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On diffused-interface models of shape memory alloys

by

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Abstract: The paper surveys mathematical models of thermomechanical evolution of shape memory alloys and related mathematical results. The survey is confined to so-called diffused-interface or phase-field models based on Landau-Ginzburg free energy as a thermodynamic potential. It includes the well-known models due to Falk, Frémond and Fried-Gurtin. The focus is on a three-dimensional (3-D) generalization of Falk's model based on the linearized strain tensor, absolute temperature and strain tensor gradient. For such model the thermodynamical basis and the recent mathematical results on its well-posedness are presented.
Keywords: shape memory alloys, diffused-interface models, Landau-Ginzburg free energy, existence and uniqueness of solutions

1. Introduction

The ability of some metallic alloys to "remember" certain predefined shapes has been the focus of extensive studies since many years. Such alloys can be deformed to a particular shape at some temperature, but after heating they revert to their original shape. This phenomenon, known as shape memory effect, is due to the ability of the material to change its lattice structure from a high symmetry phase (austenite) to a lower symmetry phase (martensite). The change of structure, activated by stress or temperature, reflects the phase transition in solid.

The goal of this paper is to review mathematical models of thermomechanical evolution of shape memory alloys and related mathematical results.

As it is well-known there are two main approaches to describe phase transitions in continuum mechanics: the sharp interface and the diffused-interface or phase-field theories, see e.g. Gurtin and Struthers (1990), Fried and Gurtin (1994, 1999), Fried and Grach (1997), Šilhavý (1985).

In the first one the interface separating the coexisting phases is considered as a two-dimensional surface of discontinuity of the first deformation gradient (strain), and in the second one the interface is treated as a thin three-dimensional region where strain changes considerably but smoothly.

The first approach corresponds to a potential of Landau form based on an order parameter, and the second one to a potential of Landau-Ginzburg form involving order parameter and its gradient. The order parameter is an internal quantity which characterizes the difference between the phases of the material.

In the present paper we shall confine ourselves to diffused-interface approach based on Landau-Ginzburg free energy as a potential. Within this approach we present the following one- and three-dimensional (1- and 3-D) models which differ in the choice of the order parameter:

(i) 1-D Falk's model (Falk, 1980, 1982, 1983, 1990) based on free energy depending on the scalar sheer strain, temperature and sheer strain gradient;

(ii) 3-D generalization of Falk's model based on the linearized strain tensor, temperature and strain tensor gradient (see Pawłow, 2000b, for thermodynamical derivation, and Pawłow and Żochowski, 2001, 2002, Pawłow and Zajączkowski, 2002a, 2000b, for mathematical results);

(iii) 3-D Frémond's model (Frémond, 1987, 1990, 2002) based on the phase ratios, the linearized strain tensor, temperature and gradient of the strain tensor trace;

(iv) 3-D isothermal Fried-Gurtin model (Fried and Gurtin, 1994) based on the deformation gradient, a multicomponent order parameter and its gradient.

We focus our attention on the second class of models, for which we present the corresponding thermodynamical framework. In discussing other models we refer, whenever possible, to this framework. We mention that the Landau-Ginzburg approach based on the strain tensor as an order parameter has been used in Barsch and Krumhansl (1984, 1988) where physically justified 2-D elastic and strain gradient energies have been proposed.

Our thermomechanical model, which constitutes a 3-D counterpart of Falk's model, is based on the elastic energy due to Falk and Konopka (1990). This 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. We mention that there are other elastic energy models for shape memory materials, e.g., the model due to 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. Such energy has been used by Klouček and Luskin (1994) for numerical simulation of shape memory alloy dynamics in 3-D, with temperature treated as a parameter.

For an account on modelling and mathematical aspects of shape memory alloys, apart from the papers cited in the text, we refer to the monographs by Brokate and Sprekels (1996) Chapter 4, 5, Frémond (2002) Chapter 13, Frémond and Miyazaki (1996), Zheng (1995) Chapter 4. For comprehensive references concerning the subject we refer to Sprekels (1990), Spies (1995), Roubíček (1999), Bonetti (2001), Müller and Seelecke (2001), Bernardini (2001). We mention also that recently a hysteresis operator approach has been applied to model the dynamics of 1-D shape memory alloy, see Aiki and Kenmochi (2001).

The plan of the paper is as follows:

In Section 2 we outline the 1-D Falk's model and review briefly the results concerning its well-posedness. We point out the methods based on parabolic decomposition of the momentum balance which can be extended to the 3-D case.

In Section 3 we outline the thermodynamically consistent constitutive equations for 3-D thermoelasticity models with free energy depending on strain tensor, its gradient and absolute temperature. We derive the availability identity, which provides the energy estimates for such class of models, and discuss a Lyapunov relation.

In Section 4 we formulate a 3-D nonlinear thermoelasticity system representing a counterpart of 1-D Falk's model. For such a system we present recent results on global in time existence and uniqueness of solutions and comment on difficulties in the mathematical treatment.

In Section 5 we outline Frémond's model, show how it fits into our thermodynamical framework, and review briefly the mathematical results.

In Section 6 we present the basic equations of Fried-Gurtin model and their specific forms corresponding to some free energy models.

We use the following notation:

$$u_{,i} = \frac{\partial u(\boldsymbol{x},t)}{\partial x_i}, \quad i = 1,\dots,n, \qquad u_t = \frac{du(\boldsymbol{x},t)}{dt}, \quad \boldsymbol{\varepsilon} = (\varepsilon_{ij})_{i,j=1,\dots,n},$$
$$F_{,\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon},\theta) = \frac{\partial F(\boldsymbol{\varepsilon},\theta)}{\partial \boldsymbol{\varepsilon}} = \left(\frac{\partial F(\boldsymbol{\varepsilon},\theta)}{\partial \varepsilon_{ij}}\right)_{i,j=1,\dots,n}, \qquad F_{,\theta}(\boldsymbol{\varepsilon},\theta) = \frac{\partial F(\boldsymbol{\varepsilon},\theta)}{\partial \theta}.$$

The symbol $(\cdot)_t$ denotes the material time derivative of the field $(\cdot)$. For simplicity we use the same notation, $u_{,i}$ and u_t, for variables corresponding to the first order space and time derivatives. Whenever there is no danger of confusion, we omit the function arguments. The specification of the range of tensor indices is omitted, as well. Vectors and tensors are denoted by bold letters. The summation convention over repeated indices is used. Moreover, for vectors $\boldsymbol{a} = (a_i)$, $\tilde{\boldsymbol{a}} = (\tilde{a}_i)$ and tensors $\boldsymbol{B} = (B_{ij})$, $\tilde{\boldsymbol{B}} = (\tilde{B}_{ij})$, $\boldsymbol{A} = (A_{ijkl})$ we write

$$\boldsymbol{a} \cdot \tilde{\boldsymbol{a}} = a_i \tilde{a}_i, \quad \boldsymbol{B} : \tilde{\boldsymbol{B}} = B_{ij}\tilde{B}_{ij},$$

$$\boldsymbol{AB} = (A_{ijkl}B_{kl}), \quad \boldsymbol{BA} = (B_{ij}A_{ijkl}),$$

$$|\boldsymbol{a}| = (a_i a_i)^{1/2}, \quad |\boldsymbol{B}| = (B_{ij}B_{ij})^{1/2}.$$

Throughout the paper all derivatives are material (Lagrangian). The symbols ∇ and $\nabla\cdot$ denote the gradient and divergence with respect to the material point $\boldsymbol{x} \in \mathbb{R}^n$: $\nabla a = (a_{,i})$, $\nabla \boldsymbol{a} = (a_{i,j})$, $\nabla \cdot \boldsymbol{a} = a_{i,i}$, $\nabla \cdot \boldsymbol{B} = (B_{ij,j})$, $\nabla \cdot \boldsymbol{A} = (A_{ijkl,l})$.

2. Review of 1-D Falk's model

The 1-D model due to Falk (1980, 1982, 1983, 1990) describes martensitic phase transitions of the sheer type. The sheer strain $\varepsilon = u_x$, where u denotes displacement, is used as an order parameter distinguishing between different configurations of the crystal lattice.

The Helmholtz free energy density $f = f(\varepsilon, \varepsilon_x, \theta)$, depending on strain ε, strain gradient ε_x and absolute temperature θ, is assumed in the Landau-Ginzburg form

$$f(\varepsilon, \varepsilon_x, \theta) = f_*(\theta) + F(\varepsilon, \theta) + \frac{\varkappa}{2}\varepsilon_x^2, \tag{1}$$

where

$$f_*(\theta) = -c_v\theta \log\left(\frac{\theta}{\theta_1}\right) + c_v\theta + \tilde{c}, \quad F(\varepsilon, \theta) = F_1(\varepsilon, \theta) + F_2(\varepsilon),$$

$$F_1(\varepsilon, \theta) = \alpha_1(\theta - \theta_c)\varepsilon^2, \quad F_2(\varepsilon) = -\alpha_2\varepsilon^4 + \alpha_3\varepsilon^6,$$

with positive physical constants θ_c, α_1, α_2, α_3, $\varkappa$, c_v, θ_1, and some constant $\tilde{c}$ immaterial from the point of view of differential equations.

The terms in (1) denote: $f_*(\theta)$ — thermal energy with thermal specific heat c_v, $F(\varepsilon, \theta)$ — elastic energy, $\varkappa\varepsilon_x^2/2$ — strain gradient energy. The elastic energy is nonconvex multiwell function of ε with the shape strongly depending on θ.

The balance laws of linear momentum and energy in a wire of length 1 and constant density $\varrho = 1$ read

$$\begin{aligned} &u_{tt} - \sigma_x + \mu_{xx} = b, \\ &e_t + q_{0x} - \sigma\varepsilon_t - \mu\varepsilon_{xt} = g \quad \text{in} \quad \Omega^T = (0,1) \times (0,T), \end{aligned} \tag{2}$$

where $T > 0$ is final time, σ — shear stress, μ — couple stress, e — internal energy, q_0 — heat flux, b — distributed body force, g — distributed heat source.

