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Professor Jakub Gutenbaum
on his 70th birthday*

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Three-dimensional model of thermomechanical evolution of shape memory materials

by

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Abstract: We derive a thermodynamically consistent model of the thermomechanical evolution of shape memory materials in three dimensions. The model is based on the linearized strain tensor and the absolute temperature as state variables. It accounts for the viscous and spatially nonlocal effects, and constitutes a generalization of the one-dimensional Falk model. The constitutive equations comply with the entropy inequality. Examples of free energies characteristic for shape memory alloys and noncrystalline materials are given.

Keywords: shape memory, thermomechanical evolution, martensitic phase transformation, thermodynamically consistent model.

1. Introduction

Beginning from the one-dimensional theory due to Falk (1982, 1990) for martensitic phase transformations of the shear type, the model of shape memory alloys (SMA) based on the Ginzburg-Landau free energy has been the subject of extensive studies, see, e.g. Niezgódka and Sprekels (1988), Sprekels and Zheng (1989), Sprekels (1990), Hoffmann and Źochowski (1992), Źochowski (1992).

The martensitic phase transformation, activated by stress or temperature, is a special type of deformation of a crystal lattice of parent phase (austenite) in a crystal lattice of product phase (martensite) without diffusion which is accompanied by a jump in the thermomechanical properties (see, e.g. Levitas, 1998). A reverse phase transformation transforms martensite into austenite.

In three dimensions there exist different approaches to the continuum description of thermomechanical evolution of SMA. The well-known model due

to Frémond (1987) is based on the linearized strain tensor, the volumetric proportions of austenite and martensite, and the absolute temperature as state variables. The interfacial structure is accounted for there by the gradient of the strain tensor trace. This model has been extensively studied, by e.g. Colli, Frémond and Visintin (1990), Hoffmann, Niezgodka and Zheng (1990), Colli and Sprekels (1992, 1993), and Colli (1995).

A different model has been derived by Fried and Gurtin (1994) in an isothermal case within a thermodynamical theory of configurational forces. It is based on the strain tensor, a multicomponent order parameter and its gradient.

To describe the characteristic stress–strain relations of three–dimensional SMA, Falk and Konopka (1990) have proposed an elastic energy density $F(\epsilon, \theta)$, dependent on the symmetric strain tensor ϵ and the absolute temperature θ , which is invariant with respect to the cubic symmetry group of the high–temperature phase. More precisely, it satisfies the isotropy condition

$$F(\epsilon, \theta) = F(\mathbf{G}\epsilon\mathbf{G}^T, \theta) \quad (1)$$

for each of the 48 matrices \mathbf{G} , which represent the corresponding symmetry operations in \mathbb{R}^3 . The proposed energy is a polynomial expansion up to sixth order with respect to the invariants, i.e. certain combinations of the strain tensor components, with temperature–dependent coefficients.

A different elastic energy, proposed by Ericksen (1986), is expressed in terms of the right Cauchy–Green strain tensor in the form of a fourth order polynomial with temperature–dependent coefficients. This energy has been used by Klouček and Luskin (1994) for numerical simulation of SMA dynamics in 3–D, with temperature treated as a parameter.

To account for the structure of moving interface boundaries Barsch and Krumhansl (1984) have proposed a strain–gradient elastic energy, derived on the basis of symmetry considerations.

For a recent survey of continuum models for the evolution of microstructure in SMA, with emphasis on "mesoscopic" models, we refer to Roubíček (1999).

We mention that in the isothermal case a phase transition model in the form of a viscoelasticity system has been studied by many authors, e.g. Ball et al. (1991), Rybka (1992, 1994, 1997).

Our goal here is to derive a thermodynamically consistent model of the thermomechanical evolution of shape memory materials in three dimensions, which corresponds to the Falk–Konopka free energy as a prototype.

The model is based on the linearized strain tensor $\epsilon(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$, where \mathbf{u} denotes the displacement vector, and the absolute temperature θ . It constitutes a generalization of the one–dimensional Falk model. The field equations correspond to the balance laws for linear momentum and energy (for constant mass density)

$$\mathbf{u}_{tt} - \nabla \cdot \boldsymbol{\sigma} = \mathbf{b}, \quad (2)$$

$$e_t + \nabla \cdot \mathbf{q} - \boldsymbol{\sigma} : \epsilon_t = r, \quad (3)$$

where the stress tensor σ , the internal energy e , and the energy flux \mathbf{q} are modeled by constitutive relations accounting for nonlocal and viscous effects. The viscous effects are represented in the constitutive variables by the strain rate tensor $\epsilon_t = \epsilon(\mathbf{u}_t)$, and the nonlocal effects by higher order strain gradients $\mathbf{D}^m \epsilon$. It turns out that in order to characterize constitutive relations for materials with first order strain-gradient free energy density

$$f = \hat{f}(\epsilon, \mathbf{D}\epsilon, \theta), \quad (4)$$

it is necessary to admit ϵ_t as the constitutive variable. The strain-gradient energy contribution corresponds to spatially nonlocal effects. It enables to describe finer effects between the regions with nearly constant strain tensor, and provides so-called diffuse (structured) interface approach to the development of phase transition.

As the main result of the paper it is proved that for such materials the stress tensor and the energy flux relations compatible with the entropy principle have the following forms

$$\sigma = \frac{\delta f}{\delta \epsilon} + \theta(\mathbf{h} - f, \mathbf{D}\epsilon) \cdot \nabla\left(\frac{1}{\theta}\right) + \sigma^v, \quad (5)$$

$$\mathbf{q} = \mathbf{q}_0 - \epsilon_t \cdot \mathbf{h}, \quad (6)$$

and the Gibbs relations hold

$$e = f + \theta s, \quad s = -f, \theta. \quad (7)$$

Here s is the entropy density, and the expression $\frac{\delta f}{\delta \epsilon}$ is the first variation of f with respect to ϵ :

$$\frac{\delta f}{\delta \epsilon} = f, \epsilon - \nabla \cdot f, \mathbf{D}\epsilon. \quad (8)$$

A third order tensor \mathbf{h} is an arbitrary quantity, which is not restricted by the entropy principle. The presence of such a quantity is characteristic for phase transition models with first order gradient free energy (see Alt and Pawlow, 1996).

Moreover, the heat flux \mathbf{q}_0 and the viscous stress tensor σ^v are subject to the dissipation inequality

$$\epsilon_t : \left(\frac{\sigma^v}{\theta}\right) + \nabla\left(\frac{1}{\theta}\right) \cdot \mathbf{q}_0 \geq 0 \quad \text{for all fields } (\mathbf{u}, \theta). \quad (9)$$

In particular, this inequality is satisfied by the standard Fourier law for heat conduction

$$\mathbf{q}_0 = -k \nabla \theta, \quad (10)$$

and Hooke's-like law for viscosity

$$\sigma^v = \nu \mathbf{A} \epsilon_t, \quad (11)$$

where $k > 0$ is the heat conductivity, $\nu = \text{const.} > 0$ is the viscosity coefficient, and \mathbf{A} is the fourth order tensor of linearized elasticity given through the relation

$$\mathbf{A}\boldsymbol{\epsilon}(\mathbf{u}) = \lambda \text{trace } \boldsymbol{\epsilon}(\mathbf{u}) \mathbf{I} + 2\mu\boldsymbol{\epsilon}(\mathbf{u}), \quad (12)$$

with λ, μ denoting Lamé constants. With the above constitutive relations, and with the particular choice of the tensor field

$$\mathbf{h} = f_{,D\boldsymbol{\epsilon}}, \quad (13)$$

the equations (2), (3) transform to the form which in 1-D is identical with the evolution model due to Falk (1982, 1990). In case the strain-gradient free energy contribution is independent of temperature (called energetic case), i.e. $f_{,\theta D\boldsymbol{\epsilon}} = 0$, the equations read

$$\mathbf{u}_{tt} - \nu \nabla \cdot (\mathbf{A}\boldsymbol{\epsilon}_t) + \nabla \cdot (\nabla \cdot f_{,D\boldsymbol{\epsilon}}) = \nabla \cdot f_{,\boldsymbol{\epsilon}}(\boldsymbol{\epsilon}, \theta) + \mathbf{b}, \quad (14)$$

$$c(\boldsymbol{\epsilon}, \theta)\theta_t - \nabla \cdot (k\nabla\theta) = \theta f_{,\theta\boldsymbol{\epsilon}}:\boldsymbol{\epsilon}_t + (\mathbf{A}\boldsymbol{\epsilon}_t):\boldsymbol{\epsilon}_t + r, \quad (15)$$

where

$$c(\boldsymbol{\epsilon}, \theta) = -\theta f_{,\theta\theta}(\boldsymbol{\epsilon}, \theta)$$

is the specific heat coefficient.

