partial f}{\partial T}, \quad \frac{\partial f}{\partial \text{Grad } T} = \mathbf{0}. \quad (26 \text{ a,b,c})$$

Second result - *Gibbs equations*:

$$\rho_0 \dot{f} = \mathbf{P} \cdot \dot{\mathbf{F}} - \rho_0 s \dot{T}, \quad \rho_0 T \dot{s} = \rho_0 \dot{u} - \mathbf{P} \cdot \dot{\mathbf{F}}. \quad (27 \text{ a,b})$$

Third result - *Heat conduction inequality (Fourier's inequality)*:

$$\frac{\mathbf{h}}{T} \cdot \text{Grad } T \leq 0 \quad \Rightarrow \quad \mathbf{h} \cdot \text{Grad } T \leq 0. \quad (28)$$

Note that in thermoelastic materials (in contrast e.g. to materials with viscosity) \mathbf{P} is always an equilibrium stress, i.e. a stress which is fully determined by the free energy (which can in this sense be called a "potential" from which the stress can be derived) and for which the Gibbs equations are valid. Note also that for other than thermoelastic materials a heat conduction inequality of the form (28) does not necessarily exist. E.g. for materials with heat conduction *and viscosity* the heat conduction inequality (28) must be replaced by the internal dissipation inequality

$$\mathbf{P}_d(\mathbf{F}, \dot{\mathbf{F}}, T, \text{Grad } T) \cdot \dot{\mathbf{F}} - \frac{\mathbf{h}(\mathbf{F}, \dot{\mathbf{F}}, T, \text{Grad } T)}{T} \cdot \text{Grad } T \geq 0, \quad (29)$$

where \mathbf{P}_d is the non-equilibrium (dynamical) part of the stress tensor, cf. [1,2,4].

Since the free energy f is independent of $\text{Grad } T$, cf. equation (26c), and at the same time f is a "potential" for \mathbf{P} and s , also the latter are independent of $\text{Grad } T$. Thus, as a consequence of the dissipation inequality (23), the constitutive equations of thermoelastic materials are

$$\mathbf{P} = \mathbf{P}(\mathbf{F}, T), \quad (30)$$

$$\mathbf{h} = \mathbf{h}(\mathbf{F}, T, \text{Grad } T), \quad (31)$$

$$f = f(\mathbf{F}, T), \quad (32)$$

$$s = s(\mathbf{F}, T). \quad (33)$$

In particular, as a consequence of the Coleman-Noll interpretation of the second law [4], the stress cannot depend on the temperature gradient. Material mod-

els for which, additionally, $\mathbf{h} \equiv \mathbf{0}$, i.e. material models which do not admit heat conduction, may be called "adiabatic materials". They are of importance in dynamical situations (fast processes); for example, in the case of "adiabatic elasticity" only shock waves can be responsible for energy dissipation, cf. [1], p. 152. For adiabatic materials it is common practice to replace the constitutive equation for the free energy f by that of the internal energy u and to use the (specific) entropy s instead of the temperature T as an independent variable, cf. [1], p. 179.

Physical linearization of the constitutive equations

In order to obtain a linear theory of thermoelasticity, we consider the series expansions about a reference state (\mathbf{F}_0, T_0) . The linear approximation of the first Piola-Kirchhoff stress tensor (for small deformation gradients and small temperature differences) is

$$\mathbf{P}(\mathbf{F}, T) = \mathbf{P}_0 + \frac{\partial \mathbf{P}}{\partial \mathbf{F}}(\mathbf{F} - \mathbf{F}_0) + \frac{\partial \mathbf{P}}{\partial T}(T - T_0) + \dots \quad (34)$$

The linear approximation of the heat flux is taken about the thermal equilibrium state with $\text{Grad } T = \mathbf{0}$, i.e. $\mathbf{h}_0 \equiv \mathbf{h}(\mathbf{F}_0, T_0, \mathbf{0})$,

$$\mathbf{h}(\text{Grad } T) \equiv \mathbf{h}(\mathbf{F}_0, T_0, \text{Grad } T) = \mathbf{h}_0 + \frac{\partial \mathbf{h}}{\partial \text{Grad } T} \cdot \text{Grad } T + \dots \quad (35)$$

and the linear approximation of the entropy is a scalar analogue of that of the stress tensor,

$$s(\mathbf{F}, T) = s_0 + \frac{\partial s}{\partial \mathbf{F}}(\mathbf{F} - \mathbf{F}_0) + \frac{\partial s}{\partial T}(T - T_0) + \dots \quad (36)$$