In addition to (2) the fields are required to comply with the second principle of thermodynamics in the form of the Clausius-Duhem inequality

$$\eta_t + \left(\frac{q_0}{\theta}\right)_x \geq \frac{g}{\theta} \quad \text{in} \ \ \Omega^T, \tag{3}$$

where η is the entropy density related to f and e by Gibbs relations

$$f = e - \theta\eta, \quad \eta = -f_{,\theta}. \tag{4}$$

It is straightforward to check (see Lemma 3.2) that in case of free energy $f = f(\varepsilon, \varepsilon_x, \theta)$, the inequality (3) is satisfied for constitutive equations

$$\begin{aligned} &\sigma = f_{,\varepsilon} + \sigma^v, \quad \sigma^v = \nu\varepsilon_t, \quad \mu = f_{,\varepsilon_x}, \\ &q_0 = -k\theta_x, \end{aligned} \tag{5}$$

where σ^v denotes viscous stress, $\nu \geq 0$ — viscosity coefficient, $k > 0$ — heat conductivity. Using (5) in (2), and taking into account the particular form (1) of f, we arrive at the system

$$\begin{aligned} &u_{tt} - \nu u_{xxt} + \varkappa u_{xxxx} = (F_{,\varepsilon}(\varepsilon, \theta))_x + b, \\ &c_0(\varepsilon, \theta)\theta_t - k\theta_{xx} = \theta F_{,\varepsilon\theta}(\varepsilon, \theta)\varepsilon_t + \nu\varepsilon_t^2 + g \quad \text{in} \ \ \Omega^T, \end{aligned} \tag{6}$$

where $\varepsilon = u_x$, and

$$c_0(\varepsilon, \theta) = c_v - \theta F_{,\theta\theta}(\varepsilon, \theta)$$

denotes the specific heat. Clearly, for F linearly dependent on θ as in (1), $c_0 = c_v$.

The system (6) is subject to initial conditions

$$u\big|_{t=0} = u_0, \ \ u_t\big|_{t=0} = u_1, \ \ \theta\big|_{t=0} = \theta_0 \ \ \text{in} \ \ \Omega,$$

and some boundary conditions.

The boundary value problems for (6) have been investigated under various structural assumptions on $F(\varepsilon, \theta)$ in the cases $\varkappa = 0$, $\nu > 0$, or $\varkappa > 0$, $\nu = 0$, or $\varkappa > 0$, $\nu > 0$. In all cases the mathematical analysis required a considerable effort despite the 1-D setting. The positivity of one of the coefficinets ν or $\varkappa$ played a regularizing role.

In case $\varkappa = 0$, $\nu > 0$ the global in time existence of solutions to (6) has been studied by Niezgódka and Sprekels (1988), Hoffman and Zheng (1988), Zheng and Sprekels (1988), Chen and Hoffmann (1994), Racke and Zheng (1997), Shen, Zheng and Zhu (1999).

The last two references address also the question of asymptotic behaviour as time tends to infinity. We emphasise that in view of $\varkappa = 0$ (no interfacial structure) the framework of these papers allows the strain ε to belong to L_∞.

For recent results concerning general thermovisco-elasticity systems related to (6), including, in particular shape memory alloys, we refer e.g. to Watson (2000), Qin (2001).

In case of $\varkappa > 0$, $\nu = 0$ the system (6) has been studied by Sprekels (1989), Zheng (1989), Sprekels and Zheng (1989), Aiki (2000). We point out that the analysis in Sprekels (1989) required restrictive growth conditions on $F(\varepsilon, \theta)$ with respect to θ, which excluded the physically relevant case in (1). This assumption has been removed in Zheng (1989), where $F(\varepsilon, \theta)$ has been admitted in the standard form (1) but $-f_*(\theta)$ has been assumed to grow at least quadratically in θ. Finally, the latter assumption has been removed in Sprekels and Zheng (1989) by means of deriving more delicate estimates. Then Aiki (2000) addresses the existence and uniqueness of weak solutions.

In case of $\varkappa > 0$, $\nu > 0$ the system (6) has been studied by Żochowski (1992), Hoffmann and Żochowski (1992 a,b) in the 1-D and 2-D cases. In these references the analysis has been based on the parabolic decomposition of momentum equation $(6)_1$.

The same type of decomposition has been applied for the 3-D model in Pawłow and Żochowski (2000, 2002) (see Section 4). In case of boundary conditions

$$u = 0, \quad u_{xx} = 0 \quad \text{on} \quad S^T = \{0\} \times (0,T) \cup \{1\} \times (0,T),$$

it is easy to see that $(6)_1$ splits into the following two systems:

$$\begin{aligned} & w_t - \beta w_{xx} = (F_{,\varepsilon}(\varepsilon, \theta))_x + b && \text{in } \Omega^T, \\ & w\big|_{t=0} = u_1 - \alpha u_{0xx} && \text{in } \Omega, \\ & w = 0 && \text{on } S^T, \end{aligned} \tag{7}$$

and

$$\begin{aligned} & u_t - \alpha u_{xx} = w && \text{in } \Omega^T, \\ & u\big|_{t=0} = u_0 && \text{in } \Omega, \\ & u = 0 && \text{on } S^T, \end{aligned} \tag{8}$$

where α, β are numbers satisfying $\alpha + \beta = \nu$, $\alpha\beta = \varkappa$, $0 < 2\sqrt{\varkappa} \le \nu$.

We point out that in the papers cited above a priori estimates on solutions depend on the time horizon T, therefore do not admit the asymptotic analysis as $T \to \infty$.

The study of system (6) in case $\varkappa > 0$, $\nu > 0$ has been continued in Sprekels, Zheng and Zhu (1998), Sprekels and Zheng (1998), where the global existence, uniqueness, the asymptotic behaviour of solution as time $T \to \infty$, and the existence of a compact maximal attractor has been established.

The analysis in these papers is based on different type of parabolic decomposition of $(6)_1$ by means of the transformation due to Pego (1987) and Andrews (1980):

$$p(x,t) = \int_1^x u_t(y,t)dy. \tag{9}$$

In view of (9),

$$\varepsilon_t = p_{xx} \quad \text{in} \ \ \Omega^T, \tag{10}$$

and system (6) ($b = 0, g = 0$) can be recast as

$$\begin{aligned} &p_t - \nu p_{xx} = -\varkappa \varepsilon_{xx} + F_{,\varepsilon}(\varepsilon, \theta), \\ &c_0\theta_t - k\theta_{xx} = \theta F_{,\varepsilon\theta}(\varepsilon, \theta) p_{xx} + \nu p_{xx}^2 \quad \text{in} \ \ \Omega^T. \end{aligned}$$

The transformation (9) has been also applied in the previously discussed case $\varkappa = 0$, $\nu > 0$ in Racke and Zheng (1997), Shen, Zheng and Zhu (1999). We point out that in all the papers, mentioned above, concerning asymptotic behaviour of solutions, the main tool was the basic lemma due to Shen and Zheng (1993).

We mention that the transformation (9) has been generalized to many space dimensions by Rybka (1992, 1997) to study isothermal viscoelasticity system, see also Swart and Holmes (1992).

System (6) with $\varkappa > 0$, $\nu > 0$, has been also investigated from the point of view of so-called state-space approach by means of expressing it as a semilinear Cauchy problem in an appropriate Hilbert space, see Speis (1994, 1995), Morin and Spies (1997).

Finally, we mention that there exists an extensive literature concerning the control problems for 1-D Falk's model where distributed or boundary inputs are used to control the system behaviour. We refer, e.g., to Hoffmann and Sprekels (1987), Sprekels (1989b), Brokate and Sprekels (1991), Sokołowski and Sprekels (1994), Bubner, Sokołowski and Sprekels (1998). Control problems for a special 2-D model of a plate activated by shape memory reinforcements have been considered by Żochowski (1992), Hoffmann and Tiba (1997), Hoffmann and Żochowski (1998). Recently, control problem for 3-D counterpart of Falk's model has been studied in Pawłow and Żochowski (2002b).

3. Thermodynamical framework of diffused-interface models with strain tensor as an order parameter

Let $\Omega \subset \mathbb{R}^n$, $n = 2$ or 3, be a bounded domain with a smooth boundary S, occupied by a body in a reference configuration. Let $\boldsymbol{u} = (u_i)$ denote the displacement vector, $\theta > 0$ — the absolute temperature, and

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\boldsymbol{u}) = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$$

be the linearized strain tensor.

We outline the field equations for thermodynamically consistent thermoelasticity models governed by Landau-Ginzburg free energy

$$f = f(\boldsymbol{\varepsilon}(\boldsymbol{u}), \nabla\boldsymbol{\varepsilon}(\boldsymbol{u}), \theta). \tag{11}$$

We confine our attention to small strain approximation, that is, the assumption of infinitesimal displacement gradient.

Assuming constant mass density ($\varrho = 1$), the balance laws of linear momentum and internal energy read:

$$\begin{aligned} &\boldsymbol{u}_{tt} - \nabla \cdot \boldsymbol{S} = \boldsymbol{b}, \\ &e_t + \nabla \cdot \boldsymbol{q} - \boldsymbol{S} : \boldsymbol{\varepsilon}_t = g \quad \text{in} \quad \Omega^T = \Omega \times (0,T), \end{aligned} \tag{12}$$

where $\boldsymbol{S}$ denotes the referential (first Piola-Kirchhoff) stress tensor, e — internal energy, $\boldsymbol{q}$ — energy flux, and $\boldsymbol{\varepsilon}_t = \boldsymbol{\varepsilon}(\boldsymbol{u}_t)$ — the strain rate tensor, and $\boldsymbol{b}$ — external body force.