The well-posedness of the system (14), (15) with appropriate initial and boundary conditions has been studied in Pawłow and Zochowski (2000). For the sake of mathematical analysis the free energy has been assumed there in the form

$$f(\boldsymbol{\epsilon}, \nabla\boldsymbol{\epsilon}, \theta) = -c_v\theta\log\theta + F(\boldsymbol{\epsilon}(\mathbf{u}), \theta) + \frac{\kappa}{8} |\nabla \cdot (\mathbf{A}\boldsymbol{\epsilon}(\mathbf{u}))|^2 \quad (16)$$

involving the particular strain-gradient contribution. Here $\kappa = \text{const.} > 0$ is a parameter corresponding to spatially nonlocal effects, and the divergence term can be interpreted as a resultant of forces acting on an elementary volume element. The first and the second term in (16) are the caloric energy and the elastic Falk-Konopka energy, respectively.

In such a case the constitutive equation for the stress takes on the form

$$\boldsymbol{\sigma} = F_{,\boldsymbol{\epsilon}}(\boldsymbol{\epsilon}(\mathbf{u}), \theta) - \frac{\kappa}{4} \mathbf{A}\boldsymbol{\epsilon}(\nabla \cdot (\mathbf{A}\boldsymbol{\epsilon}(\mathbf{u}))) + \nu \mathbf{A}\boldsymbol{\epsilon}_t, \quad (17)$$

where the first term on the right-hand side is the elastic stress tensor, the second is the hyperstress tensor and the third is the viscous stress tensor.

This relation augments the conventional constitutive law for an elastic material in such a way that the stress tensor depends not only on the strain tensor $\boldsymbol{\epsilon}$, but also on the strain rate tensor $\boldsymbol{\epsilon}_t$ and the second spatial gradients $D^2\boldsymbol{\epsilon}$. The characteristic feature of constitutive law (17) is that the dependence of the stress tensor on $\boldsymbol{\epsilon}$ is nonlinear, but $\boldsymbol{\epsilon}_t$ and $D^2\boldsymbol{\epsilon}$ enter linearly via Hooke's law. This constitutive equation generalizes to three dimensions the well-known one-dimensional viscosity-capillarity relation proposed by Slemrod (1983, 1984), and

analyzed in e.g. Abeyaratne and Knowles (1991), and Truskinovsky (1994). In such a case the elasticity equation (14) takes on the form

$$\mathbf{u}_{tt} - \nu \mathbf{Q}\mathbf{u}_t + \frac{\kappa}{4} \mathbf{Q}\mathbf{Q}\mathbf{u} = \nabla \cdot \mathbf{F}_{,\epsilon}(\epsilon, \theta) + \mathbf{b}, \quad (18)$$

where \mathbf{Q} stands for the second order differential operator of linearized elasticity

$$\mathbf{u} \mapsto \mathbf{Q}\mathbf{u} = \nabla \cdot (\mathbf{A}\epsilon(\mathbf{u})).$$

The mathematical analysis in Pawłow and Źochowski (2000) is based on the parabolic decomposition of the system (18). Such a procedure is possible due to the particular structure of (18) involving operators \mathbf{Q} and $\mathbf{Q}\mathbf{Q}$, which correspond to the viscous and the nonlocal term, respectively.

It should be pointed out that with the selection (13) of the quantity \mathbf{h} the internal energy dynamics is not influenced by the strain–gradient contribution of the free energy. In the context of van der Waals–Korteweg gradient theory of phase transitions such a postulate has been suggested by Felderhof (1970), and applied by Slemrod (1984) to study the coupled effects of viscosity, capillarity and heat conduction in 1–D case. Then the energy equation (3) in the energetic case, $f_{,\theta D\epsilon} = 0$, reduces to the form

$$e_0(\epsilon, \theta)_t + \nabla \cdot \mathbf{q}_0 = f_{,\epsilon} : \epsilon_t + \sigma^v : \epsilon_t + r, \quad (19)$$

where $e_0(\epsilon, \theta) = e(\epsilon, 0, \theta)$ is the volumetric internal energy. For Fourier and Hooke's laws this yields (15).

We add here a comment related to the frame–indifference question, which is not considered in this paper. We point out that the constitutive relations of the model have been derived under the small strain assumption of linearized elasticity. Therefore, the proposed model is in its origin an approximation to what must be a more complicated description.

As known (see Fosdick and Serrin, 1979), the linear stress response function is incompatible with the principle of frame–indifference, therefore an exact linear constitutive theory for elastic solids is impossible. This implies, in particular, that the constitutive relation (17), assumed in Pawłow and Źochowski (2000) for the sake of a mathematical analysis, is not physically meaningful. It should be pointed out, however, that Hooke's law satisfies the invariance condition of an isotropic function (see, e.g., Gurtin, 1981, p.235). In particular, for viscosity the following condition holds

$$\mathbf{R}\sigma^v(\epsilon_t)\mathbf{R}^T = \sigma^v(\mathbf{R}\epsilon_t\mathbf{R}^T)$$

for any proper orthogonal tensor \mathbf{R} of the second order.

The investigation of invariance conditions imposed by the axiom of frame–indifference in the framework of strain–gradient theory requires a separate study.

The paper is organized as follows. In Section 2 we recall the balance laws, the entropy principle, and the basic thermodynamic relations.

In Section 3 we present a constitutive theory for strain–gradient thermo-viscoelastic materials. The constitutive relations involve dependencies of the internal energy, the stress tensor and the heat flux on the strain tensor, its gradients, the strain rate tensor, and the entropy and its gradients as thermodynamic variables. We deduce restrictions placed on the constitutive relations by the entropy inequality with undetermined multipliers.

The linear momentum and energy balances in conjunction with the constitutive relations lead to the field equations, which are presented in Section 4. The independent variables in these equations are the displacement vector, the entropy and the multiplier conjugated with the energy equation. In case of thermal stability, i.e. positive specific heat coefficient, by duality relations, this multiplier can be identified with the inverse of the absolute temperature. In such a case the relation between the temperature and the entropy defines a transformation. Consequently, the problem can be alternatively expressed in terms of the displacement vector and the entropy, or the displacement vector and the temperature as independent variables. With the latter choice we arrive at the system (14), (15).

Section 5 contains the examples of free energy densities for shape memory alloys and noncrystalline materials in the 2-D and 3-D cases.

The proofs are presented in Section 6.

Throughout this paper tensor notation is used. Vectors and tensors are denoted by bold letters. For $\mathbf{a} = (a_i)$, $\mathbf{b} = (b_i)$, $\mathbf{A} = (A_{ij})$, $\mathbf{B} = (B_{ij})$, $\mathbf{C} = (C_{ijk})$ we denote

$$\begin{aligned} \mathbf{a} \cdot \mathbf{b} &= a_i b_i, \quad \mathbf{a} \cdot \mathbf{A} = (a_i A_{ij}), \quad \mathbf{A} \cdot \mathbf{a} = (A_{ij} a_j), \\ \mathbf{B} \cdot \mathbf{C} &= (B_{ij} C_{ijk}), \quad \mathbf{C} \cdot \mathbf{B} = (C_{ijk} B_{jk}), \quad \mathbf{A} : \mathbf{B} = A_{ij} B_{ij}. \end{aligned}$$

The summation convention over repeated indices is used. The expression $\nabla \cdot \mathbf{A}(x)$ denotes the divergence,

$$\nabla \cdot \mathbf{A}(x) = \left(\frac{\partial}{\partial x_j} A_{ij}(x) \right),$$

where the convention of the contraction over the last index is used. The superscript T denotes the transposition, and subscript s symmetrization of the tensor, ∇ is the gradient operator.

We write $f_{,A} = \partial_A f$ for the partial derivative of the function f with respect to the variable A . In particular, for f scalar-valued and \mathbf{A}^m a tensor of order m , $f_{,\mathbf{A}^m}$ is a tensor of order m with components $f_{,A_{i_1 \dots i_m}^m}$. Moreover, we denote

$$f_{,i} = \frac{\partial f}{\partial x_i}, \quad f_t = \frac{\partial f}{\partial t}.$$

2. Balance laws and basic relations

Let $\Omega \subset \mathbb{R}^n$, $n > 1$, be an open bounded domain with a smooth boundary $\partial\Omega$, occupied by a body in the current configuration at time t . The behaviour of the body is described by the following fields: mass density ρ , velocity $\mathbf{v} = (v_i)$, stress tensor $\boldsymbol{\sigma} = (\sigma_{ij})$, body force $\mathbf{b} = (b_i)$, internal energy e , energy flux $\mathbf{q} = (q_i)$, heat supply r , which depend on time t and position x in Ω , and are assumed to comply with the balance laws and the entropy principle.