Note that in order to achieve consistency with the thermostatic relations above, equations (26 a,b), the free energy must contain quadratic terms:

$$f(\mathbf{F}, T) = f_0 + \frac{\partial f}{\partial \mathbf{F}}(\mathbf{F} - \mathbf{F}_0) + \frac{\partial f}{\partial T}(T - T_0) + \frac{1}{2}(\mathbf{F} - \mathbf{F}_0)^T \cdot \frac{\partial^2 f}{\partial \mathbf{F}^2} \cdot (\mathbf{F} - \mathbf{F}_0) + \frac{\partial^2 f}{\partial \mathbf{F} \partial T} \cdot (\mathbf{F} - \mathbf{F}_0)(T - T_0) + \frac{1}{2} \frac{\partial^2 f}{\partial T^2} (T - T_0)^2 + \dots \quad (37)$$

Based on these approximations (series expansions), we can now identify the following thermoelastic properties as the coefficients occurring in the linear terms:

1. Elasticity or stiffness tensor (more precisely, the referential tensor of isothermal elasticities):

$$\mathbf{C} \equiv \frac{\partial \mathbf{P}}{\partial \mathbf{F}} = \rho_0 \frac{\partial^2 f}{\partial \mathbf{F}^2}. \quad (38)$$

Note that, with a slight abuse of terminology, we will use \mathbf{C} interchangeably to denote also the spatial and the Cauchy-Hooke tensor of isothermal elasticities

for the purpose of this article, since after introducing the small strain approximation (i.e. the geometric linearization of the kinematic measures) below, this distinction is without concern. Thus, we can assume \mathbf{C} to be a fully symmetric fourth-order tensor. However, the difference between the three types of elasticity tensors plays a role in *nonlinear* thermoelasticity, cf. [1], p. 174. When the (specific) entropy s is used instead of the temperature T as an independent variable, adiabatic (or "isentropic") elasticities $\tilde{\mathbf{C}}$ can be defined in complete analogy to equation (38), cf. [1], pp. 179-180.

2. Stress-temperature tensor (more precisely, the referential stress-temperature tensor, also called thermal coefficient of stress):

$$\mathbf{M} \equiv \frac{\partial \mathbf{P}}{\partial T} = \rho_0 \frac{\partial^2 f}{\partial \mathbf{F} \partial T} . \quad (39)$$

The stress-temperature tensor is intimately connected to the latent heat with respect to deformation \mathbf{L}_F (a symmetric second-order tensor corresponding to the heat that must be supplied to the body to achieve unit relative deformation while maintaining the temperature fixed, cf. [1], p. 180):

$$\mathbf{L}_F = -\frac{T_0}{\rho_0} \mathbf{M} \mathbf{F}^T = -T_0 \frac{\partial^2 f}{\partial \mathbf{F} \partial T} \mathbf{F}^T . \quad (40)$$

Although redundant, the latent heat tensor is sometimes preferred, e.g. in connection with phase transformations. Further, the stress-temperature tensor \mathbf{M} is related to the thermal expansion tensor \mathbf{A} via the relation

$$\mathbf{A} = -\mathbf{C}^{-1} \mathbf{M} , \quad (41)$$

where \mathbf{C}^{-1} is the fourth-order compliance tensor (i.e. the inverse of the stiffness tensor), cf. [11-13]. From the above it is evident that the information contained in the stress-temperature tensor and the latent heat tensor is equivalent to that contained in the thermal expansion tensor. Only one of these quantities is necessary to describe the thermoelastic response of solids. With respect to practical measurability, the thermal expansion tensor turns usually out to be the most convenient one.

3. Heat conductivity tensor (referential heat conductivity tensor):

$$\mathbf{K} \equiv -\frac{\partial \mathbf{h}}{\partial \text{Grad } T} . \quad (42)$$

4. Specific heat at constant deformation (a scalar corresponding to the heat supplied to unit mass of a body in order to achieve a unit temperature change while keeping the deformation constant):

$$c_F \equiv T_0 \frac{\partial s}{\partial T} = -T_0 \frac{\partial^2 f}{\partial T^2} . \quad (43)$$

Note that, although the Clausius-Duhem inequality (22) says nothing about the sign of c_F ([1], p. 181), the positivity of c_F can be derived from the requirement of thermodynamic stability of the body ([1], p. 279).