The corresponding thermodynamically consistent constitutive relations for e, $\boldsymbol{S}$ and $\boldsymbol{q}$ have been established in Pawłow (2000b). In order to construct theory with first order strain gradient free energy f it is necessary to admit as constitutive variables not only the strain tensor $\boldsymbol{\varepsilon}$, its higher gradients $\nabla^M \boldsymbol{\varepsilon}$, $M \in \mathbb{N}$, and absolute temperature θ (or, by duality, entropy η or internal energy e) but also the strain rate tensor $\boldsymbol{\varepsilon}_t$. By assuming such constitutive dependence and exploiting the entropy inequality with multipliers it has been proved in the above mentioned reference that the constitutive dependence of f is restricted to the variables as in (11), e and η are linked by the Gibbs relations (4), and $\boldsymbol{S}$, $\boldsymbol{q}$ are defined by

$$\begin{aligned} &\boldsymbol{S} = \frac{\delta f}{\delta \boldsymbol{\varepsilon}} + \theta(\boldsymbol{h} - f_{,\nabla\boldsymbol{\varepsilon}})\nabla\left(\frac{1}{\theta}\right) + \boldsymbol{S}^v, \\ &\boldsymbol{q} = \boldsymbol{q}_0 + \boldsymbol{q}_1, \quad \boldsymbol{q}_1 = -\boldsymbol{\varepsilon}_t \boldsymbol{h}, \end{aligned} \tag{13}$$

where $\delta f/\delta\boldsymbol{\varepsilon}$ denotes the first variation of f with respect to $\boldsymbol{\varepsilon}$, given by

$$\frac{\delta f}{\delta \boldsymbol{\varepsilon}} = f_{,\boldsymbol{\varepsilon}} - \nabla \cdot f_{,\nabla\boldsymbol{\varepsilon}}.$$

A third order tensor $\boldsymbol{h} = (h_{ijk})$ is an arbitrary constitutive quantity. It is not constrained by the second principle but, as conventional, required to be frame indifferent. The presence of such quantity is characteristic for phase transition models with first order gradient free energy (Alt and Pawłow, 1996). It contributes to nonstationary energy and entropy fluxes associated with evolving non-zero width phase interfaces.

In (13), $\boldsymbol{q}_1$ denotes a nonstationary energy flux. Furhermore, $\boldsymbol{S}^v$ is the viscous stress tensor and $\boldsymbol{q}_0$ is the heat flux which are subject to the dissipation inequality

$$\boldsymbol{\varepsilon}_t : \left(\frac{\boldsymbol{S}^v}{\theta}\right) + \nabla\left(\frac{1}{\theta}\right) \cdot \boldsymbol{q}_0 \geq 0 \quad \text{for all fields} \quad \boldsymbol{u}, \theta. \tag{14}$$

The standard examples of constitutive equations for $\boldsymbol{S}^v$ and $\boldsymbol{q}_0$ are Hooke's and Fourier's laws:

$$\boldsymbol{S}^v = \nu \boldsymbol{A} \boldsymbol{\varepsilon}_t, \quad \boldsymbol{q}_0 = -k\nabla\theta, \tag{15}$$

where $\nu > 0$ is the viscosity, $k > 0$ the heat conductivity, and $\boldsymbol{A} = (A_{ijkl})$ the fourth order elasticity tensor

$$\boldsymbol{A}\boldsymbol{\varepsilon}(\boldsymbol{u}) = \lambda tr\boldsymbol{\varepsilon}(\boldsymbol{u})\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon}(\boldsymbol{u}), \tag{16}$$

with $\boldsymbol{I} = (\delta_{ij})$ identity tensor and λ, μ Lamé constants.

The thermodynamical compatibility of relations (13), (14) is assured by the following

Lemma 3.1 *(Pawłow, 2000b) The solutions of system of balance laws (3.2) with constitutive relations (13), (14) satisfy the entropy inequality*

$$\eta_t + \nabla\cdot\boldsymbol{\psi} = \boldsymbol{\varepsilon}_t : \left(\frac{\boldsymbol{S}^v}{\theta}\right) + \nabla\left(\frac{1}{\theta}\right)\cdot\boldsymbol{q}_0 + \frac{g}{\theta} \geq \frac{g}{\theta} \quad \text{for all} \quad \boldsymbol{u}, \theta, \tag{17}$$

where η is the entropy obeying Gibbs relations (4), and $\boldsymbol{\psi}$ is the entropy flux given by

$$\boldsymbol{\psi} = \boldsymbol{\psi}_0 + \boldsymbol{\psi}_1, \quad \boldsymbol{\psi}_0 = \frac{1}{\theta}\boldsymbol{q}_0, \quad \boldsymbol{\psi}_1 = \frac{1}{\theta}\boldsymbol{\varepsilon}_t(f_{,\nabla\boldsymbol{\varepsilon}} - \boldsymbol{h}). \tag{18}$$

For special selection

$$\boldsymbol{h} = f_{,\nabla\boldsymbol{\varepsilon}}, \tag{19}$$

the constitutive equations for $\boldsymbol{S}$, $\boldsymbol{q}$ and $\boldsymbol{\psi}$ become

$$\begin{aligned} &\boldsymbol{S} = \frac{\delta f}{\delta\boldsymbol{\varepsilon}} + \boldsymbol{S}^v, \quad \boldsymbol{q} = \boldsymbol{q}_0 + \boldsymbol{q}_1, \quad \boldsymbol{q}_1 = -\boldsymbol{\varepsilon}_t f_{,\nabla\boldsymbol{\varepsilon}}, \\ &\boldsymbol{\psi} = \boldsymbol{\psi}_0 + \boldsymbol{\psi}_1, \quad \boldsymbol{\psi}_0 = \frac{1}{\theta}\boldsymbol{q}_0, \quad \boldsymbol{\psi}_1 = 0. \end{aligned} \tag{20}$$

Is is straightforward to check that for such constitutive equations, for $\boldsymbol{S}^v$, $\boldsymbol{q}_0$ defined by (15) and f by (11) the system (12) in 1-D case is identical to Falk's model (2), (5). We note also that the third order tensor $f_{,\nabla\boldsymbol{\varepsilon}} = (f_{,\varepsilon_{ij,k}})$ represents the couple stress.

The mathematical results reported in Section 4 concern system (12) with $\boldsymbol{h}$ specified by (19). For discussion of other choices of $\boldsymbol{h}$, for example $\boldsymbol{h} = 0$, and the related field equations we refer to Pawłow (2000b). Here, we present the general properties of the system (12) with the constitutive equations (20). First, for further convenience, we collect the equivalent forms of energy equation in this system.

Lemma 3.2 *Consider system (12) with constitutive equations satisfying (20) and (14). Then the energy equation* $(12)_2$ *admits the following equivalent formulations:*

$$\begin{aligned} &e_t + \nabla\cdot(\boldsymbol{q}_0 - \boldsymbol{\varepsilon}_t f_{,\nabla\boldsymbol{\varepsilon}}) - \boldsymbol{S} : \boldsymbol{\varepsilon}_t = g, \\ &\theta\eta_t + \nabla\cdot\boldsymbol{q}_0 - \boldsymbol{S}^v : \boldsymbol{\varepsilon}_t = g, \\ &c_0\theta_t + \nabla\cdot\boldsymbol{q}_0 = \theta f_{,\theta\boldsymbol{\varepsilon}} : \boldsymbol{\varepsilon}_t + \theta f_{,\theta\nabla\boldsymbol{\varepsilon}} : \nabla\boldsymbol{\varepsilon}_t + \boldsymbol{S}^v : \boldsymbol{\varepsilon}_t + g, \end{aligned} \tag{21}$$

where

$$c_0 = -\theta f_{,\theta\theta}, \tag{22}$$

and e, η obey the Gibbs relations (4).

Proof. The equivalence of $(21)_1$ and $(21)_2$ follows in view of the identity

$$\begin{aligned} &e_t - \nabla\cdot(\boldsymbol{\varepsilon}_t f_{,\nabla\boldsymbol{\varepsilon}}) - \boldsymbol{S} : \boldsymbol{\varepsilon}_t \\ &= (\theta\eta_t + f_{,\boldsymbol{\varepsilon}} : \boldsymbol{\varepsilon}_t + f_{,\nabla\boldsymbol{\varepsilon}} : \nabla\boldsymbol{\varepsilon}_t) \\ &\qquad - ((\nabla\cdot f_{,\nabla\boldsymbol{\varepsilon}}) : \boldsymbol{\varepsilon}_t + f_{,\nabla\boldsymbol{\varepsilon}} : \nabla\boldsymbol{\varepsilon}_t) \\ &\qquad - (f_{,\boldsymbol{\varepsilon}} - \nabla\cdot f_{,\nabla\boldsymbol{\varepsilon}} + \boldsymbol{S}^v) : \boldsymbol{\varepsilon}_t = \theta\eta_t - \boldsymbol{S}^v : \boldsymbol{\varepsilon}_t, \end{aligned}$$

where we have used that, by virtue of Gibbs relations,

$$\theta\eta_t = e_t + f_{,\theta}\theta_t - f_{,t} = e_t - f_{,\varepsilon} : \varepsilon_t - f_{,\nabla\varepsilon} : \nabla\varepsilon_t.$$

Clearly, the equivalance of $(3.11)_2$ and $(3.11_3$ results from the identity

$$\theta\eta_t = -\theta f_{,\theta\varepsilon} : \varepsilon_t - \theta f_{,\theta\nabla\varepsilon} : \nabla\varepsilon_t + c_0\theta_t.$$

■

Now we present the availability identity for the system (12) with constitutive equations satisfying (20), (14). In mathematical analysis such identity provides energy estimates.

LEMMA 3.3 *For solutions of system (12) with (20), (14) the following identity is satisfied*

$$\begin{aligned} &\frac{d}{dt}\int\limits_\Omega \left(e + \frac{1}{2}|\boldsymbol{u}_t|^2 - \bar{\theta}\eta\right)dx \\ &\qquad + \int\limits_S \left[-(\boldsymbol{S}\boldsymbol{n})\cdot\boldsymbol{u}_t - \boldsymbol{n}\cdot(\boldsymbol{\varepsilon}_t f_{,\nabla\boldsymbol{\varepsilon}}) + \left(1 - \frac{\bar{\theta}}{\theta}\right)\boldsymbol{n}\cdot\boldsymbol{q}_0\right]dS \\ &\qquad + \int\limits_\Omega \left[\nabla\left(\frac{\bar{\theta}}{\theta}\right)\cdot\boldsymbol{q}_0 + \frac{\bar{\theta}}{\theta}\boldsymbol{\varepsilon}_t : \boldsymbol{S}^v\right]dx \\ &\quad = \int\limits_\Omega \left[\boldsymbol{b}\cdot\boldsymbol{u}_t + \left(1 - \frac{\bar{\theta}}{\theta}\right)g\right]dx \quad \text{for} \quad t \in (0,T), \end{aligned} \tag{23}$$

where $\bar{\theta} = \bar{\theta}(x) > 0$ is a given function, and $\boldsymbol{n}$ denotes the unit outward normal to S.