The balance of mass, linear momentum, moment of momentum and the total (internal plus kinetic) energy are at regular points of Ω locally expressed by the following equations (see, e.g., Müller, 1985):

$$\rho_t + \rho \nabla \cdot \mathbf{v} = 0, \quad (20)$$

$$\rho \mathbf{v}_t - \nabla \cdot \boldsymbol{\sigma} = \rho \mathbf{b}, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}^T, \quad (21)$$

$$\rho \left(e + \frac{|\mathbf{v}|^2}{2} \right)_t + \nabla \cdot (-\mathbf{v} \cdot \boldsymbol{\sigma} + \mathbf{q}) = \rho \mathbf{b} \cdot \mathbf{v} + \rho r, \quad (22)$$

where subscript t denotes the material time derivative

$$\phi_t = \partial_t \phi + \nabla \phi \cdot \mathbf{v}.$$

Multiplying scalarly the first equation in (21) by \mathbf{v} and using the identity

$$\mathbf{v} \cdot (\nabla \cdot \boldsymbol{\sigma}) = v_i (\partial_j \sigma_{ij}) = \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\sigma}) - \boldsymbol{\sigma} : (\nabla \mathbf{v})_s,$$

where

$$(\nabla \mathbf{v})_s = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T),$$

leads to the balance equation for the kinetic energy

$$\rho \left(\frac{|\mathbf{v}|^2}{2} \right)_t - \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\sigma}) + \boldsymbol{\sigma} : (\nabla \mathbf{v})_s = \rho \mathbf{b} \cdot \mathbf{v}. \quad (23)$$

Subtraction of (23) from (22) gives the balance equation for the internal energy

$$\rho e_t + \nabla \cdot \mathbf{q} - \boldsymbol{\sigma} : (\nabla \mathbf{v})_s = \rho r. \quad (24)$$

The balance laws (20) - (22) are considered together with constitutive relations reflecting material properties. The entropy principle is used to find out restrictions on these relations, in other words - to select a class of thermodynamically consistent models.

Let Y denote the set of constitutive variables for the quantities in balance laws. The entropy principle (see Müller, 1985, Alt and Pawłow, 1996) asserts the existence of the entropy $s = \hat{s}(Y)$ and the entropy flux $\boldsymbol{\psi} = \hat{\boldsymbol{\psi}}(Y)$, which are smooth functions of Y , with the following property:

For all smooth local solutions of balance equations the entropy source τ , defined by

$$s_t + \nabla \cdot \psi = \tau, \quad (25)$$

satisfies the condition

$$\tau \geq \tau_0, \quad \text{where } \tau_0 = \hat{\tau}_0(Y, r), \quad \text{and } \hat{\tau}_0(Y, 0) = 0 \text{ for all } Y. \quad (26)$$

Let $\mathbf{u} = (u_i)$ denote the displacement vector and $\epsilon = (\epsilon_{ij})$ the strain tensor. Further on we confine ourselves to linear thermoelasticity. We assume the small strain approximation, that is – the relations

$$\epsilon = (\nabla \mathbf{u})_s, \quad \text{and } \mathbf{v} = \mathbf{u}_t.$$

This implies that the strain rate tensor satisfies the equality $\epsilon_t = (\nabla \mathbf{v})_s$.

We assume also that the mass density ρ is constant, normalized to unity. Consequently, we restrict the description of the process to the linear momentum balance

$$\mathbf{u}_{tt} - \nabla \cdot \boldsymbol{\sigma} - \mathbf{b} = 0, \quad (27)$$

and the internal energy balance

$$e_t + \nabla \cdot \mathbf{q} - \boldsymbol{\sigma} : \epsilon_t = r, \quad (28)$$

which together yield the total energy balance

$$\left(e + \frac{|\mathbf{u}_t|^2}{2} \right)_t + \nabla \cdot (-\mathbf{u}_t \cdot \boldsymbol{\sigma} + \mathbf{q}) - \mathbf{b} \cdot \mathbf{u}_t = r. \quad (29)$$

For further use we recall here the duality relations (Legendre transformations) for non-homogeneous continua characterized by an order parameter and its gradient (see Alt and Pawłow, 1996).

Let $\theta > 0$ denote the absolute temperature and $w := \frac{1}{\theta}$ the inverse temperature. Within the first order theory with the strain tensor ϵ as an order parameter the Helmholtz free energy density is given by a constitutive equation $f = \hat{f}(\epsilon, \mathbf{D}\epsilon, \theta)$, where $\mathbf{D}\epsilon = (\epsilon_{ij,k})$ denotes the third order tensor corresponding to space derivatives $\nabla \epsilon = (\partial_k \epsilon_{ij})$. Let $\varphi = \hat{\varphi}(\epsilon, \mathbf{D}\epsilon, \frac{1}{\theta}) = \frac{1}{\theta} \hat{f}(\epsilon, \mathbf{D}\epsilon, \theta)$ denote the reduced free energy density.

The Gibbs relations read

$$f = e - \theta s, \quad s = -f_{,\theta}, \quad (30)$$

or equivalently,

$$s + \varphi = w e, \quad e = \varphi_{,w}. \quad (31)$$

The specific heat coefficient is defined by

$$c = \hat{c}(\epsilon, \mathbf{D}\epsilon, \theta) := e_{,\theta}(\epsilon, \mathbf{D}\epsilon, \frac{1}{\theta}). \quad (32)$$

Hence, by Gibbs relations,

$$c = -\theta f_{,\theta\theta} = \theta s_{,\theta}. \quad (33)$$

Under assumption of thermal stability, i.e. positive specific heat coefficient, $c > 0$, it follows from (30) that $\theta \mapsto -\hat{f}(\epsilon, \mathbf{D}\epsilon, \theta)$ is a strictly convex function and $w \mapsto \hat{\varphi}(\epsilon, \mathbf{D}\epsilon, w)$ a strictly concave function. Therefore the duality relations take place. In particular, there is the well defined conjugate convex function

$$\hat{\tilde{e}}(\epsilon, \mathbf{D}\epsilon, s) := \sup_{0 < \theta < \infty} (\bar{\theta}s + \hat{f}(\epsilon, \mathbf{D}\epsilon, \bar{\theta})) \leq +\infty, \quad (34)$$

which is a lower semicontinuous strictly convex function of $s \in \mathbb{R}$. Similarly, there, is the well defined conjugate concave function of φ with e as dual variable.

By (33) the map $\theta \mapsto \hat{s}(\epsilon, \mathbf{D}\epsilon, \frac{1}{\theta})$ is then strictly increasing, therefore the inverse map $s \mapsto \hat{\theta}(\epsilon, \mathbf{D}\epsilon, s)$ exists. The property $0 < \theta < \infty$ is equivalent to $s_* < s < s^*$ with $s_* = \hat{s}_*(\epsilon, \mathbf{D}\epsilon) \geq -\infty$ and $s^* = \hat{s}^*(\epsilon, \mathbf{D}\epsilon) \leq \infty$. If $s_* < s < s^*$ the supremum in (34) is uniquely attained at $\bar{\theta} = \theta = \hat{\theta}(\epsilon, \mathbf{D}\epsilon, s)$ with

$$\hat{\tilde{e}}(\epsilon, \mathbf{D}\epsilon, s) - \hat{f}(\epsilon, \mathbf{D}\epsilon, \theta) = \theta s, \quad \tilde{e}_{,s}(\epsilon, \mathbf{D}\epsilon, s) = \theta. \quad (35)$$

Then, by (30),

$$\hat{e}(\epsilon, \mathbf{D}\epsilon, \frac{1}{\theta}) = \hat{\tilde{e}}(\epsilon, \mathbf{D}\epsilon, \hat{s}(\epsilon, \mathbf{D}\epsilon, \frac{1}{\theta})),$$

that is $-\tilde{e}$ is the internal energy expressed as a function of the entropy s .

The duality relations allow to use alternatively the absolute temperature θ (or the inverse temperature w), the entropy s , or the internal energy e as independent variables.

We note that the heat capacity in terms of s is

$$\tilde{c} = \hat{c}(\epsilon, \mathbf{D}\epsilon, s) = \hat{c}(\epsilon, \mathbf{D}\epsilon, \hat{\theta}(\epsilon, \mathbf{D}\epsilon, s)) = \hat{\theta} \frac{1}{\tilde{\theta}_{,s}} = \tilde{e}_{,s} \frac{1}{\tilde{e}_{,ss}}. \quad (36)$$

For further use we recall also the following relation (see Alt and Pawłow, 1996, Proposition 1, Sec.11)

$$\frac{\delta f}{\delta \epsilon} = \frac{\delta \tilde{e}}{\delta \epsilon}, \quad (37)$$

which follows from (35). Actually, since

$$\hat{f}(\epsilon, \mathbf{D}\epsilon, \theta) = \hat{\tilde{e}}(\epsilon, \mathbf{D}\epsilon, \hat{s}(\epsilon, \mathbf{D}\epsilon, \frac{1}{\theta})) - \theta \hat{s}(\epsilon, \mathbf{D}\epsilon, \frac{1}{\theta}),$$

the second identity in (35) implies that

$$f_{,\epsilon} = \tilde{e}_{,\epsilon}, \quad f_{,\mathbf{D}\epsilon} = \tilde{e}_{,\mathbf{D}\epsilon} \quad (38)$$

with appropriate arguments.

3. Constitutive equations

We represent the material non-homogeneity (nonlocality) by the strain gradients and the viscosity by the strain rate tensor as constitutive variables. To embed the modelling into thermodynamic theory we supplement the list of constitutive variables by the entropy and its gradients. The choice of entropy as an independent variable is convenient for exploiting the entropy inequality. Then, the internal energy \tilde{e} in the canonical representation as a constitutive function of the strain tensor and entropy plays the role of a thermodynamical potential.