The stress-temperature tensor (and therefore the latent heat tensor and the thermal expansion tensor as well) is a symmetric tensor of second order. Although the general validity of the Onsager reciprocity relations [14] has been seriously questioned by Truesdell [15], also the heat conductivity tensor is usually assumed to be symmetric. Truesdell has convincingly shown that this is not the case in general. Wang [16], however, has proved that at least for isotropic materials, cubic crystals, orthorhombic crystals and trigonal, tetragonal and hexagonal crystals of classes 32, 3m, $\bar{3}m$, 422, 4mm, $\bar{4}2m$, 4/m mm and 622, 6mm, $\bar{6}m2$, 6/m mm, respectively, the heat conductivity tensor is indeed necessarily symmetric.

Note that the adiabatic elasticities $\tilde{\mathbf{C}}$ are related to the isothermal elasticities via the relation

$$\tilde{\mathbf{C}} = \mathbf{C} + \frac{T}{\rho_0 c_F} \mathbf{M} \otimes \mathbf{M} , \quad (44)$$

where \otimes denotes a tensor product of two second-order tensors, resulting in a fourth-order tensor (cf. [1], p. 180). Similarly, the specific heats at constant stress and constant deformation, respectively, are related via the relations

$$c_T - c_F = \frac{\rho}{T} \mathbf{C} [\mathbf{L}_T, \mathbf{L}_T] , \quad (45)$$

where $\mathbf{C} [\mathbf{L}_T, \mathbf{L}_T]$ is a scalar product of two fourth-order tensors (cf. [1], pp. 28 and 181) and \mathbf{L}_T is the latent heat tensor with respect to stress (i.e. the heat that must be supplied to the body to achieve a unit change of the Cauchy stress while maintaining the temperature fixed), which is related to the latent heat tensor with respect to deformation \mathbf{L}_F by

$$\mathbf{L}_T = \mathbf{C} \mathbf{L}_F . \quad (46)$$

Further, the following relation is valid between the specific heats (cf. [1], p. 181):

$$\frac{c_T}{c_F} = \frac{\det \tilde{\mathbf{C}}}{\det \mathbf{C}} . \quad (47)$$

In terms of specific heats and latent heat tensors the (rate of external specific) heat supply is (cf. [1], p. 180)

$$Q = c_F \dot{T} + \mathbf{L}_F \cdot \mathbf{D} = c_T \dot{T} + \mathbf{L}_T \cdot \dot{\mathbf{T}} . \quad (48)$$

Additional simplifications, usually tacitly adopted in the linear theory of thermoelasticity, are introduced as follows: Obviously, without loss of generality we can

assume zero free energy and zero entropy in the reference state (\mathbf{F}_0, T_0) , i.e.

$$f_0 = 0 \quad (49)$$

and

$$s_0 = 0. \quad (50)$$

Further we assume the reference state to be a natural (preferred) state with zero initial stress (residual stress), i.e. we assume absence of stress when strain is absent (at the reference temperature), i.e.

$$\mathbf{P}_0 = \mathbf{O} \quad \text{if} \quad \mathbf{F}_0 = \mathbf{O}. \quad (51)$$

Finally, it is evident that the heat conduction inequality in the form

$$\mathbf{h}_0 \cdot \text{Grad } T - \text{Grad } T \cdot \mathbf{K} \text{ Grad } T \leq 0 \quad (52)$$

(obtained by inserting the linearized constitutive equation (35), together with definition (42), into equation (28)) is valid for arbitrary temperature gradients $\text{Grad } T$ if and only if

$$\mathbf{h}_0 = \mathbf{0} \quad (53)$$

and

$$\text{Grad } T \cdot \mathbf{K} \text{ Grad } T \geq 0, \quad (54)$$

i.e. firstly, the heat flux vanishes whenever the temperature gradient vanishes and secondly, the heat conductivity tensor is positive semi-definite. The latter is the tensorial counterpart of the statement that the scalar heat conductivity cannot be negative.