Proof. Multiplication of $(21)_2$ by $\bar{\theta}/\theta$ (it is assumed that $\theta > 0$) and integration over Ω yields the identity for the entropy

$$\begin{aligned} &\frac{d}{dt}\int\limits_\Omega \bar{\theta}\eta dx - \int\limits_\Omega \nabla\left(\frac{\bar{\theta}}{\theta}\right)\cdot\boldsymbol{q}_0 dx + \int\limits_S \boldsymbol{n}\cdot\boldsymbol{q}_0\frac{\bar{\theta}}{\theta}dS \\ &\qquad - \int\limits_\Omega \frac{\bar{\theta}}{\theta}\boldsymbol{\varepsilon}_t : \boldsymbol{S}^v dx = \int\limits_\Omega \frac{\bar{\theta}}{\theta}g dx. \end{aligned} \tag{24}$$

Next, integration of $(21)_1$ over Ω yields the identity for the internal energy

$$\frac{d}{dt}\int_\Omega e dx + \int_S [\boldsymbol{n}\cdot\boldsymbol{q}_0 - \boldsymbol{n}\cdot(\boldsymbol{\varepsilon}_t f_{,\nabla\boldsymbol{\varepsilon}})]\, dS - \int_\Omega \boldsymbol{S} : \varepsilon_t dx = \int_\Omega g dx. \tag{25}$$

Furthermore, by multiplying (12) by $\boldsymbol{u}_t$ and integrating over Ω we get the identity for the kinetic energy

$$\frac{d}{dt}\int_\Omega \frac{1}{2}|\boldsymbol{u}_t|^2 dx + \int_\Omega \boldsymbol{S} : \boldsymbol{\varepsilon}_t dx - \int_S (\boldsymbol{S}\boldsymbol{n})\cdot \boldsymbol{u}_t dS = \int_\Omega \boldsymbol{b}\cdot\boldsymbol{u}_t dx. \tag{26}$$

By adding (25) and (26) we obtain the identity for the total energy

$$\frac{d}{dt}\int_\Omega \left(e + \frac{1}{2}|\boldsymbol{u}_t|^2\right) dx + \int_S [-(\boldsymbol{S}\boldsymbol{n})\cdot\boldsymbol{u}_t - \boldsymbol{n}\cdot(\boldsymbol{\varepsilon}_t f_{,\nabla\boldsymbol{\varepsilon}}) + \boldsymbol{n}\cdot\boldsymbol{q}_0] dS$$
$$= \int_\Omega (\boldsymbol{b}\cdot\boldsymbol{u}_t + g) dx. \tag{27}$$

Finally, subtracting (24) from (27) yields (23). ■

In view of the dissipation inequality (14), if external sources vanish

$$\boldsymbol{b} = 0, \quad g = 0,$$

if boundary conditions on S imply that

$$(\boldsymbol{S}\boldsymbol{n})\cdot\boldsymbol{u}_t = 0, \quad \boldsymbol{n}\cdot(\varepsilon_t f_{,\nabla\boldsymbol{\varepsilon}}) = 0, \quad \boldsymbol{n}\cdot\boldsymbol{q}_0 = 0,$$

and if $\bar{\theta} = \text{const} > 0$, identity (23) implies the Lyapunov relation

$$\frac{d}{dt}\int_\Omega \left(e + \frac{1}{2}|\boldsymbol{u}_t|^2 - \bar{\theta}\eta\right) dx \le 0,$$

where the function under the integral is known as the equilibrium free energy.

4. 3-D counterpart of Falk's model and its well-posedness

Let $\boldsymbol{A} = (A_{ijkl})$ be the elasticity tensor given by (16), where Lamé constants λ, μ are specified below in assumption (A2). We recall that $\boldsymbol{A}$ satisfies the following symmetry conditions:

$$A_{ijkl} = A_{jikl}, \quad A_{ijkl} = A_{ijlk}, \quad A_{ijkl} = A_{klij}.$$

Moreover, let $\boldsymbol{Q}$ stand for the second order differential operator of linearized elasticity, defined by

$$\boldsymbol{u} \mapsto \boldsymbol{Q}\boldsymbol{u} = \nabla\cdot(\boldsymbol{A}\boldsymbol{\varepsilon}(\boldsymbol{u})) = \mu\Delta\boldsymbol{u} + (\lambda+\mu)\nabla(\nabla\cdot\boldsymbol{u}). \tag{28}$$

Correspondingly, the operator $\boldsymbol{Q}^2 = \boldsymbol{Q}\boldsymbol{Q}$ is given by

$$\boldsymbol{u} \mapsto \boldsymbol{Q}^2\boldsymbol{u} = \mu\Delta(\boldsymbol{Q}\boldsymbol{u}) + (\lambda+\mu)\nabla(\nabla\cdot(\boldsymbol{Q}\boldsymbol{u})).$$

The Landau-Ginzburg free energy (11) is assumed in the form

$$f(\boldsymbol{\varepsilon}(\boldsymbol{u}), \nabla\boldsymbol{\varepsilon}(\boldsymbol{u}), \theta) = f_*(\theta) + F(\boldsymbol{\varepsilon}(\boldsymbol{u}), \theta) + \frac{\varkappa_0}{8}|\boldsymbol{Q}\boldsymbol{u}|^2, \tag{29}$$

with $f_*(\theta)$ as in (1).

The special form of strain gradient term with constant $\varkappa_0 > 0$ is chosen for the sake of mathematical analysis.

The meaning of the quantities in (29) is the same as in (1). The representative model of the elastic energy $F(\varepsilon,\theta)$ is due to Falk and Konopka (1990):

$$F(\boldsymbol{\varepsilon}, \theta) = \sum_{i=1}^{3} a_i^2(\theta)J_i^2(\boldsymbol{\varepsilon}) + \sum_{i=1}^{5} a_i^4(\theta)J_i^4(\boldsymbol{\varepsilon}) + \sum_{i=1}^{2} a_i^6(\theta)J_i^6(\boldsymbol{\varepsilon}), \tag{30}$$

where $a_i^k(\theta)$ are experimentally determined material coefficients, and $J_i^k(\boldsymbol{\varepsilon})$ are crystal invariants in the form of k-th order polynomials in ε_{ij}. In particular, for CuAlNi alloy Falk and Konopka (1990) have proposed

$$\begin{aligned} &a_i^k(\theta) = \alpha_i^k + \tilde{\alpha}_i^k(\theta - \theta_c), \quad k = 2,4, \\ &a_i^6(\theta) = \alpha_i^6, \end{aligned} \tag{31}$$

with constants

$$\begin{aligned} &\alpha_1^2, \alpha_2^2, \alpha_3^2 > 0, \quad \tilde{\alpha}_1^2 = 0, \quad \tilde{\alpha}_2^2 > 0, \quad \tilde{\alpha}_3^2 < 0, \\ &\alpha_1^4, \alpha_4^4, \alpha_5^4 < 0, \quad \alpha_2^4, \alpha_3^4 > 0, \quad \tilde{\alpha}_1^4 > 0, \quad \tilde{\alpha}_2^4 = \tilde{\alpha}_3^4 = \tilde{\alpha}_4^4 = \tilde{\alpha}_5^4 = 0, \\ &\alpha_1^6, \alpha_2^6 > 0, \quad \theta_c > 0. \end{aligned}$$

Here, in contrast to elastic energy $F(\varepsilon,\theta)$ in Falk's model (1), not only second order, a_i^2, but also fourth order coefficient a_1^4 are dependent on temperature.

We consider the system of balance laws (12) governed by free energy (29), with constitutive equations for $\boldsymbol{S}$, $\boldsymbol{q}$ given by (20), and for $\boldsymbol{S}^v$, $\boldsymbol{q}_0$ by (15). In such a case

$$f_{,\nabla\boldsymbol{\varepsilon}} = (f_{,\varepsilon_{pq,r}}) = \frac{\varkappa_0}{4}((\boldsymbol{Q}\boldsymbol{u})_i A_{irpq}) = \frac{\varkappa_0}{4}(A_{pqri}(\boldsymbol{Q}\boldsymbol{u})_i) = \frac{\varkappa_0}{4}\boldsymbol{A}\boldsymbol{Q}\boldsymbol{u},$$

$$\nabla\cdot f_{,\nabla\boldsymbol{\varepsilon}} = \frac{\varkappa_0}{4}(A_{pqri}\varepsilon_{ri}(\boldsymbol{Q}\boldsymbol{u})) = \frac{\varkappa_0}{4}\boldsymbol{A}\boldsymbol{\varepsilon}(\boldsymbol{Q}\boldsymbol{u}),$$

$$\frac{\delta f}{\delta\boldsymbol{\varepsilon}} = F_{,\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon},\theta) - \frac{\varkappa_0}{4}\boldsymbol{A}\boldsymbol{\varepsilon}(\boldsymbol{Q}\boldsymbol{u}),$$

$$\boldsymbol{q}_1 = -\frac{\varkappa_0}{4}\boldsymbol{\varepsilon}_t(\boldsymbol{A}\boldsymbol{Q}\boldsymbol{u}).$$

Inserting the above equations into (12) leads to the following system, which is a 3-D generalization of the Falk's model (6):

$$\boldsymbol{u}_{tt} - \nu \boldsymbol{Q} \boldsymbol{u}_t + \frac{\varkappa_0}{4} \boldsymbol{Q}^2 \boldsymbol{u} = \nabla \cdot F_{,\boldsymbol{\varepsilon}}(\varepsilon, \theta) + \boldsymbol{b}, \tag{32}$$

$$c_0(\boldsymbol{\varepsilon}, \theta)\theta_t - k\Delta\theta = \theta F_{,\theta\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \theta) : \boldsymbol{\varepsilon}_t + \nu(\boldsymbol{A}\boldsymbol{\varepsilon}_t) : \boldsymbol{\varepsilon}_t + g \tag{33}$$

in $\Omega^T = \Omega \times (0, T)$, where

$$c_0(\boldsymbol{\varepsilon}, \theta) = c_v - \theta F_{,\theta\theta}(\boldsymbol{\varepsilon}, \theta). \tag{34}$$

The above system is considered with the following initial and boundary conditions

$$\boldsymbol{u}\big|_{t=0} = \boldsymbol{u}_0, \quad \boldsymbol{u}_t\big|_{t=0} = \boldsymbol{u}_1 \quad \text{in} \quad \Omega, \tag{35}$$

$$\boldsymbol{u} = 0, \quad \boldsymbol{Q}\boldsymbol{u} = 0 \quad \text{on} \quad S^T = S \times (0, T), \tag{36}$$

$$\theta\big|_{t=0} = \theta_0 \quad \text{in} \quad \Omega, \tag{37}$$

$$\boldsymbol{n} \cdot \nabla\theta = 0 \quad \text{on} \quad S^T, \tag{38}$$

where $\boldsymbol{n}$ is the unit outward normal to S.