The constitutive set is assumed in the following form

$$Y := (Y^0, Y^t),$$

where

$$Y^0 := (\epsilon, D\epsilon, \dots, D^{M_0}\epsilon, s, Ds, \dots, D^{K_0}s), \quad M_0 \geq 2, \quad K_0 \geq 1$$

is the stationary part associated with material non-homogeneity, and

$$Y^t := (\epsilon_t)$$

is the nonstationary part related to material viscosity. Here

$$D^m \epsilon := (\epsilon_{i_1 \dots i_m})_{i,j,i_1, \dots, i_m=1, \dots, n}, \quad 0 \leq m \leq M_0$$

is $(2+m)$ -th order tensor of variables corresponding to space derivatives

$$\nabla^m \epsilon = (\partial_{i_1} \dots \partial_{i_m} \epsilon_{i_1 \dots i_m})_{i,j,i_1, \dots, i_m=1, \dots, n}.$$

We use the convention $D^0 \epsilon = \epsilon$. We shall show that the set Y describes models with the first order strain-gradient internal energy \tilde{e} , characteristic for materials of grade 2 (see, e.g., Toupin, 1964). Higher strain rate gradients in the set Y^t would allow for higher order energies.

We consider the balance equations (27), (28) with constitutive equations

$$\tilde{e} = \hat{\tilde{e}}(Y), \quad \mathbf{q} = \hat{\mathbf{q}}(Y), \quad \boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}(Y). \quad (39)$$

In order to select a class of thermodynamically consistent models we apply the method based on evaluating the entropy inequality with undetermined multipliers (see Müller, 1985, Alt and Pawlow, 1996, and Pawlow, 2000, for application to phase transition models).

In particular, for the system (27), (29), (39) the entropy inequality asserts that:

$$s_t + \nabla \cdot \boldsymbol{\psi} - \boldsymbol{\lambda}_u \cdot (\mathbf{u}_{tt} - \nabla \cdot \boldsymbol{\sigma} - \mathbf{b}) - \lambda \left((\tilde{e} + \frac{|\mathbf{u}_t|^2}{2})_t + \nabla \cdot (-\mathbf{u}_t \cdot \boldsymbol{\sigma} + \mathbf{q}) - \mathbf{b} \cdot \mathbf{u}_t \right) \geq 0, \quad (40)$$

is satisfied for all fields \mathbf{u} , s , where $\boldsymbol{\psi} = \hat{\boldsymbol{\psi}}(Y)$ is the entropy flux, $\lambda = \hat{\lambda}(Y)$ and $\boldsymbol{\lambda}_u := -\hat{\lambda}(Y)\mathbf{u}_t$ are undetermined multipliers conjugated with the total

energy balance and the linear momentum balance, respectively. We note that inequality (40) is equivalent to

$$s_t + \nabla \cdot \boldsymbol{\psi} - \lambda(\tilde{e}_t + \nabla \cdot \mathbf{q} - \boldsymbol{\sigma} : \boldsymbol{\epsilon}_t) \geq 0. \quad (41)$$

Clearly, (41) implies that for system (27), (28), (39) the entropy principle is satisfied with the entropy source $\tau = \hat{\lambda}(Y)r$.

We impose the following structural assumptions:

(A1) Nondegeneracy condition

$$\hat{\tilde{e}}_{,s}(Y) > 0 \text{ for all } Y.$$

(A2) Relation between stationary energy and entropy fluxes

$$\boldsymbol{\psi}^{(0)} = \lambda^{(0)} \mathbf{q}^{(0)}$$

where

$$\mathbf{q}^{(0)} := \hat{\mathbf{q}}(Y^0, Y^t) |_{Y^t=0}$$

denotes the stationary energy flux, and other quantities are defined similarly.

In addition, without loss of generality, we assume that

(A3) the energy flux

$$\mathbf{q} = \mathbf{q}_0 - \boldsymbol{\epsilon}_t \cdot \mathbf{h}$$

splits into a heat flux $\mathbf{q}_0 = \hat{\mathbf{q}}_0(Y^0)$ and a nonstationary flux $\boldsymbol{\epsilon}_t \cdot \mathbf{h}$, where $\mathbf{h} = \hat{\mathbf{h}}(Y)$ is a certain third order tensor.

We shall prove the following

PROPOSITION 3.1 (*Consequences of the entropy inequality*) *Assume that for balance equations (27), (28) with constitutive relations (39) the entropy inequality (41) is satisfied, and (A1)–(A3) hold. Then $\tilde{e}, \lambda, \boldsymbol{\sigma}, \mathbf{q}$ and $\boldsymbol{\psi}$ obey the following relations:*

(i) *Internal energy relation*

$$\tilde{e} = \hat{\tilde{e}}(\boldsymbol{\epsilon}, \mathbf{D}\boldsymbol{\epsilon}, s);$$

(ii) *Multiplier relation*

$$\lambda = \hat{\lambda}(\boldsymbol{\epsilon}, \mathbf{D}\boldsymbol{\epsilon}, s) = \frac{1}{\hat{\tilde{e}}_{,s}} > 0;$$

(iii) *Entropy flux relation*

$$\boldsymbol{\psi} = \lambda \mathbf{q} \mathbf{q}_0 + \lambda \boldsymbol{\epsilon}_t \cdot (\tilde{e}_{, \mathbf{D}\boldsymbol{\epsilon}} - \mathbf{h});$$

(iv) *There exists a second order tensor $\boldsymbol{\sigma}^v = \hat{\boldsymbol{\sigma}}^v(Y)$ such that following are satisfied:*

(iv-1) *Stress tensor relation*

$$\boldsymbol{\sigma} = \frac{\delta \tilde{e}}{\delta \boldsymbol{\epsilon}} + \frac{1}{\lambda} (\mathbf{h} - \tilde{e}_{,D\boldsymbol{\epsilon}}) \cdot \nabla \lambda + \boldsymbol{\sigma}^v,$$

where

$$\frac{\delta \tilde{e}}{\delta \boldsymbol{\epsilon}} = \tilde{e}_{, \boldsymbol{\epsilon}} - \nabla \cdot \tilde{e}_{, D\boldsymbol{\epsilon}};$$

(iv-2) *Residual inequality*

$$\boldsymbol{\epsilon}_t : (\lambda \boldsymbol{\sigma}^v) + \nabla \lambda \cdot \mathbf{q}_0 \geq 0$$

for all fields \mathbf{u}, s .

The proof is given in Section 6.

Further, for simplicity, we denote

$$\boldsymbol{\sigma}^e = \tilde{e}_{, \boldsymbol{\epsilon}} = (\tilde{e}_{, \epsilon_{ij}}), \quad \boldsymbol{\sigma}^h = \tilde{e}_{, D\boldsymbol{\epsilon}} = (\tilde{e}_{, \epsilon_{ij,k}}).$$

Here $\boldsymbol{\sigma}^e$ is the elastic stress tensor, $\boldsymbol{\sigma}^h$ corresponds to the strain-gradient energy, $\nabla \cdot \boldsymbol{\sigma}^h = (\partial_k \sigma_{ijk}^h)$ is called the hyperstress tensor (see, e.g., Toupin, 1964), and $\boldsymbol{\sigma}^v = (\sigma_{ij}^v)$ is the viscous (dissipative) stress tensor.

We note that in case $c > 0$, due to (38), the following equalities (with appropriate arguments) take place

$$\boldsymbol{\sigma}^e = f_{, \boldsymbol{\epsilon}}, \quad \boldsymbol{\sigma}^h = f_{, D\boldsymbol{\epsilon}}.$$

We complement Proposition 3.1 by the following

REMARK 3.1 • *Assertions (i) - (iv) provide thermodynamical state laws for thermoviscoelastic materials of grade 2.*

- *The constitutive set Y is associated with internal energy \tilde{e} , which can depend only on the strain tensor, its gradient, and the entropy.*
- *Under thermal stability assumption, $c > 0$, by virtue of the duality relations (35), the multiplier λ can be identified with the inverse temperature. Hence, assumption (A1) is equivalent to the positivity of temperature. This property is satisfied for typical phase transitions models (see Section 5).*
- *The energy and entropy fluxes are unconventional. They contain nonequilibrium fluxes involving the tensor \mathbf{h} , and are related by the condition*

$$\boldsymbol{\psi} - \lambda \mathbf{q} = \lambda \boldsymbol{\epsilon}_t \cdot \boldsymbol{\sigma}^h.$$

Therefore, at least one of the fluxes must contain nonequilibrium part. Entropy flux relation (iii) generalizes the standard relation valid in equilibrium

$$\boldsymbol{\psi} = \lambda \mathbf{q}_0.$$

The entropy inequality imposes no restrictions on the tensor \mathbf{h} .