Geometric linearization
of the kinematic measures

What has been performed up to now may be called physical linearization of the constitutive equations. For real materials such a linearization is justified for small deviations from the reference state (\mathbf{F}_0, T_0) , i.e. for deformation gradients close to the reference value \mathbf{F}_0 and for small temperature changes $(T - T_0)$. Note that in a consistent linear theory, the material coefficients cannot depend on the actual temperature T but only on the (uniform) reference temperature T_0 . This has to be kept in mind when the temperature dependence of elastic and thermoelastic properties is discussed. The deformation gradient \mathbf{F} itself, however, is a nonlinear deformation measure, similar to the finite strain tensor (Green-Lagrange strain tensor) \mathbf{G} , cf. equations (2) and (5) above. Strains are small when the (referential) displacement gradients $\text{Grad } \mathbf{u}$ are in some sense small compared to the unit tensor $\mathbf{1}$, i.e.

$$\text{Grad } \mathbf{u} \ll \mathbf{1}. \quad (55)$$

Usually this criterion is formalized by stating that its norm (magnitude) is small compared to unity:

$$\sqrt{\text{Grad } \mathbf{u} \cdot (\text{Grad } \mathbf{u})^T} \ll 1 \quad (56)$$

Some of the consequences of this condition are

$$\mathbf{F} \approx \mathbf{1} \quad (57)$$

and

$$|J| \approx 1. \quad (58)$$

Therefore e.g. the referential gradient and divergence (Grad and Div) reduce to the usual spatial gradient and divergence (grad and div) and $\rho_0 = \rho$. Consequently, the Piola-Kirchhoff stress tensors \mathbf{P} and \mathbf{S} coincide with the Cauchy stress tensor \mathbf{T} ,

$$\mathbf{P} \approx \mathbf{S} \approx \mathbf{T}, \quad (59)$$

and the referential heat flux \mathbf{h} with the spatial heat flux \mathbf{q}

$$\mathbf{h} \approx \mathbf{q}. \quad (60)$$

In other words, the difference between referential (Lagrangian) and spatial (Eulerian) description vanishes. Concomitantly with this, the balance equations (16), (17), (18), (21), including the entropy inequality (22), adopt the following more common forms, cited in most textbooks in hydromechanics and undergraduate continuum mechanics:

Mass balance:

$$\dot{\rho} + \rho \text{div } \mathbf{v} = 0. \quad (61)$$

Linear momentum balance:

$$\rho \mathbf{v} = \text{div } \mathbf{T} + \rho \mathbf{b}, \quad (62)$$

where div is the spatial divergence operator $\text{div } \mathbf{T} \equiv \text{tr}(\text{grad } \mathbf{T})$.

Angular momentum balance:

$$\mathbf{T} = \mathbf{T}^T. \quad (63)$$

Energy balance:

$$\rho \dot{u} = \mathbf{T} \cdot \mathbf{D} - \text{div } \mathbf{q} + \rho Q, \quad (64)$$

where the stretching tensor (deformation rate tensor) \mathbf{D} is the symmetric part of the velocity gradient (irrelevant in the absence of viscosity)

$$\mathbf{D} = \frac{1}{2}(\text{grad } \mathbf{v} + \text{grad } \mathbf{v}^T). \quad (65)$$

Entropy inequality (Clausius-Duhem inequality):

$$\rho s \geq -\text{div } \frac{\mathbf{q}}{T} + \rho \frac{Q}{T}. \quad (66)$$

In the geometrically linearized theory of thermoelasticity the small strain tensor

$$\mathbf{E} \equiv \frac{1}{2}(\text{grad } \mathbf{u} + \text{grad } \mathbf{u}^T) \quad (67)$$

is used as a measure of deformation, cf. equation (6). Before we now proceed to formulate the physically and geometrically linearized theory of thermoelasticity, which corresponds rather closely to more traditional treatments (e.g. [17]) and should serve as a guide for the reader to easily recognize the analogies to classical thermodynamics, we would like to emphasize at this point the approximate character of the above expressions, equations (57) through (60), and all constitutive equations which follow below. A theory for which these approximate expressions would be exact is inconsistent - it violates the Clausius-Duhem inequality, cf. [1], p. 183. For the exact treatment of the completely linearized theory the reader should consult Šilhavý's book [1], especially pp. 461-465 and 474-477.