The initial boundary value problem (32)–(38) has been studied under various structural assumptions in Pawłow and Żochowski (2000, 2002a, b), Pawłow and Zajączkowski (2002a, b).

The main structural assumption has been concerned with the behaviour of the elastic energy $F(\boldsymbol{\varepsilon}, \theta)$ as a function of θ. Namely, in all the above papers $F(\boldsymbol{\varepsilon}, \theta)$ has been assumed to satisfy growth condition

$$|F(\boldsymbol{\varepsilon}, \theta)| \leq c + c\theta^s |\boldsymbol{\varepsilon}|^{K_1}$$

for large values of θ and ε_{ij}, with exponents $0 < s < 1$ and $0 < K_1 < \infty$ linked by an appropriate relation.

Under such condition the specific heat coefficient $c_0(\boldsymbol{\varepsilon}, \theta)$, by definition, contains the nonlinear contribution $-\theta F_{,\theta\theta}(\boldsymbol{\varepsilon}, \theta)$. The presence of such nonlinearity causes essential difficulties in the mathematical analysis of the problem. They are related to the necessity of deriving Hölder bounds on $\boldsymbol{\varepsilon}$ and θ in application of the classical parabolic theory.

In Pawłow and Żochowski (2002a) the problem (32)–(38) has been studied in the 3-D case, by means of the Leray-Schauder fixed point theorem, under structural simplification of energy equation (33). The simplification consisted in neglecting the nonlinear term in $c_0(\boldsymbol{\varepsilon}, \theta)$, that is, by setting

$$c_0(\boldsymbol{\varepsilon}, \theta) = c_v = \text{const} > 0.$$

The reference Pawłow and Zajączkowski (2002a) generalizes Pawłow and Żochowski (2002a) by removing the above mentioned simplification. However, the proof of existence result in that reference is intrinsically two-dimensional, based on Sobolev's imbeddings and interpolation inequalities in 2-D.

The subsequent paper of Pawłow and Zajączkowski (2002b) offers a different proof of a priori estimates which, with the help of the Leray-Schauder fixed point theorem, allows for the establishment of existence of solutions in the 2-D and 3-D cases.

The proof of a priori estimates consists in recursive improvement of energy estimates with the help of Sobolev's imbedding theorems and the regularity theory of parabolic systems. The key estimates are $L_\infty(\Omega^T)$-norm bound and Hölder-norm bound for a solution of heat conduction equation (33) with nonlinear specific heat $c_0(\varepsilon,\theta)$.

In all above mentioned references the idea of the existence proof is similar to that in Żochowski (1992), where 1-D Falk's model has been considered. It is based on parabolic decomposition of (32) and the application of the Leray-Schauder fixed point theorem. The elasticity system (32) admits the decompositon into two parabolic systems, for vector field $\boldsymbol{w}$:

$$\begin{aligned}&\boldsymbol{w}_t - \beta Q\boldsymbol{w} = \nabla\cdot F_{,\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon},\theta) + \boldsymbol{b} \quad \text{in} \quad \Omega^T,\\ &\boldsymbol{w}\big|_{t=0} = \boldsymbol{w}_0 \equiv \boldsymbol{u}_1 - \alpha\boldsymbol{Q}\boldsymbol{u}_0 \quad \text{in} \quad \Omega,\\ &\boldsymbol{w} = 0 \quad \text{on} \quad S^T,\end{aligned} \tag{39}$$

and for vector field $\boldsymbol{u}$:

$$\begin{aligned}&\boldsymbol{u}_t - \alpha\boldsymbol{Q}\boldsymbol{u} = \boldsymbol{w} \quad \text{in} \quad \Omega^T,\\ &\boldsymbol{u}\big|_{t=0} = \boldsymbol{u}_0 \quad \text{in} \quad \Omega,\\ &\boldsymbol{u} = 0 \quad \text{on} \quad S^T,\end{aligned} \tag{40}$$

where α,β are numbers satisfying

$$\alpha+\beta=\nu, \quad \alpha\beta = \frac{\varkappa_0}{4}.$$

Further on, we assume the condition $0<\sqrt{\varkappa_0}\le\nu$, which assures that $\alpha,\beta\in\mathbb{R}_+$. Systems (39), (40) are coupled with problem (33),(37), (38) for θ.

We present now the existence and uniqueness results for the problem (32)–(38) proved in Pawłow and Zajączkowski (2002b). First we list the assumptions:

(A1) Domain $\Omega\subset\mathbb{R}^n$, $n=2$ or 3, with the boundary of class C^4. The C^4-regularity is needed in order to apply the classical regularity theory for parabolic systems.

(A2) The coefficients of the operator $\boldsymbol{Q}$ satisfy

$$\mu>0, \quad n\lambda+2\mu>0.$$

These conditions assure the following properties:

(i) Coercivity and boundedness of the algebraic operator $\boldsymbol{A}$:

$$\underline{c}|\varepsilon|^2 \leq (\boldsymbol{A\varepsilon}) : \boldsymbol{\varepsilon} \leq \bar{c}|\boldsymbol{\varepsilon}|^2,$$

where

$$\underline{c} = \min\{n\lambda + 2\mu, 2\mu\}, \quad \bar{c} = \max\{n\lambda + 2\mu, 2\mu\}.$$

(ii) Strong ellipticity of the operator $\boldsymbol{Q}$ (see Pawłow and Żochowski, 2002a). Thanks to this property the following estimate holds true

$$c\|\boldsymbol{u}\|_{\boldsymbol{W}_2^2(\Omega)} \leq \|\boldsymbol{Qu}\|_{\boldsymbol{L}_2(\Omega)} \quad \text{for} \quad \{\boldsymbol{u} \in \boldsymbol{W}_2^2(\Omega)|\ \boldsymbol{u}|_S = 0\}.$$

(iii) Parabolicity in the general (Solonnikov) sense of system (32) (see Pawłow and Żochowski (2002a)).

The subsequent assumption concerns the structure of elastic energy.

(A3) Function $F(\boldsymbol{\varepsilon}, \theta) : S^2 \times [0, \infty) \to \mathbb{R}$ is of class C^3, where S^2 denotes the set of symmetric second order tensors in $\mathbb{R}^n$. We assume the splitting

$$F(\boldsymbol{\varepsilon}, \theta) = F_1(\boldsymbol{\varepsilon}, \theta) + F_2(\boldsymbol{\varepsilon}),$$

where F_1 and F_2 are subject to the following conditions:

(A3-1) Conditions on $F_1(\boldsymbol{\varepsilon}, \theta)$

(i) Concavity with respect to θ

$$-F_{1,\theta\theta}(\boldsymbol{\varepsilon}, \theta) \geq 0 \quad \text{for} \quad (\boldsymbol{\varepsilon}, \theta) \in S^2 \times [0, \infty). \tag{41}$$

(ii) Nonnegativity

$$F_1(\boldsymbol{\varepsilon}, \theta) \geq 0 \quad \text{for} \quad (\boldsymbol{\varepsilon}, \theta) \in S^2 \times [0, \infty).$$

(iii) Boundedness of the norm

$$\|F_1\|_{C^3(S^2 \times [0,\infty))} < \infty.$$

(iv) Growth conditions. There exist a positive constant c and numbers $s, K_1 \in (0, \infty)$ such that

$$\begin{aligned}
&|F_1(\boldsymbol{\varepsilon}, \theta)| \leq c(1 + \theta^s|\boldsymbol{\varepsilon}|^{K_1}),\\
&|F_{1,\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \theta)| \leq c(1 + \theta^s|\boldsymbol{\varepsilon}|^{K_1-1}),\\
&|F_{1,\boldsymbol{\varepsilon\varepsilon}}(\boldsymbol{\varepsilon}, \theta)| \leq c(1 + \theta^s|\boldsymbol{\varepsilon}|^{K_1-2}),\\
&|F_{1,\theta\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \theta)| \leq c(1 + \theta^{s-1}|\boldsymbol{\varepsilon}|^{K_1-1}),\\
&|F_{1,\theta\theta}(\boldsymbol{\varepsilon}, \theta)| \leq c(1 + \theta^{s-2}|\boldsymbol{\varepsilon}|^{K_1}),\\
&|F_{1,\theta\theta\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \theta)| \leq c(1 + \theta^{s-2}|\boldsymbol{\varepsilon}|^{K_1-1})
\end{aligned}$$

for large values of θ and ε_{ij}, where admissible ranges of s and K_1 are given by

$$0 < s < \frac{n+1}{2n} = \begin{cases} 3/4 & \text{if } n = 2\\ 2/3 & \text{if } n = 3, \end{cases}$$

$$0 < K_1 < 1 + \frac{q_n}{2}\left[\frac{n+2}{2n} + \frac{1}{n(n+1)}\right] = \begin{cases} \text{any finite number} & \text{if } n = 2\\ 15/4 & \text{if } n = 3. \end{cases}$$

Moreover, in case of $K_1 > 1$ the numbers s and K_1 are linked by the equality

$$\frac{2sn}{n+1} + \frac{4n(K_1-1)}{q_n(n+2)} = 1 + \frac{2}{(n+1)(n+2)}.$$

Here, q_n is the Sobolev exponent for which the imbedding of $W_2^1(\Omega)$ into $L_{q_n}(\Omega)$ is continuous, i.e., $q_n = 2n/(n-2)$ for $n \ge 3$ and q_n is any finite number for $n = 2$.