- *The difference $(\mathbf{h} - \boldsymbol{\sigma}^h)$ contributes to the stress part due to temperature gradient.*
- *(iv-2) is the residual inequality, which determines the constitutive equations for the heat flux \mathbf{q}_0 and the viscous stress tensor $\boldsymbol{\sigma}^v$.*

4. The model equations

Motivated by the previous result we consider here an augmented model with the multiplier as an additional independent variable. Let us set

$$\theta = \frac{1}{\lambda} > 0,$$

and treat the equation

$$\theta - \tilde{\epsilon}_{,s} = 0 \quad (42)$$

as an additional constraint. This equation defines a nonequilibrium temperature. Then, the residual inequality takes on the form of a standard dissipation inequality

$$\Sigma(\mathbf{X}; \omega) := \mathbf{X} \cdot \mathbf{J}(\mathbf{X}; \omega) \geq 0 \quad \text{for all } (\mathbf{X}; \omega) \quad (43)$$

where

$$\mathbf{X} := (\epsilon_t, \mathbf{D}(\frac{1}{\theta})), \quad \mathbf{J}(X, \omega) := (\frac{\sigma^v}{\theta}, \mathbf{q}_0), \quad \omega := (\epsilon, \mathbf{D}\epsilon, s, \frac{1}{\theta})$$

are thermodynamical forces, thermodynamical fluxes and state variables, respectively.

Σ is a dissipation scalar.

For a given potential $\tilde{\epsilon} = \tilde{\epsilon}(\epsilon, \mathbf{D}\epsilon, s)$, satisfying assumption (A1), the model consists of the linear momentum balance (27) and the energy balance (28), with equation (A3) for the energy flux \mathbf{q} , the stress tensor equation

$$\sigma = \frac{\delta \tilde{\epsilon}}{\delta \epsilon} + \theta(\mathbf{h} - \sigma^h) \cdot \nabla(\frac{1}{\theta}) + \sigma^v, \quad (44)$$

temperature equation (42), and dissipation inequality (43).

The solution of (43) can be characterized by means of the decomposition theorem due to Edelen (1973, 1974). It asserts that any mapping $J(X; \omega)$ from $E_n \times E_p$ into E_n , with E_n, E_p vector spaces of dimension n and p , respectively, which is continuous in ω and C^1 in X can be uniquely decomposed in the following way:

$$\mathbf{J}(\mathbf{X}; \omega) = \nabla_{\mathbf{X}} \mathcal{D}(\mathbf{X}; \omega) + \mathbf{U}(X; \omega), \quad (45)$$

$$\mathbf{X} \cdot \mathbf{U}(\mathbf{X}; \omega) = 0, \quad (46)$$

where $\mathcal{D}(\mathbf{X}; \omega)$ is a dissipation potential and $\mathbf{U}(\mathbf{X}; \omega)$ is an anomaly vector, given by

$$\mathcal{D}(\mathbf{X}; \omega) = \int_0^1 \mathbf{X} \cdot \mathbf{J}(\tau \mathbf{X}; \omega) d\tau + d(\omega), \quad (47)$$

$$U_k(\mathbf{X}; \omega) = \int_0^1 \tau \sum_{l=1}^n X_l \left(\frac{\partial J_k(\tau \mathbf{X}; \omega)}{\partial(\tau X_l)} - \frac{\partial J_l(\tau \mathbf{X}; \omega)}{\partial(\tau X_k)} \right) d\tau. \quad (48)$$

$\nabla_{\mathbf{X}}$ denotes the gradient with respect to \mathbf{X} ; $\mathbf{U}(\mathbf{X}; \omega)$ is unique and $\mathcal{D}(\mathbf{X}; \omega)$ is unique within an additive function of ω (physically irrelevant). With such a decomposition the dissipation inequality (43) reduces to

$$\Sigma(\mathbf{X}; \omega) = \mathbf{X} \cdot \nabla_{\mathbf{X}} \mathcal{D}(\mathbf{X}; \omega) \geq 0. \quad (49)$$

The equality $\mathbf{U} = 0$ is equivalent to Onsager's reciprocity relations. $\mathcal{D}(\mathbf{X}; \omega)$ is convex in \mathbf{X} and $\mathcal{D}(0; \omega)$ yields the absolute minimum of $\mathcal{D}(\mathbf{X}; \omega)$ for fixed ω . If $\mathbf{X} = 0$ then (provided $\mathbf{J} \in C^{1,0}$) $\Sigma(0; \omega) = 0$ and $\mathbf{J}(0; \omega) = 0$.

In our case the decomposition theorem, excluding anomalies (i.e. for $\mathbf{U} = 0$), provides the existence of a dissipation potential \mathcal{D} which is convex, nonnegative and homogeneous of a certain degree in the variables $\mathbf{D}(\frac{1}{\theta})$ and ϵ_t , and the following thermodynamic relationships

$$\mathbf{q}_0 = \frac{\partial \mathcal{D}}{\partial \mathbf{D}(\frac{1}{\theta})}, \quad \frac{\sigma^v}{\theta} = \frac{\partial \mathcal{D}}{\partial \epsilon_t}, \quad (50)$$

The standard example of a dissipation potential for the heat conduction is

$$\mathcal{D} = \frac{1}{2} k |\nabla \log \theta|^2 = \frac{1}{2} k \theta^2 |\nabla(\frac{1}{\theta})|^2$$

where $k > 0$ is the heat conductivity coefficient. It governs the Fourier law for an isotropic continuum

$$\mathbf{q}_0 = -k \nabla \theta. \quad (51)$$

The standard dissipation potential for the viscosity is analogous to the elastic free energy of an isotropic continuum (see Landau and Lifshytz, 1987, Chap.V)

$$\mathcal{D} = \frac{1}{\theta} \left\{ \eta [(\epsilon_t)_{ik} - \frac{1}{3} \delta_{ik} (\epsilon_t)_{ll}]^2 + \frac{\xi}{2} (\epsilon_t)_{ll}^2 \right\}$$

where $\eta > 0$ and $\xi > 0$ are two viscosity coefficients. By virtue of (50), σ^v is given by

$$\sigma_{ik}^v = (\mathbf{A} \epsilon_t)_{ik} := \xi (\epsilon_t)_{ll} \delta_{ik} + 2\eta [(\epsilon_t)_{ik} - \frac{1}{3} \delta_{ik} (\epsilon_t)_{ll}], \quad (52)$$

where \mathbf{A} corresponds to the fourth order tensor of linearized elasticity. Equation (52) expressed in the inverted form

$$(\epsilon_t)_{ik} = \frac{1}{9\xi} \delta_{ik} \sigma_{ll}^v + \frac{1}{2\eta} (\sigma_{ik}^v - \frac{1}{3} \delta_{ik} \sigma_{ll}^v) \quad (53)$$

represents linear Hooke's-like law.

We shall show now that the augmented model is thermodynamically consistent:

PROPOSITION 4.1 Consider the system of balance laws (27), (29) with temperature given by equation (42), and stress tensor by (44). We assume that internal energy $\tilde{e} = \tilde{e}(\epsilon, \mathbf{D}\epsilon, s)$ satisfies assumption (A1), and that the heat flux \mathbf{q}_0 and the viscous stress σ^v satisfy inequality (43). Then the entropy inequality

$$\begin{aligned} s_t + \nabla \cdot \psi &- \lambda_u \cdot (\mathbf{u}_{tt} - \nabla \cdot \sigma - \mathbf{b}) \\ &- \lambda_1 \left(\left(\tilde{e} + \frac{|\mathbf{u}_t|^2}{2} \right)_t + \nabla \cdot (-\mathbf{u}_t \cdot \sigma + \mathbf{q}) - \mathbf{b} \cdot \mathbf{u}_t \right) \\ &- \lambda_2 (\theta - \tilde{e}_{,s}) \\ &= \epsilon_t : \left(\frac{\sigma^v}{\theta} \right) + \nabla \cdot \left(\frac{1}{\theta} \right) \cdot \mathbf{q}_0 =: \Sigma \geq 0 \end{aligned} \quad (54)$$

is satisfied for all fields $\mathbf{u}, s, \frac{1}{\theta}$, where the entropy flux ψ is given in Proposition 3.1 (iii) with $\lambda = \frac{1}{\theta}$, and the multipliers are

$$\lambda_u = -\lambda_1 \mathbf{u}_t, \quad \lambda_1 = \frac{1}{\theta}, \quad \lambda_2 = \frac{s_t}{\theta}. \quad (55)$$

The proof is given in Section 6.