Linear thermoelasticity of anisotropic solids

Within the completely (i.e. physically and geometrically) linearized theory the constitutive equation for the stress tensor can be written in the form of a generalized Hooke's law, extended to include thermal effects:

$$\mathbf{T} = \mathbf{C} \mathbf{E} + \mathbf{M} (T - T_0) . \quad (68)$$

Evidently, the stress-temperature tensor \mathbf{M} gives the stress resulting from a given temperature distribution when the strain vanishes, i.e.

$$\mathbf{T} = \mathbf{M} (T - T_0) , \quad (69)$$

when $\mathbf{E} = \mathbf{O}$. For invertible elasticity or stiffness tensors \mathbf{C} (with \mathbf{C}^{-1} being the compliance tensor) the strain tensor can be expressed in terms of the stress tensor as

$$\mathbf{E} = \mathbf{C}^{-1} \mathbf{T} + \mathbf{A} (T - T_0) , \quad (70)$$

where $\mathbf{A} = \mathbf{C}^{-1} \mathbf{M}$ is the thermal expansion tensor, cf. equation (41), which gives the strain resulting from a given temperature distribution when the stress vanishes, i.e.

$$\mathbf{E} = \mathbf{A} (T - T_0) , \quad (71)$$

when $\mathbf{T} = \mathbf{O}$. The constitutive equation for the heat flux vector (Fourier's law) is

$$\mathbf{q} = -\mathbf{K} \text{grad } T , \quad (72)$$

where \mathbf{K} is the heat conductivity tensor. The remaining constitutive equations are

$$s = \frac{c_F}{T_0} (T - T_0) - \frac{1}{\rho} \mathbf{M} \cdot \mathbf{E} \quad (73)$$

for the entropy and

$$f = \frac{1}{2\rho} \mathbf{E}^T \cdot \mathbf{C} \mathbf{E} + \frac{1}{\rho} \mathbf{M} \cdot \mathbf{E} (T - T_0) - \frac{1}{2} \frac{c_F}{T_0} (T - T_0)^2 \quad (74)$$

for the free energy. Since all three second-order property tensors (the stress-temperature tensor \mathbf{M} , the thermal expansion tensor \mathbf{A} and, with the aforementioned reservations, the heat conductivity tensor \mathbf{K}) are symmetric they can be transformed to principal axes, so that the maximum number of independent components is three (for triclinic, monoclinic and orthorhombic monocystals and for orthotropic composites). For materials of higher symmetry the number is further reduced. For all materials with an axis of rotational symmetry (i.e. trigonal, tetragonal and hexagonal monocystals as well as transversely isotropic composites) there are two independent components, while for cubic monocystals and isotropic materials there is only one [11]. Of course, with respect to the heat conductivity tensor \mathbf{K} the reader should keep in mind the aforementioned fact that the assumed symmetry is not guaranteed, in particular not for triclinic, monoclinic and transversely isotropic materials [16]. Generally, with respect to second-order tensor properties cubic monocystals behave like isotropic materials, but not with respect to tensorial properties of higher order, e.g. elasticity, cf. [10].

Linear thermoelasticity of isotropic solids

For isotropic materials the following simplifications result: The generalized Hooke law of linear elasticity,

$$\mathbf{T} = \mathbf{C} \mathbf{E} , \quad (75)$$

with its fourth-order elasticity tensor \mathbf{C} (with 21 independent components in the case of triclinic monocystals) can be replaced by the Cauchy-Hooke law,

$$\mathbf{T} = \lambda (\text{tr } \mathbf{E}) \mathbf{1} + 2 \mu \mathbf{E} , \quad (76)$$

where the scalar coefficients λ and μ (this is all that remains for isotropic materials) are the isothermal Lamé constants (cf. [10,12]). Further, the stress-temperature tensor \mathbf{M} , the thermal expansion tensor \mathbf{A} and the heat conductivity tensor \mathbf{K} (all second-order) reduce to isotropic tensors, determined by one scalar component, i.e.