Concerning the part $F_2(\boldsymbol{\varepsilon})$ we impose:

(A3-2) Conditions on $F_2(\boldsymbol{\varepsilon})$

(i) Nonnegativity

$$F_2(\boldsymbol{\varepsilon}) \ge 0 \quad \text{for} \quad \boldsymbol{\varepsilon} \in S^2.$$

(ii) Boundedness of the norm

$$\|F_2\|_{C^2(S^2)} < \infty.$$

(iii) Growth conditions

$$|F_2(\boldsymbol{\varepsilon})| \le c(1 + |\boldsymbol{\varepsilon}|^{K_2}),$$
$$|F_{2,\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon})| \le c(1 + |\boldsymbol{\varepsilon}|^{K_2-1}),$$
$$|F_{2,\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon})| \le c(1 + |\boldsymbol{\varepsilon}|^{K_2-2})$$

for large values of ε_{ij}, where

$$0 < K_2 \le 1 + \frac{q_n(n+4)}{4n} = \begin{cases} \text{any finite number} & \text{if } n = 2 \\ 9/2 & \text{if } n = 3. \end{cases}$$

We point out the consequences of assumption (A3), which are of importance in the proof of existence of solutions. In view of (A3-1) (i), the coefficient $c_0(\boldsymbol{\varepsilon}, \theta)$ is bounded from below

$$0 < c_v \le c_0(\boldsymbol{\varepsilon}, \theta) \quad \text{for} \quad (\boldsymbol{\varepsilon}, \theta) \in S^2 \times [0, \infty).$$

Moreover, (A3-1) (iii) and (iv) imply that the bounds on the coefficient $c_0(\boldsymbol{\varepsilon}, \theta)$ and its derivatives with respect to $\boldsymbol{\varepsilon}$ and θ are independent of θ, more precisely,

$$|c_0(\boldsymbol{\varepsilon}, \theta)|,\ |c_{0,\theta}(\boldsymbol{\varepsilon}, \theta)| \le c(1 + |\boldsymbol{\varepsilon}|^{K_1}),$$
$$|c_{0,\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \theta)| \le c(1 + |\boldsymbol{\varepsilon}|^{\max\{0, K_1-1\}}) \quad \text{for} \quad (\boldsymbol{\varepsilon}, \theta) \in S^2 \times [0, \infty).$$

From (A3-1) (i) and (ii) it follows that

$$F_1(\boldsymbol{\varepsilon}, \theta) - \theta F_{1,\theta}(\boldsymbol{\varepsilon}, \theta) \ge 0 \quad \text{for} \quad (\boldsymbol{\varepsilon}, \theta) \in S^2 \times [0, \infty)$$

what, according to Gibbs relations (4), means that the internal energy corresponding to F_1 is nonnegative. Furthermore, owing to (A3-2) (i),

$$(F_1(\boldsymbol{\varepsilon}, \theta) - \theta F_{1,\theta}(\boldsymbol{\varepsilon}, \theta)) + F_2(\boldsymbol{\varepsilon}) \ge 0 \quad \text{for} \quad (\boldsymbol{\varepsilon}, \theta) \in S^2 \times [0, \infty),$$

what means that the internal energy is nonnegative. This bound is of importance in derivation of energy estimates.

We are looking for the solution in the Sobolev space

$$\boldsymbol{V}(p, q) = \{(\boldsymbol{u}, \theta) |\ \boldsymbol{u} \in \boldsymbol{W}_p^{4,2}(\Omega^T),\ \theta \in W_q^{2,1}(\Omega^T),\ \ n + 2 < p \le q < \infty\}.$$

The assumptions on the source terms and data correspond to this space.

(A4) Source terms satisfy

$$\boldsymbol{b} \in \boldsymbol{L}_p(\Omega^T), \quad n+2 < p < \infty,$$
$$g \in L_q(\Omega^T), \quad n+2 < q < \infty, \quad \text{and} \quad g \geq 0 \quad \text{a.e. in } \Omega^T.$$

Initial data satisfy

$$\boldsymbol{u}_0 \in \boldsymbol{W}_p^{4-2/p}(\Omega), \quad \boldsymbol{u}_1 \in W_p^{2-2/p}(\Omega), \quad n+2 < p < \infty,$$
$$\theta_0 \in W_q^{2-2/q}(\Omega), \quad n+2 < q < \infty, \quad \text{and} \quad \theta_* \equiv \min_{\Omega} \theta_0 > 0.$$

Moreover, initial data are supposed to satisfy compatibility conditions for the classical solvability of parabolic problems.

Before formulating the existence result we give an example of the function $F_1(\boldsymbol{\varepsilon}, \theta)$ which satisfies the structure assumptions (A3-1) (i)–(iv). This example is motivated by the Falk-Konopka energy model (30), (31).

Example 4.1 *Let*

$$F_1(\boldsymbol{\varepsilon}, \theta) = \sum_{i=1}^{N} \tilde{F}_{1i}(\theta) \tilde{F}_{2i}(\boldsymbol{\varepsilon}),$$

with functions $\tilde{F}_{1i} \in C^3([0,\infty))$ *given by*

$$\tilde{F}_{1i}(\theta) = \begin{cases} \theta & \text{for } 0 \leq \theta \leq \theta_1 \\ \varphi_i(\theta) & \text{for } \theta_1 < \theta < \theta_2 \\ \theta^{s_i} & \text{for } \theta_2 \leq \theta < \infty. \end{cases}$$

Here $N \in \mathcal{N}$, $0 < s_i < s < 1$, θ_1, θ_2 *are numbers satisfying* $0 < \theta_1 < \theta_2$, $s_i \theta_2^{s_i - 1} < 1$, *and functions* φ_i *are nondecreasing, concave such that* $\tilde{F}_{1i} \in C^3([0,\infty))$. *Moreover, functions* $F_{2i} \in C^3(S^2)$ *are supposed to satisfy*

$$\tilde{F}_{2i}(\boldsymbol{\varepsilon}) \geq 0,$$
$$|\tilde{F}_{2i}(\boldsymbol{\varepsilon})| \leq c(1 + |\boldsymbol{\varepsilon}|^{K_1}),$$
$$|\tilde{F}_{2i,\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon})| \leq c(1 + |\boldsymbol{\varepsilon}|^{\max\{0, K_1 - 1\}}),$$
$$|\tilde{F}_{2i,\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon})| \leq c(1 + |\boldsymbol{\varepsilon}|^{\max\{0, K_1 - 2\}})$$

for all $\boldsymbol{\varepsilon} \in S^2$, *where numbers* s *and* K_1 *are subject to conditions specified in (A3-1) (iv).*

Under the above formulated assumptions the following holds true:

Theorem 4.1 *(Pawłow and Zajączkowski, 2002b). Let assumptions (A1)–(A4) be satisfied and the coefficients* $\varkappa_0, \nu$ *fulfil the condition*

$$0 < \sqrt{\varkappa_0} \leq \nu.$$

Then, for any $T > 0$ there exists a solution $(\boldsymbol{u}, \theta)$ to problem (32)–(38) in the space $\boldsymbol{V}(p,q)$, such that

$$\|\boldsymbol{u}\|_{\boldsymbol{W}_p^{4,2}(\Omega^T)} \le c(T), \quad \|\theta\|_{W_q^{2,1}(\Omega^T)} \le c(T),$$

with a positive constant $c(T)$ depending on the data of the problem and T^a, $a \in \mathbb{R}_+$. Moreover, there exists a positive finite number ω, satisfying

$$[g + \nu(\boldsymbol{A}\varepsilon_t) : \boldsymbol{\varepsilon}_t] \exp(\omega t) + [\omega c_0(\boldsymbol{\varepsilon}, \theta) + F_{,\theta\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \theta) : \boldsymbol{\varepsilon}_t]\theta_* \ge 0 \quad \text{in} \quad \Omega^T,$$

such that

$$\theta \ge \theta_* \exp(-\omega T) \quad \text{in} \quad \Omega^T.$$

The second theorem concerns the uniqueness of solutions.

THEOREM 4.2 *(Pawłow and Zajączkowski, 2002a). Let the assumptions of Theorem 4.1 be satisfied and in addition suppose that*
(A5)

$$F(\boldsymbol{\varepsilon}, \theta) : S^2 \times [0, \infty) \text{ is of class } C^4, \text{ and } g \in L_\infty(\Omega^T).$$

Then the solution $(\boldsymbol{u}, \theta) \in \boldsymbol{V}(p,q)$ to problem (32)–(38) is unique.

We comment briefly on the main steps of the existence proof.

In order to apply the Leray-Schauder fixed point theorem we make use of the parabolic decomposition (39), (40). We introduce a solution map $T(\tau, \cdot) : \boldsymbol{V}(p,q) \to \boldsymbol{V}(p,q)$, with parameter $\tau \in [0,1]$, corresponding to decomposed elasticity system (39), (40), and problem (33), (37), (38) for θ. In the subsequent steps we check the assumptions of the Leray-Schauder fixed point theorem, i.e., the following properties of the solution map: the complete continuity, the uniform equicontinuity with respect to the parameter, a priori bounds for a fixed point and the uniqueness property for the parameter τ equal to zero.

The central, most difficult part of the proof is constitute by a priori bounds for a fixed point. Their derivation requires a lot of technical work. Here the central steps concern:

— proof of the positivity of temperature within the assumed class of solutions;

— energy estimates;

— procedure of recursive improvement of energy estimates;

— proof of the crucial $L_\infty(\Omega^T)$ – estimate on θ; the idea consists in deriving a bound in $L_r(\Omega^T)$ – norm and passing to the limit with $r \to \infty$;

— proof of the Hölder continuity of θ; to this end, we apply the method presented in Ladyzhenskaya, Solonnikov and Ural'tseva (1967), which consists in showing that $\theta \in \mathcal{B}_2(\Omega^T, M, \gamma, r, \delta, \varkappa)$;

— application of the classical parabolic theory.

The proof of Theorem 4.2 is based on direct comparison of two solutions to problem (32)–(38) corresponding to the same data. Thanks to the regularity of solutions it is possible to derive energy estimates for the difference of solutions and next, with the help of Gronwall's inequality, to conclude the uniqueness.