We shall show that the above assertion implies the Lyapunov property for the Gibbs function, defined by

$$V = \alpha_0 \left(\tilde{e} + \frac{|\mathbf{u}_t|^2}{2} \right) - s,$$

where $\alpha_0 = \text{const.} > 0$. By Proposition 4.1 it follows that for solutions of system (27), (29), (42), (44) the following identity is satisfied

$$V_t + \nabla \cdot \left(\left(\alpha_0 - \frac{1}{\theta} \right) (\mathbf{q}_0 - \epsilon_t \cdot \mathbf{h}) - \frac{1}{\theta} \epsilon_t \cdot \sigma^h - \alpha_0 \mathbf{u}_t \cdot \sigma \right) + \left(\frac{1}{\theta} - \alpha_0 \right) r - \alpha_0 \mathbf{b} \cdot \mathbf{u}_t + \Sigma = 0. \quad (56)$$

Assuming vanishing heat source and body forces, $r = 0$, $\mathbf{b} = 0$, we obtain from (56) the growth relation

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} V dx + \int_{\partial\Omega} \left(\alpha_0 - \frac{1}{\theta} \right) (\mathbf{q}_0 - \epsilon_t \cdot \mathbf{h}) \cdot \mathbf{n} dS - \int_{\partial\Omega} \frac{1}{\theta} (\epsilon_t \cdot \sigma^h) \cdot \mathbf{n} dS \\ - \int_{\partial\Omega} \alpha_0 (\mathbf{u}_t \cdot \sigma) \cdot \mathbf{n} dS = - \int_{\Omega} \Sigma dx \leq 0. \end{aligned}$$

Hence, if boundary conditions

$$(\mathbf{q}_0 - \epsilon_t \cdot \mathbf{h}) \cdot \mathbf{n} = 0, \quad (\epsilon_t \cdot \sigma^h) \cdot \mathbf{n} = 0, \quad (\mathbf{u}_t \cdot \sigma) \cdot \mathbf{n} = 0$$

are satisfied on $\partial\Omega$, the Lyapunov relation follows

$$\frac{d}{dt} \int_{\Omega} V dx = - \int_{\Omega} \Sigma dx \leq 0.$$

Under assumption of thermal stability, $c > 0$, the formulation of the model can be simplified. Due to (36), the internal energy \tilde{e} is then strictly convex in the entropy s . Consequently, relation (42) between entropy s and temperature θ defines a transformation. Therefore, in such a case one can use alternatively (\mathbf{u}, s) or (\mathbf{u}, θ) as independent variables.

We summarize here the governing equations: In terms of (\mathbf{u}, s) variables the governing potential is the internal energy $\tilde{e} = \tilde{e}(\epsilon, D\epsilon, s)$ with the properties in (A1). The field equations are balance laws of linear momentum (27) and energy (28), with the stress tensor σ , the energy flux \mathbf{q} and the temperature θ given by (44), (A3), and (42), respectively. The heat flux \mathbf{q}_0 and the viscous stress tensor σ^v are given correspondingly by Fourier and Hooke's law.

The advantage of (\mathbf{u}, s) -formulation is that there is no sign constraint on the solution. However, the disadvantage is the lack of boundedness of the leading coefficients of the energy equation.

In terms of (\mathbf{u}, θ) variables the potential is the free energy $f = \hat{f}(\epsilon, D\epsilon, \theta)$ related to $\tilde{e} = \tilde{e}(\epsilon, D\epsilon, s)$ by the first equality in duality relations (35). We note that the second equality in (35) is equivalent to the second equality in Gibbs relations (30).

Due to relationship (37), the stress equation (44) turns into the form

$$\sigma = \frac{\delta f}{\delta \epsilon} + \theta(\mathbf{h} - f_{,D\epsilon}) \cdot \nabla\left(\frac{1}{\theta}\right) + \sigma^v. \quad (57)$$

Two extreme cases for the strain-gradient term of f are of interest: the energetic case, $f_{,\theta D\epsilon} = 0$, and the entropic case $(\frac{f}{\theta})_{,\theta D\epsilon} = 0$, i.e. f with the strain-gradient term independent of θ and linearly dependent on θ , respectively. The energetic case is typical for shape memory alloys (see, e.g. Falk, 1982, 1990). The entropic case is characteristic for polymer materials (see examples in Alt and Pawłow, 1996).

In the energetic case the choice $\mathbf{h} = \sigma^h$ gives σ independent of $\nabla\theta$. Then the energy flux is

$$\mathbf{q} = \mathbf{q}_0 - \epsilon_t \cdot \sigma^h,$$

and the entropy flux is stationary,

$$\psi = \lambda \mathbf{q}_0.$$

In the entropic case the choice $\mathbf{h} = 0$ gives σ independent of $\nabla\theta$. Then the equation for the stress tensor becomes

$$\frac{\sigma}{\theta} = \frac{\delta}{\delta \epsilon} \left(\frac{f}{\theta} \right) + \frac{\sigma^v}{\theta}, \quad (58)$$

and the nonstationary flux appears in the entropy equation.

By Gibbs relations (30) it follows that

$$e_t = f_{,;\epsilon} : \epsilon_t + f_{,D\epsilon} : \nabla \epsilon_t + \theta s_t,$$

and

$$s_t = -f_{,\theta\epsilon} : \epsilon_t - f_{,\theta D\epsilon} : \nabla \epsilon_t - f_{,\theta\theta} \theta_t.$$

Hence, using expression (33) for the specific heat, the energy equation can be recast into the form

$$c(\epsilon, \theta)\theta_t + \nabla \cdot (\mathbf{q}_0 - \epsilon_t \cdot \mathbf{h}) = \sigma : \epsilon_t - (f - \theta f_{,\theta})_{,\epsilon} : \epsilon_t - (f - \theta f_{,\theta})_{,D\epsilon} : \nabla \epsilon_t + r.$$

One can see that with the choice $\mathbf{h} = \sigma^h$ the above equation simplifies to the form

$$c(\epsilon, \theta)\theta_t + \nabla \cdot \mathbf{q}_0 = \theta f_{,\theta\epsilon} : \epsilon_t + \theta f_{,\theta D\epsilon} : \nabla \epsilon_t + \sigma^v : \epsilon_t + r. \quad (59)$$

In consequence, in such a case the system takes on the form of the elasticity equation

$$\mathbf{u}_{tt} - \nabla \cdot (f_{,\epsilon} - \nabla \cdot f_{,D\epsilon} + \sigma^v) = \mathbf{b} \quad (60)$$

coupled to the energy equation (59), with \mathbf{q}_0 and σ^v given by Fourier's and Hook's laws, respectively.

We note also that in the energetic case equations (60), (59) provide system (14), (15), which has been studied in Pawłowski and Źochowski (2000).

The system should be completed by the initial conditions

$$\mathbf{u}(0, x) = \mathbf{u}_0(x), \quad \mathbf{u}_t(0, x) = \mathbf{u}_1(x), \quad \theta(0, x) = \theta_0(x) \text{ in } \Omega,$$

and appropriate boundary conditions, for example

$$\begin{aligned} \mathbf{u} &= 0 \text{ on } \Gamma_0, & \sigma \cdot \mathbf{n} &= \mathbf{b}_1 \text{ on } \Gamma_1, \\ & & \sigma^h \cdot \mathbf{n} &= 0 \text{ on } \partial\Omega, \\ \nabla \theta \cdot \mathbf{n} &= p_0 k_0 (\theta_{ext} - \theta) \text{ on } \partial\Omega, \end{aligned}$$

where Γ_0 and Γ_1 are disjoint parts of the boundary $\partial\Omega = \Gamma_0 \cup \Gamma_1$, $\Gamma_0 \cap \Gamma_1 = \emptyset$, and \mathbf{n} is the unit outward normal to $\partial\Omega$. The above boundary conditions express, respectively, that the body is fixed on the part Γ_0 , subject to a boundary force \mathbf{b}_1 on Γ_1 , the normal of the strain-gradient tensor σ^h vanishes on $\partial\Omega$, and there is heat exchange through $\partial\Omega$ with external temperature θ_{ext} and heat exchange coefficient p_0 .

Finally, we note that the field equations corresponding to the entropic case, with the specific choice $\mathbf{h} = 0$ and σ given by (58) read as follows

$$\begin{aligned} \mathbf{u}_{tt} - \nabla \cdot (\mathbf{A}\epsilon_t) + \nabla \cdot \left(\theta \nabla \cdot \left(\frac{f_{,D\epsilon}}{\theta} \right) \right) &= \nabla \cdot f_{,\epsilon} + \mathbf{b}, \\ c(\epsilon, \theta)\theta_t - \nabla \cdot (k\nabla\theta) &= \theta f_{,\theta\epsilon} : \epsilon_t - \theta \left(\nabla \cdot \left(\frac{f_{,D\epsilon}}{\theta} \right) \right) : \epsilon_t + (\mathbf{A}\epsilon_t) : \epsilon_t + r. \end{aligned} \quad (61)$$

In this case energy equation includes contribution due to the hyperstress tensor. As far as we know, such class of thermoelastic systems has not been considered in the literature.

5. Examples of free energy density

Example 1. The Falk model for 1-D shape memory alloys (SMA) (see Falk, 1982, 1990). The free energy density has the Ginzburg-Landau-Devonshire form

$$f(\epsilon, \mathbf{D}\epsilon, \theta) = f_0(\epsilon, \theta) + f^G(\mathbf{D}\epsilon) \quad (62)$$

where f_0 and f^G denote the volumetric and strain-gradient contributions, given by

$$\begin{aligned} f_0(\epsilon, \theta) &= f_*(\theta) + f_1(\theta)f_2(\epsilon) + f_3(\epsilon), & f^G(\mathbf{D}\epsilon) &= \frac{1}{2}\kappa |\mathbf{D}\epsilon|^2, \\ f_*(\theta) &= -c_v\theta \log \theta, & f_1(\theta) &= \theta, & f_2(\epsilon) &= \frac{1}{2}a_2\epsilon^2, \\ f_3(\epsilon) &= -\theta_1 f_2(\epsilon) - \frac{1}{4}a_4\epsilon^4 + \frac{1}{6}a_6\epsilon^6. \end{aligned} \quad (63)$$

Here $c_v, a_2, a_4, a_6, \theta_1, \kappa$ are nonnegative constants; $\epsilon = u_x$ is the strain, $c_v > 0$ is the caloric specific heat coefficient, $\kappa > 0$ is the surface energy coefficient.