$$\mathbf{M} = m \mathbf{1} , \quad (77)$$

$$\mathbf{A} = \alpha \mathbf{1} , \quad (78)$$

$$\mathbf{K} = k \mathbf{1} , \quad (79)$$

where k is the heat conductivity and the stress-temperature modulus (thermal coefficient of stress) m is con-

nected with the coefficient of linear thermal expansion α via the relation

$$m = -\alpha (3\lambda + 2\mu) . \quad (80)$$

Due to the small strain assumption at the outset of this and the preceding section $\text{tr } \mathbf{E}$ turns out to be approximately equivalent to the relative volume change ($\text{tr } \mathbf{E} \approx \Delta V/V$) and the coefficient of volumetric thermal expansion $\alpha_{\text{volumetric}}$ is approximately 3α . The constitutive equation for the stress tensor of isotropic solids within the completely linearized theory of thermoelasticity (Duhamel-Neumann law) is

$$\mathbf{T} = \lambda (\text{tr } \mathbf{E}) \mathbf{1} + 2 \mu \mathbf{E} + m (T - T_0) \mathbf{1} . \quad (81)$$

When the strain vanishes ($\mathbf{E} = \mathbf{0}$) stress equals pressure in an isotropic body, i.e.

$$\mathbf{T} = m (T - T_0) \mathbf{1} . \quad (82)$$

Conversely, when the stress vanishes ($\mathbf{T} = \mathbf{0}$) strain equals omnidirectional dilatation or hydrostatic compression in an isotropic body, i.e.

$$\mathbf{E} = \alpha (T - T_0) \mathbf{1} . \quad (83)$$

The latter, of course, is possible only when the following inverse Duhamel-Neumann law exists:

$$\mathbf{E} = -\frac{\lambda}{2\mu(3\lambda + 2\mu)} (\text{tr } \mathbf{T}) \mathbf{1} + \frac{1}{2\mu} \mathbf{T} + \alpha (T - T_0) \mathbf{1} . \quad (84)$$

The remaining constitutive equations are

$$\mathbf{q} = -k \text{grad } T \quad (85)$$

for the heat flux (Fourier's law),

$$s = \frac{c_F}{T_0} (T - T_0) - \frac{m}{\rho} (\text{tr } \mathbf{E}) \quad (86)$$

for the entropy (Biot's law) and

$$f = \frac{1}{2\rho} \lambda (\text{tr } \mathbf{E})^2 + \mu \text{tr } (\mathbf{E}^2) + m (\text{tr } \mathbf{E}) (T - T_0) - \frac{1}{2} \frac{c_F}{T_0} (T - T_0)^2 \quad (87)$$

for the free energy. Note that the adiabatic Lamé constants $\tilde{\lambda}$ and $\tilde{\mu}$ of isotropic solids are

$$\tilde{\lambda} = \lambda + \frac{Tm^2}{\rho c_F} \quad (88)$$

and

$$\tilde{\mu} = \mu , \quad (89)$$

cf. [1], p. 189. All other (isothermal or adiabatic) elasticity moduli (tensile modulus E , shear modulus G , bulk modulus K) and the Poisson ratio ν can be calculated from the two Lamé constants (isothermal and adiabatic, respectively), according to the standard relations of

elasticity theory, cf. [10,12]. E.g. the adiabatic bulk modulus is

$$\tilde{K} = \frac{3\tilde{\lambda} + 2\tilde{\mu}}{3} . \quad (90)$$

For real bodies $c_F > 0$ and therefore $\tilde{\lambda} > \lambda$ (cf. [1], p. 189). Further we have

$$c_T - c_F = \frac{3 T m^2}{(3\lambda + 2\mu)\rho} = 9\alpha^2 K V T \quad (91)$$

(with the specific volume $V = \rho^{-1} = |J|/\rho_0$) and

$$\frac{c_T}{c_F} = \frac{\tilde{K}}{K} . \quad (92)$$

The latent heat tensors (with respect to deformation \mathbf{L}_F and with respect to stress \mathbf{L}_T , respectively) are

$$\mathbf{L}_F = -\frac{Tm}{\rho} \mathbf{1} \quad (93)$$

and

$$\mathbf{L}_T = -\frac{Tm}{(3\lambda + 2\mu)\rho} \mathbf{1} . \quad (94)$$

Linear thermoelasticity of fluids

Common fluids are isotropic materials of a very special type, in a subtle sense more symmetric than isotropic solids, cf. [2]. For reasons of this symmetry the deformation gradient \mathbf{F} as an independent variable is replaced by the density ρ or its inverse, the specific volume $V = \rho^{-1} = |J|/\rho_0$. That means, all information about the deformation of an elastic fluid (e.g. a gas) is contained in a single scalar variable. Therefore e.g. the free energy function $f(\mathbf{F}, T)$ becomes $f(V, T)$ and the Cauchy stress $\mathbf{T}(\mathbf{F}, T)$ is fully determined by the pressure $p(V, T)$:

$$\mathbf{T}(\mathbf{F}, T) = -p(V, T) \mathbf{1} . \quad (95)$$

In the case of elastic fluids the constitutive equation $p(V, T)$ is also called equation of state, the simplest and most famous example being that of an ideal gas. As a consequence of the first and second law, equations (21) and (22), one obtains the well-known thermodynamic relations

$$p = -\frac{\partial f}{\partial V} \quad (96)$$

and

$$s = -\frac{\partial f}{\partial T} . \quad (97)$$

Accordingly, the total differential of the free energy function is

$$df = -pdV - sdT . \quad (98)$$

These expressions should be compared with equations (26a), (26b) and (27a), respectively. Since shear strains (corresponding in solid bodies to changes of shape) are not sustained in fluids, the Duhamel-Neumann law reduces for fluids to the constitutive relation

$$\mathbf{T} = -V \frac{\partial p}{\partial V} (\text{tr } \mathbf{E}) \mathbf{1} - \frac{\partial p}{\partial T} (T - T_0) \mathbf{1}, \quad (99)$$

where $\partial p / \partial T = -m$ is the thermal coefficient of pressure, i.e. for fluids

$$\mathbf{M} = -\frac{\partial p}{\partial T} \mathbf{1}. \quad (100)$$

The coefficient of volumetric thermal expansion is

$$\alpha_{\text{volumetric}} = \frac{\partial p / \partial T}{V \partial p / \partial V} = \frac{\partial V}{V \partial T} \quad (101)$$

(defined only if $\partial p / \partial V \neq 0$), in accordance with classical thermodynamics, cf. [17,18]. Generally the coefficient of volumetric thermal expansion $\alpha_{\text{volumetric}}$ is connected to that of linear thermal expansion α via the relation

$$\alpha_{\text{volumetric}} = 3\alpha + 3\alpha^2 + \alpha^3. \quad (102)$$

Already for gases, however, the coefficient of volumetric thermal expansion is quite small (and nearly the same for all gases, viz. $\alpha_{\text{volumetric}} \approx T^{-1}$, i.e. approx. 0.003 K^{-1} at room temperature), for condensed phases (liquids) even smaller, cf. [17,18]. Therefore, the coefficient of linear thermal expansion can be calculated from $\alpha_{\text{volumetric}} \approx 3\alpha$, as above for isotropic solids.

In the case of fluids the specific heats at constant deformation c_F and at constant stress c_T are denoted c_V and c_p , respectively. For the specific heat at constant (specific) volume we have

$$c_V = -T \frac{\partial^2 f}{\partial T^2} \quad (103)$$

and for the specific heat at constant pressure (defined only if $\partial p / \partial V \neq 0$)

$$c_p - c_V = -T \frac{(\partial p / \partial T)^2}{\partial p / \partial V}. \quad (104)$$

In terms of adiabatic and isothermal bulk moduli their ratio is

$$\frac{c_p}{c_V} = \frac{\tilde{K}}{K} = \frac{\partial \bar{p} / \partial V}{\partial p / \partial V}. \quad (105)$$

Finally, for fluids the latent heat tensors (with respect to deformation \mathbf{L}_F and with respect to stress \mathbf{L}_T , respectively) are both isotropic,

$$\mathbf{L}_F = V l_V \mathbf{1}, \quad (106)$$

$$\mathbf{L}_T = -\frac{1}{3} l_p \mathbf{1}. \quad (107)$$

with the scalar coefficients

$$l_V = T \partial p / \partial T \quad (108)$$

(latent heat with respect to volume) and

$$l_p = T \frac{\partial p / \partial T}{\partial p / \partial V} \quad (109)$$

(latent heat with respect to pressure, defined only if $\partial p / \partial V \neq 0$). In terms of specific heats and latent heats the (rate of external specific) heat supply for fluids is