5. 3-D Frémond's model

The Frémond model (Frémond, 1987, 1990, 1996) is based on the Landau-Ginzburg free energy of the form

$$\tilde{f} = \tilde{f}(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \theta, \tilde{\boldsymbol{\beta}}) = \sum_{i=1}^{3} \beta_i f_i(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \theta) + \theta \tilde{I}_B(\tilde{\boldsymbol{\beta}}), \tag{42}$$

where $\boldsymbol{\varepsilon}$ is the linearized strain tensor, θ — absolute temperature, $\tilde{\boldsymbol{\beta}} = (\beta_1, \beta_2, \beta_3)$ — vector representing local ratios of two martensitic, β_1, β_2, and the austenitic phase, β_3.

The density is assumed constant $\varrho = 1$. The free energies f_i of the individual phases are given by

$$\begin{aligned}
f_1 &= f_1(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \theta) = -c_v\theta\log\theta + \frac{1}{2}\boldsymbol{\varepsilon} : (\boldsymbol{A}\boldsymbol{\varepsilon}) + \frac{\varkappa}{2}|\nabla tr\boldsymbol{\varepsilon}|^2 - \alpha(\theta) tr\boldsymbol{\varepsilon}, \qquad (43)\\
f_2 &= f_2(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \theta) = -c_v\theta\log\theta + \frac{1}{2}\boldsymbol{\varepsilon} : (\boldsymbol{A}\boldsymbol{\varepsilon}) + \frac{\varkappa}{2}|\nabla tr\boldsymbol{\varepsilon}|^2 + \alpha(\theta) tr\boldsymbol{\varepsilon},\\
f_3 &= f_3(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \theta) = -c_v\theta\log\theta + \frac{1}{2}\boldsymbol{\varepsilon} : (\boldsymbol{A}\boldsymbol{\varepsilon}) + \frac{\varkappa}{2}|\nabla tr\boldsymbol{\varepsilon}|^2 - \frac{l}{\theta^*}(\theta - \theta^*),
\end{aligned}$$

where c_v denotes thermal specific heat, $\boldsymbol{A}$ — rigidity matrix defined by (16), $\varkappa$ — positive coefficient, θ^* — critical temperature, l — latent heat of the austenite-martensite phase transition, $\alpha(\theta)$ — function proportional to the thermal expansion coefficient, nonnegative, nonincreasing and vanishing for temperatures above the Curie temperature $\theta_C > \theta^*$. Furthermore, $\theta\tilde{I}_B(\tilde{\boldsymbol{\beta}})$ represents a mixture energy, where

$$\tilde{I}_B(\tilde{\boldsymbol{\beta}}) := \begin{cases} 0 & \text{if } \tilde{\boldsymbol{\beta}} \in B, \\ +\infty & \text{if } \tilde{\boldsymbol{\beta}} \notin B, \end{cases}$$

is the indicator function of the closed convex set

$$B := \{\tilde{\boldsymbol{\beta}} \in \mathbb{R}^3 |\ 0 \le \beta_i \le 1,\ i = 1, 2, 3,\ \sum_{i=1}^{3} \beta_i = 1\}.$$

We point out that free energy (42), in contrast to (29), is convex in $\boldsymbol{\varepsilon}$. The strain gradient term is a special case of that in (29) (viz., operator $\boldsymbol{Q}$ with $\mu = 0$).

Upon elimination of β_3 the free energy $\tilde{f}$ takes the form

$$f(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \theta, \boldsymbol{\beta}) = f_0(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \theta, \boldsymbol{\beta}) + \theta I_T(\boldsymbol{\beta}), \tag{44}$$

where

$$f_0 = \beta_1(f_1 - f_3) + \beta_2(f_2 - f_3) + f_3$$

stands for a smooth part of f, $\boldsymbol{\beta} = (\beta_1, \beta_2)$, and $I_{\mathcal{T}}(\cdot)$ denotes the indicator function of the triangle

$$\mathcal{T} = \{\boldsymbol{\beta} \in \mathbb{R}^2 |\ \beta_1 \geq 0,\ \beta_2 \geq 0,\ \beta_1 + \beta_2 \leq 1\}.$$

The field equations in terms of $\boldsymbol{u}, \theta$ and $\boldsymbol{\beta} = (\beta_1, \beta_2)$ are (Frémond, 1990, Colli, Frémond and Visintin, 1990, Frémond and Miyazaki, 1996):

$$\begin{aligned}
&\boldsymbol{u}_{tt} - \nabla \cdot (\lambda tr\boldsymbol{\varepsilon}\boldsymbol{I} + 2\mu\boldsymbol{\varepsilon} + \alpha(\theta)(\beta_2 - \beta_1)\boldsymbol{I}) + \varkappa\nabla \cdot (\Delta tr\boldsymbol{\varepsilon}\boldsymbol{I}) = \boldsymbol{b}, \qquad (45)\\
&(c_v - \theta\alpha_{,\theta\theta}(\theta)tr\boldsymbol{\varepsilon}(\beta_2 - \beta_1))\theta_t - k\Delta\theta - \theta\alpha_{,\theta}(\theta)tr\boldsymbol{\varepsilon}_t(\beta_2 - \beta_1)\\
&\quad -l(\beta_1 + \beta_2)_t + (\alpha(\theta) - \theta\alpha_{,\theta}(\theta))tr\boldsymbol{\varepsilon}(\beta_2 - \beta_1)_t = g,\\
&-\gamma\partial_t\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} + \begin{pmatrix} \alpha(\theta)tr\boldsymbol{\varepsilon} - l(\theta - \theta^*)/\theta^* \\ -\alpha(\theta)tr\boldsymbol{\varepsilon} - l(\theta - \theta^*)/\theta^* \end{pmatrix} \in \partial I_{\mathcal{T}}(\boldsymbol{\beta}),
\end{aligned}$$

where $\boldsymbol{\varepsilon} = (\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)/2$, γ is a nonnegative viscosity constant, and $\partial I_{\mathcal{T}}(\cdot)$ denotes the subdifferential of $I_{\mathcal{T}}(\cdot)$. We note that $\theta\partial I_{\mathcal{T}} = \partial I_{\mathcal{T}}$.

Originally, the system (45) has been proposed on the basis of the principle of virtual power and a second gradient theory. It is worth to point out that it turns out to fall into a general setting presented in Section 3. In fact, it represents balance laws of linear momentum and energy (12), and a relaxation law for phase ratios in the form of differential inclusion

$$-\gamma\partial_t\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} - f_{0,\boldsymbol{\beta}}(\boldsymbol{\varepsilon}, \nabla\boldsymbol{\varepsilon}, \theta, \boldsymbol{\beta}) \in \partial I_{\mathcal{T}}(\boldsymbol{\beta}), \qquad (46)$$

with constitutive equations for $\boldsymbol{S}$ and $\boldsymbol{q}$ defined by (20), $\boldsymbol{S}^v = 0$, and $\boldsymbol{q}_0$ given by Fourier law (15), i.e.,

$$\begin{aligned}
&\boldsymbol{S} = f_{,\boldsymbol{\varepsilon}} - \nabla \cdot f_{,\nabla\boldsymbol{\varepsilon}}, \qquad (47)\\
&\boldsymbol{q} = \boldsymbol{q}_0 + \boldsymbol{q}_1, \quad \boldsymbol{q}_0 = -k\nabla\theta, \quad \boldsymbol{q}_1 = -\boldsymbol{\varepsilon}_t f_{,\nabla\boldsymbol{\varepsilon}}.
\end{aligned}$$

Actually, for f defined by (44) we have

$$\begin{aligned}
&f_{,\boldsymbol{\varepsilon}} = \boldsymbol{A}\boldsymbol{\varepsilon} + \alpha(\theta)(\beta_2 - \beta_1)\boldsymbol{I}, \qquad (48)\\
&f_{,\nabla\boldsymbol{\varepsilon}} = (f_{,\varepsilon_{ij,k}}) = \varkappa(\varepsilon_{pq,k}\delta_{pq}\delta_{ij}) = \varkappa(tr\boldsymbol{\varepsilon}_{,k}\delta_{ij}),\\
&\nabla \cdot f_{,\nabla\boldsymbol{\varepsilon}} = \partial_k(\varkappa tr\boldsymbol{\varepsilon}_{,k}\delta_{ij}) = \varkappa\Delta tr\boldsymbol{\varepsilon}\boldsymbol{I},\\
&f_{,\nabla\boldsymbol{\varepsilon}} : \nabla\boldsymbol{\varepsilon}_t = \varkappa(tr\boldsymbol{\varepsilon}_{,k}\delta_{ij})\varepsilon_{tij,k} = \varkappa\nabla tr\boldsymbol{\varepsilon} \cdot \nabla tr\boldsymbol{\varepsilon}_t,\\
&f_{0,\boldsymbol{\beta}} = \begin{pmatrix} f_1 - f_3 \\ f_2 - f_3 \end{pmatrix} = \begin{pmatrix} -\alpha(\theta)tr\boldsymbol{\varepsilon} + l(\theta - \theta^*)/\theta^* \\ \alpha(\theta)tr\boldsymbol{\varepsilon} + l(\theta - \theta^*)/\theta^* \end{pmatrix}.
\end{aligned}$$

Clearly, in view of (47), (48), the momentum balance $(12)_1$ yields $(45)_1$, and the relaxation law (46) equation $(45)_3$.

Furthermore, proceeding as in Lemma 3.2, it is straightforward to show that the energy balance $(12)_2$ with $\boldsymbol{S}, q$ defined by (47) admits formally the following equivalent forms:

$$
\begin{aligned}
&e_t + \nabla \cdot \boldsymbol{q}_0 - f_{,\boldsymbol{\varepsilon}} : \boldsymbol{\varepsilon}_t - f_{,\nabla\boldsymbol{\varepsilon}} : \nabla\boldsymbol{\varepsilon}_t = g, \\
&\theta\eta_t + \nabla \cdot \boldsymbol{q}_0 + f_{0,\boldsymbol{\beta}} \cdot \boldsymbol{\beta}_t + \theta\partial I_{\mathcal{T}}(\boldsymbol{\beta}) \cdot \boldsymbol{\beta}_t \ni g \\
&c_0\theta_t + \nabla \cdot \boldsymbol{q}_0 - \theta f_{,\theta\boldsymbol{\varepsilon}} : \boldsymbol{\varepsilon}_t - \theta f_{,\theta\nabla\boldsymbol{\varepsilon}} : \nabla\boldsymbol{\varepsilon}_t + (f_{0,\boldsymbol{\beta}} - \theta f_{0,\theta\boldsymbol{\beta}}) \cdot \boldsymbol{\beta}_t = g,
\end{aligned}
\tag{49}
$$

where $c_0 = -\theta f_{,\theta\theta}$.