According to Gibbs relations, the corresponding expressions for the internal energy e and the entropy s are

$$e = \hat{e}(\epsilon, \mathbf{D}\epsilon, \frac{1}{\theta}) = c_v\theta + (f_1(\theta) - \theta f_1'(\theta))f_2(\epsilon) + f_3(\epsilon) + \frac{1}{2}\kappa |\mathbf{D}\epsilon|^2, \quad (64)$$

$$-s = \hat{s}(\epsilon, \mathbf{D}\epsilon, \frac{1}{\theta}) = -c_v(\log \theta + 1) + f_1'(\theta)f_2(\epsilon). \quad (65)$$

The corresponding specific heat coefficient is

$$c = \hat{c}(\epsilon, \mathbf{D}\epsilon, \theta) = c_v - \theta f_1''(\theta)f_2(\epsilon). \quad (66)$$

Assume that f_1 is concave, so that $c > 0$ for all arguments. Consequently, by duality relations, the temperature expressed as a function of entropy, $\theta = \hat{\theta}(\epsilon, \mathbf{D}\epsilon, s)$, is given by

$$\theta = \exp\left(\frac{1}{c_v}s + \frac{1}{c_v}f_1'(\theta)f_2(\epsilon) - 1\right). \quad (67)$$

In the standard case, $f_1(\theta) = \theta$, so that

$$\theta = \exp\left(\frac{s + f_2(\epsilon)}{c_v} - 1\right).$$

Note that since s does not depend on $\mathbf{D}\epsilon$ the transformation between s and θ does not involve $\mathbf{D}\epsilon$. Moreover, the constraint $0 < \theta < \infty$ is equivalent to $s_* < s < s^*$ with $s_*(\epsilon, \mathbf{D}\epsilon) = -\infty$ and $s^*(\epsilon, \mathbf{D}\epsilon) = +\infty$, that is - for this example there are no constraints on the entropy s . The expression for $\bar{e} = \hat{e}(\epsilon, \mathbf{D}\epsilon, s)$ follows by setting in (64) $\theta = \hat{\theta}(\epsilon, \mathbf{D}\epsilon, s)$.

Example 2. A model for noncrystalline shape memory material in the 2-D case (see Źochowski, 1992, 1993).

The corresponding expression for the free energy in 2-D has been derived by averaging the 1-D Falk free energy. The model is justified for a polymer consisting of long molecular chains which exhibit one-dimensional shape memory effect and point in random directions with negligible interactions at a microscopic level.

The idea is of averaging based on considering a single cell of unit size on a plane with a string connecting opposite sides, and having the elastic energy

$$F_s(\epsilon_{11}, \theta) = \frac{1}{2}a_2 f_1(\theta) \epsilon_{11}^2 - \frac{1}{4}a_4 \epsilon_{11}^4 + \frac{1}{6}a_6 \epsilon_{11}^6. \quad (68)$$

An application of the following 2-D transformation rule for the strain ϵ

$$\epsilon_{11}(\alpha) = \boldsymbol{\tau}^T(\alpha) \boldsymbol{\epsilon} \boldsymbol{\tau}(\alpha),$$

where $\boldsymbol{\tau}(\alpha) = (\cos\alpha, -\sin\alpha)^T$, and α denotes the inclination angle of the string with respect to x_1 -axis, gives

$$\epsilon_{11}(\alpha) = (\cos^2\alpha)\epsilon_{11} + (\sin^2\alpha)\epsilon_{22} - 2(\sin\alpha\cos\alpha)\epsilon_{12}.$$

The averaged elastic energy density is

$$F(\epsilon, \theta) = \frac{1}{2\pi} \int_0^{2\pi} F_s(\epsilon_{11}(\alpha), \theta) d\alpha.$$

Thus, the volumetric free energy density, which is the sum of the caloric and the elastic energy, is given by

$$f_0 = \hat{f}_0(\epsilon, \theta) = f_*(\theta) + F(\epsilon, \theta). \quad (69)$$

Example 3. The 3-D Falk-Konopka model for SMA (see Falk and Konopka, 1990).

An elastic free energy density, dependent on the full strain tensor and the temperature, which is invariant with respect to the cubic symmetry of the high temperature phase, has been proposed in the form of a sixth order expansion

$$F(\epsilon, \theta) = \sum_{i=1}^3 F_i^2 J_i^2 + \sum_{i=1}^5 F_i^4 J_i^4 + \sum_{i=1}^2 F_i^6 J_i^6 \quad (70)$$

expressed in terms of invariants J_i^k , $i = 1, \dots, i^k$, of k -th order corresponding to material parameters F_i^k . J_i^k are given by

$$\begin{aligned} J_1^2 &= \epsilon_1^2, & J_2^2 &= 3\epsilon_2^2 + \epsilon_3^2, & J_3^2 &= \epsilon_4^2 + \epsilon_5^2 + \epsilon_6^2, \\ J_1^4 &= (J_2^2)^2, & J_2^4 &= \epsilon_4^4 + \epsilon_5^4 + \epsilon_6^4, & J_3^4 &= (J_3^2)^2, & J_4^4 &= J_2^2 J_3^2, \\ J_5^4 &= \epsilon_4^2(\epsilon_2 - \epsilon_3)^2 + \epsilon_5^2(\epsilon_2 + \epsilon_3)^2 + 4\epsilon_6^2\epsilon_2^2, \\ J_1^6 &= (J_2^2)^3, & J_2^6 &= \epsilon_2^2(\epsilon_2^2 - \epsilon_3^2)^2, \end{aligned}$$

where

$$\begin{aligned}\epsilon_1 &= (\epsilon_1 + \epsilon_2 + \epsilon_3)/3, & \epsilon_2 &= (2\epsilon_3 - \epsilon_1 - \epsilon_2)/6, \\ \epsilon_3 &= (\epsilon_1 - \epsilon_2)/2, & \epsilon_4 &= \epsilon_4/2, & \epsilon_5 &= \epsilon_5/2, & \epsilon_6 &= \epsilon_6/2,\end{aligned}$$

and the following strain notation is used

$$\begin{aligned}\epsilon_1 &= \epsilon_{11}, & \epsilon_2 &= \epsilon_{22}, & \epsilon_3 &= \epsilon_{33}, \\ \epsilon_4 &= 2\epsilon_{23}, & \epsilon_5 &= 2\epsilon_{13}, & \epsilon_6 &= 2\epsilon_{12}.\end{aligned}$$

Here, in contrast to 1-D SMA, not only a second order but also higher order material parameters F_i^k can depend on temperature. For a CuAlNi alloy a linear dependence on temperature of a fourth order coefficient is determined by comparison with experiment (see Falk and Konopka, 1990, Sec. 5).

Example 4. Model for ferroelastic material in 2-D (see Barsch and Krumhansl, 1984).

Heterogeneous structures in ferroelastic materials where a cubic prototype phase may deform into three tetragonal variants are described by the Ginzburg-Landau free energy density of the form

$$\begin{aligned}f(\epsilon, \mathbf{D}\epsilon, \theta) &= f_0(\epsilon, \theta) + f^G(\mathbf{D}\epsilon), & (71) \\ f_0 &= A(e_2^2 + e_3^2) + Be_3(e_2^2 - 3e_3^2) + C(e_2^2 + e_3^2)^2, \\ f^G &= g[(\partial_1 e_2)^2 + (\partial_2 e_2)^2 + ((\partial_1 e_3)^2 + (\partial_2 e_3)^2)/3 \\ &\quad + 2(\partial_1 e_2 \partial_1 e_3 - \partial_2 e_2 \partial_2 e_3)/\sqrt{3}] \\ &\quad + h[(\partial_1 e_3)^2 + (\partial_2 e_3)^2 - \sqrt{3}(\partial_1 e_2 \partial_1 e_3 - \partial_2 e_2 \partial_2 e_3)]\end{aligned}$$

where

$$\begin{aligned}e_1 &= (\epsilon_{11} + \epsilon_{22} + \epsilon_{33})/\sqrt{3}, & e_2 &= (\epsilon_{11} - \epsilon_{22})/\sqrt{2}, \\ e_3 &= (\epsilon_{11} + \epsilon_{22} - 2\epsilon_{33})/\sqrt{6}, & e_4 &= \epsilon_{23}, & e_5 &= \epsilon_{13}, & e_6 &= \epsilon_{12}\end{aligned}$$

are symmetry strains appropriate for cubic symmetry, ϵ_{ij} are components of the strain tensor, A, B and $C > 0$ are elastic constants, g, h are strain gradient coefficients describing nonlocal elastic behaviour. The coefficient A depends linearly on temperature θ .

The assumption underlying (71) is that the phase transformation is described by the two-component order parameter (e_2, e_3) and is independent of x_3 .