$$\dot{Q} = c_V \dot{T} + l_V \dot{V} = c_p \dot{T} + l_p \dot{p}, \quad (110)$$

cf. [1], p. 195. With these examples it should be evident that the complete structure of classical thermodynamics (thermodynamics) arises in a natural way from the more general relations of the preceding sections. In other words, the linear theory of thermoelasticity, as sketched in this paper, comprises the whole classical thermodynamics of elastic (i.e. inviscid) fluids as a special case. Viscous fluids, however, are included in this theory only in special situations (equilibrium). Also note, that with this theory alone it is not possible to treat the specific features of mixtures. "Miscible" or single-phase mixtures (i.e. fluid or solid solutions) are the main issue of chemical thermodynamics or the thermodynamics of reacting mixtures [18,19], while "immiscible" or multi-phase mixtures are in the focus of micromechanics or composite theory [20,21]. The thermoelastic properties of the latter mixtures, including composites, porous media and other materials with microstructure (e.g. polycrystals) will be treated in forthcoming papers.

CONCLUSIONS

The linear theory of thermoelasticity has been summarized for materials scientists and engineers from the viewpoint of exact theory (rational thermomechanics). Following modern treatments of rational thermomechanics, the physically linearized theory has been derived in referential formulation, using the first Piola-Kirchhoff stress tensor \mathbf{P} , the referential heat flux \mathbf{h} , the free energy f and the entropy s as the material responses (dependent variables), for which constitutive equations are given. The deformation gradient \mathbf{F} , the temperature T and the referential temperature gradient $\text{Grad } T$ have been used as independent variables (simple thermoelastic materials). Linear approximations of the series expansions about a natural reference state (\mathbf{F}_0, T_0) and thermal equilibrium (with $\text{Grad } T = \mathbf{0}$) have been invoked to define the fourth-order elasticity tensor \mathbf{C} , the stress-temperature tensor \mathbf{M} , the thermal expansion tensor \mathbf{A} , the latent heat tensors \mathbf{L}_F and \mathbf{L}_T (with respect to deformation and stress, respectively), the heat con-

ductivity tensor \mathbf{K} and the specific heats c_F and c_T (at constant deformation and constant stress, respectively) for anisotropic solids. It has been shown that the second-order tensors \mathbf{M} , \mathbf{A} and \mathbf{L}_F (or \mathbf{L}_T) contain essentially the same information. For the completely (physically and geometrically) linearized theory the constitutive equations and linear thermoelastic properties of isotropic solids and fluids, including the scalar coefficients of thermal expansion and heat conductivity, have been derived as special cases of the theory for anisotropic materials in order to demonstrate the scope of this theory and its connection to traditional thermodynamics. The assumptions underlying each step of simplification and the physical meaning of the coefficients have been emphasized throughout. Following the spirit of rational thermomechanics as far as possible, but avoiding mathematical formalities wherever possible, this shortcut is intended to provide a relatively sound basis for the future discussion of thermoelastic properties of heterogeneous materials from the viewpoint of micromechanics. Subsequent papers will concern the thermoelastic properties of alumina-zirconia composites and other ceramics.

Acknowledgement

This work was part of the project "Mechanics and Thermomechanics of Disperse Systems, Porous Materials and Composites", supported by the Grant Agency of the Czech Republic (Grant No. 106/00/D086). The support is gratefully acknowledged.

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LINEÁRNÍ TEORIE TERMOELASTICITY Z HLEDISKA RACIONÁLNÍ TERMOMECHANIKY

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V tomto příspěvku je shrnuta lineární termoelastická teorie materiálové vědy a inženýry z hlediska exaktní teorie (tj. racionální termomechaniky). Je zde odvozena v tzv. referenční formulaci, tj. pomocí prvního Piolova-Kirchhoffova tenzoru napětí, referenčního toku tepla, volné energie a entropie. Pro všechny tyto materiálové odezvy jsou uvedeny konstitutivní rovnice. Nezávislými proměnnými jsou gradient deformace, teplota a referenční gradient teploty (tzv. "prosté" termoelastické materiály). Lineární aproximací řadových rozvoji okolo referenčního stavu (tj. elasticky "přirozené" konfigurace a tepelné rovnováhy) jsou definovány tenzor elasticity, tenzor teplotní roztažnosti, tenzor tepelné vodivosti a specifické tepelné kapacity pro anizotropní pevné látky libovolné symetrie. Z těchto obecných vztahů jsou nakonec jako speciální případy odvozeny konstitutivní rovnice a lineární termoelastické vlastnosti izotropních pevných látek a tekutin, které jsou známé z klasické termodynamiky.