6. Proofs of Propositions 3.1 and 4.1

Proof of Proposition 3.1. We use the method of exploiting the entropy inequality with undetermined multipliers, presented in detail in Pawłow (2000). A constitutive function on the set Y is defined as the following extension

$$\begin{aligned}\hat{q}(\epsilon_{ij}, \dots, \mathbf{A}_{ij}^m + (\mathbf{A}_{ij}^m)^{skew}, \dots, s, \dots, \mathbf{B}^m + (\mathbf{B}^m)^{skew}, \dots) \\ =: \hat{q}(\epsilon_{ij}, \dots, (\mathbf{A}_{ij}^m), \dots, s, \mathbf{B}^m, \dots)\end{aligned}$$

for all tensors \mathbf{A}_{ij}^m and \mathbf{B}^m denoting $\mathbf{D}^m \epsilon_{ij}$ for $2 \leq m \leq M_0$ and $\mathbf{D}^m s$ for $2 \leq m \leq K_0$, respectively. We are doing so, because e.g. in the case of $\mathbf{D}^2 \epsilon_{ij}$ the variables $\epsilon_{ij,kl}$ and $\epsilon_{ij,lk}$ are treated as independent despite the equality $\partial_k \partial_l \epsilon_{ij} = \partial_l \partial_k \epsilon_{ij}$.

For $f = \hat{f}(Y)$ a smooth scalar-valued function of its arguments, we denote the algebraic version of spatial derivative restricted to stationary variables Y^0 by

$$\partial_i^{Y^0} f := \sum_{m=0}^{M_0} f_{, \mathbf{D}^m \epsilon} : \mathbf{D}^m \epsilon_{,i} + \sum_{m=0}^{K_0} f_{, \mathbf{D}^m s} : \mathbf{D}^m s_{,i} \quad i = 1, \dots, n,$$

and by $\nabla^{Y^0} f$ the corresponding gradient. Similarly, for a smooth vector-valued function $\psi = \hat{\psi}(Y)$ with values in \mathbb{R}^n the algebraic version of the divergence restricted to stationary variables Y^0 is denoted by $\nabla^{Y^0} \cdot \psi$.

By inserting the constitutive equations into the entropy inequality (41) and applying chain rule we get

$$\begin{aligned} & s_t + \psi_{, \epsilon_t} : \mathbf{D} \epsilon_t + \nabla^{Y^0} \cdot \psi - \lambda \tilde{e}_{, \epsilon_t} : \epsilon_{tt} \\ & - \lambda \sum_{k=0}^{M_0} \tilde{e}_{, \mathbf{D}^k \epsilon} : \mathbf{D}^k \epsilon_t - \lambda \sum_{k=0}^{K_0} \tilde{e}_{, \mathbf{D}^k s} : \mathbf{D}^k s_t \\ & - \lambda \mathbf{q}_{, \epsilon_t} : \mathbf{D} \epsilon_t - \lambda \nabla^{Y^0} \cdot \mathbf{q} + \lambda \sigma : \epsilon_t \geq 0 \end{aligned} \quad (72)$$

for all variables (Z, Y) . Here

$$Z := (\epsilon_{tt}, (\mathbf{D}^k \epsilon_t)_{1 \leq k \leq M_0}, (\mathbf{D}^k s_t)_{0 \leq k \leq K_0}, \mathbf{D}^{M_0+1} \epsilon, \mathbf{D}^{K_0+1} s).$$

denotes the set of variables in which the left-hand side of (72) is linear. By the linearity in ϵ_{tt} , $\mathbf{D}^k \epsilon_t$ for $2 \leq k \leq M_0$ and in $\mathbf{D}^k s_t$ for $1 \leq k \leq K_0$, it follows that the corresponding coefficients have to vanish. This implies assertion (i). The linearity in s_t together with assumption (A1) implies assertion (ii). The terms linear in $\mathbf{D} \epsilon_t$ yield the equality

$$\psi_{, \epsilon_t} - \lambda \mathbf{q}_{, \epsilon_t} - \lambda \tilde{e}_{, \mathbf{D} \epsilon} = 0. \quad (73)$$

Let us set

$$\tilde{\psi} := \psi - \lambda \mathbf{q}. \quad (74)$$

Owing to assumption (A2), $\tilde{\psi}^{(0)} = 0$. Since λ is independent of ϵ_t , (73) gives

$$\tilde{\psi}_{, \epsilon_t} = \lambda \tilde{e}_{, \mathbf{D} \epsilon}.$$

Hence,

$$\tilde{\psi} = \lambda \epsilon_t \cdot \tilde{e}_{, \mathbf{D} \epsilon}, \quad (75)$$

which together with (74) shows assertion (iii).

With the above conclusions inequality (72) is reduced to

$$\epsilon_t : (\lambda \sigma - \lambda \tilde{e}_{,\epsilon}) + \nabla^{Y^0} \cdot \psi - \lambda \nabla^{Y^0} \cdot \mathbf{q} \geq 0. \quad (76)$$

We have the following easily verified identities

$$\begin{aligned} \nabla^{Y^0} \cdot \psi - \lambda \nabla^{Y^0} \cdot \mathbf{q} &= \nabla^{Y^0} \cdot \tilde{\psi} + \nabla \lambda \cdot \mathbf{q}, \\ \nabla^{Y^0} \cdot \tilde{\psi} &= \epsilon_t : (\tilde{e}_{,D\epsilon} \cdot \nabla \lambda + \lambda \nabla \cdot \tilde{e}_{,D\epsilon}), \end{aligned}$$

where we have used the fact that, due to (ii), $\nabla \lambda = \nabla^{Y^0} \lambda$.

With these identities the equality (76) becomes

$$\epsilon_t : (\lambda \sigma - \lambda \tilde{e}_{,\epsilon} + \lambda \nabla \cdot \tilde{e}_{,D\epsilon} + \tilde{e}_{,D\epsilon} \cdot \nabla \lambda) + \nabla \lambda \cdot \mathbf{q} \geq 0. \quad (77)$$

We note that, by assumption on M_0, K_0 , the left-hand side of (77) depends on the variables in Y . Using assumption (A3), the identity

$$\nabla \lambda \cdot (\epsilon_t \cdot \mathbf{h}) = \epsilon_t : (\mathbf{h} \cdot \nabla \lambda),$$

and defining the second order tensor σ^v , dependent on the variables in Y , by

$$\lambda \sigma^v = \lambda \sigma - \lambda \frac{\delta \tilde{e}}{\delta \epsilon} + (\tilde{e}_{,D\epsilon} - \mathbf{h}) \cdot \nabla \lambda, \quad (78)$$

we obtain inequality (77) in the form

$$\epsilon_t : (\lambda \sigma^v) + \nabla \lambda \cdot \mathbf{q}_0 \geq 0. \quad (79)$$

Together with (78) this shows assertion (iv). ■

Proof of Proposition 4.1. Let $\mathbf{u}, s, w = \frac{1}{\theta}$ be any fields. We multiply the left-hand sides of equations (27), (29), and (42) by λ_u, λ_1 , and λ_2 , which are defined in (55), respectively. Then we get from (27) and (29),

$$\begin{aligned} &\lambda_u \cdot (\mathbf{u}_{tt} - \nabla \cdot \sigma - \mathbf{b}) + \lambda_1 \left((\tilde{e} + \frac{|\mathbf{u}_t|^2}{2})_t + \nabla \cdot (-\mathbf{u}_t \cdot \sigma + \mathbf{q}) - \mathbf{b} \cdot \mathbf{u}_t \right) \\ &= w \tilde{e}_t + w \nabla \cdot \mathbf{q} - w \epsilon_t : \frac{\delta \tilde{e}}{\delta \epsilon} - \epsilon_t : ((\mathbf{h} - \sigma^h) \cdot \nabla w) - w \sigma^v : \epsilon_t, \end{aligned} \quad (80)$$

and from (42),

$$\lambda_2 (\theta - \tilde{e}_{,s}) = s_t - w \tilde{e}_{,s} s_t. \quad (81)$$

Note that for the first term on the right-hand side of (80) we have

$$w \tilde{e}_t = w \sigma^e : \epsilon_t + w \sigma^h : \nabla \epsilon_t + w \tilde{e}_{,s} s_t. \quad (82)$$

The second term on the right-hand side of (80) we write in the form

$$w \nabla \cdot \mathbf{q} = \nabla \cdot (w \mathbf{q}) - \nabla w \cdot (\mathbf{q}_0 - \epsilon_t \cdot \mathbf{h}). \quad (83)$$

The third term on the right-hand side of (80) equals to

$$\begin{aligned} -w\epsilon_t : \frac{\delta \tilde{e}}{\delta \epsilon} &= -w\epsilon_t : (\sigma^e - \nabla \cdot \sigma^h) \\ &= -w\sigma^e : \epsilon_t - w\sigma^h : \nabla \epsilon_t + \nabla \cdot (w\epsilon_t \cdot \sigma^h) - \nabla w \cdot (\epsilon_t \cdot \sigma^h). \end{aligned} \quad (84)$$

Hence, by adding (80) and (81) it follows that the sum of the last three terms on the left-hand side of (54) is equal to $-(s_t + \nabla \cdot \psi - \Sigma)$. Together with inequality (43) this shows inequality (54). ■

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