We note that since the term $\theta I_{\mathcal{T}}(\boldsymbol{\beta})$ is proportional to temperature its contribution in energy equation $(49)_3$ drops out. Consequently, in view of equalities

$$
\begin{aligned}
&c_0 = c_v - \theta\alpha_{,\theta\theta} tr\boldsymbol{\varepsilon}(\beta_2 - \beta_1), \\
&-\theta f_{,\theta\boldsymbol{\varepsilon}} : \boldsymbol{\varepsilon}_t = -\theta\alpha_{,\theta} tr\boldsymbol{\varepsilon}_t(\beta_2 - \beta_1), \quad -\theta f_{,\theta\nabla\boldsymbol{\varepsilon}} : \nabla\boldsymbol{\varepsilon}_t = 0, \\
&(f_{0,\boldsymbol{\beta}} - \theta f_{0,\theta\boldsymbol{\beta}}) \cdot \boldsymbol{\beta}_t = (\alpha - \theta\alpha_{,\theta}) tr\boldsymbol{\varepsilon}(\beta_2 - \beta_1)_t - l(\beta_1 + \beta_2)_t,
\end{aligned}
\tag{50}
$$

equation $(49)_3$ yields $(45)_2$.

The system (45) is usually written in terms of the variables

$$
\chi_1 := \beta_1 + \beta_2, \quad \chi_2 := \beta_2 - \beta_1. \tag{51}
$$

It reads then

$$
\boldsymbol{u}_{tt} - \nabla \cdot (\lambda(\nabla \cdot \boldsymbol{u})\boldsymbol{I} + 2\mu\varepsilon(\boldsymbol{u}) + \alpha(\theta)\chi_2\boldsymbol{I}) + \varkappa\nabla \cdot (\Delta(\nabla \cdot \boldsymbol{u})\boldsymbol{I}) = \boldsymbol{b}, \tag{52}
$$

$$
\begin{aligned}
c_v\theta_t - k\Delta\theta \;&=\; g + l\chi_{1t} - (\alpha(\theta) - \theta\alpha_{,\theta}(\theta))(\nabla \cdot \boldsymbol{u})\chi_{2t} \\
&+\; c_v\theta_t - k\Delta\theta + \theta\alpha_{,\theta}(\theta)\chi_2\nabla \cdot \boldsymbol{u}_t + \theta\alpha_{,\theta\theta}(\theta)\chi_2(\nabla \cdot \boldsymbol{u})\theta_t,
\end{aligned}
$$

$$
\gamma\partial_t \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} + \begin{pmatrix} 2l(\theta - \theta^*)/\theta^* \\ 2\alpha(\theta)\nabla \cdot \boldsymbol{u} \end{pmatrix} + \partial I_{\mathcal{K}}(\chi_1, \chi_2) \ni \begin{pmatrix} 0 \\ 0 \end{pmatrix},
$$

where

$$
I_{\mathcal{K}}(\chi_1, \chi_2) = \begin{cases} 0 & \text{if } (\chi_1, \chi_2) \in \mathcal{K} = \{(\bar{\chi}_1, \bar{\chi}_2) \in \mathbb{R}^2 |\; |\bar{\chi}_2| \le \bar{\chi}_1 \le 1\}, \\ +\infty & \text{if } (\chi_1, \chi_2) \notin \mathcal{K}. \end{cases}
$$

The system is supplemented with appropriate initial and boundary conditions.

The system (52) and various variants close to it have been studied in 1-D and 3-D cases. Most of the papers deal with quasistationary form of linear momentum equation $(52)_1$, i.e., neglecting the inertial term $\boldsymbol{u}_{tt}$.

For the study of 1-D quasistationary case we refer to Colli and Sprekels (1995), Colli, Laurençot and Stefanelli (2000). The full 1-D system (52) has been investigated in Chemetov (1988), Shemetov (1998).

The mathematical analysis of 3-D system (52) has faced the difficulties arising from nonlinear terms in energy equation $(52)_2$. By neglecting all or some of the nonlinearities in $(52)_2$ the existence results for quasistationary system (52) have been established , e.g., in Colli, Frémond and Visintin (1990), Colli and Sprekels (1992), Hoffmann, Niezgódka and Zheng (1990).

In the latter reference a mollified version of the equation for phase ratios, accounting for diffusion effects, has been assumed. More precisely, a technically useful term involving Laplacian operator appears on the left-hand side of $(45)_3$. The presence of such a term is associated with additional phase ratio gradient term in free energy (42).

The existence result for the full system (52) in the quasistationary form has been established by Colli (1995). The maximum principle for Frémond's model, asserting that temperature is positive, has been proved in Colli and Sprekels (1993).

Recently, Frémond's model accounting for diffusive effects and with Cattaneo-Maxwell heat flux law has been studied by Bonetti (2001, 2002).

The model is considered there in the simplified form neglecting nonlinear terms in energy equation and with quasistationary form of momentum equation. The results concerning well-posedness of such a model and the convergence as relaxation and diffusive parameters tend to zero are proved in the above mentioned references.

Finally, we mention recent references of Pagano, Alart and Maisonneuve (1998), Balandraud, Ernst and Soós (2000), Timofte and Timofte (2001a, b), where some variants of Frémond's model have been investigated. These variants neglect strain gradient term in free energy (42), i.e., do not account for interfacial structure of phase boundaries.

6. 3-D Fried-Gurtin model

Fried and Gurtin (1994) have proposed a general theory of solid-solid phase transitions, based on a microforce balance, which describes deformational effects neglecting heat and mass transport. In this theory the order parameter is not identified with the strain tensor but represents a new quantity which can have different physical status.

In case of diffusive transitions it describes atomic arrangements within unit cells of crystal lattice. For pure martensitic transitions, in which the lattice undergoes a mechanical strain but there are no rearrangements of atoms within cells, the order parameter might be viewed as an artifice that yields a regularization of mechanical equations.

As discussed in Fried and Gurtin (1994), Fried and Grach (1997), such regularization models interfacial structure of phase boundaries. Namely, it has been shown there that, granted appropriate scaling, the governing equations of the order-parameter-based theory are asymptotic to governing equations that arise in sharp-interface theory by Gurtin and Struthers (1990).

The approach based on an order parameter has been applied also for diffusive and ordering phase transitions in solids (Gurtin, 1996) and solid-liquid phase transitions in the presence of heat conduction (Fried and Gurtin, 1993).

We mention that the field equations generated by the Fried-Gurtin theory based on a microforce balance can be recovered by exploiting the entropy inequality with multipliers, see Pawłow (2000a) for examples and discussion.

The Fried-Gurtin theory is based on the first order gradient free energy

$$f = f(\boldsymbol{F}, \boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}), \tag{53}$$

where

$$\boldsymbol{F} = \boldsymbol{I} + \nabla\boldsymbol{u}$$

is the deformation gradient, and $\boldsymbol{\varphi} = (\varphi_1, \dots, \varphi_A)$ denotes vector-order parameter subject to constraint, for example,

$$\varphi_a \in [0,1], \qquad \sum_{a=1}^{A} \varphi_a = 1. \tag{54}$$

The underlying laws of the theory are: linear momentum balance, angular momentum balance, microforce balance and the second principle of thermodynamics in the form of a dissipation inequality. Assuming constitutive functions depending on $(\boldsymbol{F}, \boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}, \boldsymbol{\varphi}_t)$ it is shown that the field equations compatible with the dissipation inequality have the form:

$$\begin{aligned} &\varrho\boldsymbol{u}_{tt} = \nabla\cdot f_{,\boldsymbol{F}}(\boldsymbol{F}, \boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}) + \boldsymbol{b}, \\ &\boldsymbol{B}(\boldsymbol{F}, \boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}, \boldsymbol{\varphi}_t)\boldsymbol{\varphi}_t = -\frac{\delta f}{\delta\boldsymbol{\varphi}}(\boldsymbol{F}, \boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}) + \boldsymbol{\gamma} \\ &= -f_{,\varphi}(\boldsymbol{F}, \boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}) + \nabla\cdot f_{,\nabla\boldsymbol{\varphi}}(\boldsymbol{F}, \boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}) + \boldsymbol{\gamma}, \end{aligned} \tag{55}$$

where $\boldsymbol{b}$, $\boldsymbol{\gamma}$ are external forces, and $\boldsymbol{B}$ is a matrix of kinetic coefficients B_{ij}, consistent with the inequality

$$\boldsymbol{\varphi}_t \cdot (\boldsymbol{B}(\boldsymbol{F}, \boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}, \boldsymbol{\varphi}_t)\boldsymbol{\varphi}_t) \geq 0. \tag{56}$$

When order parameter has two components $\boldsymbol{\varphi} = (\varphi_1, \varphi_2)$ constrained via $\varphi_1 + \varphi_2 = 1$ then, writing $\varphi = \varphi_2 = 1 - \varphi_1$ and expressing free energy as a function of $\boldsymbol{F}, \varphi, \nabla\varphi$ through

$$\tilde{f}(\boldsymbol{F}, \varphi, \nabla\varphi) = f(\boldsymbol{F}, \varphi_1, \varphi_2, \nabla\varphi_1, \nabla\varphi_2),$$

the system $(55)_2$ can be reduced to one equation for φ with scalar kinetic coefficient $\beta = \beta(\boldsymbol{F}, \varphi, \nabla\varphi, \varphi_t) \geq 0$, provided that $B_{11} = B_{22}$. In such a case $\beta = B_{22} - B_{12}$.

As a special case the Fried-Gurtin theory includes also the situation of small displacement gradient where the constitutive functions depend on $\boldsymbol{F}$ only through the linearized strain $\boldsymbol{\varepsilon}(\boldsymbol{u})$. We cite now some examples corresponding to such a case. A typical form of the free energy is

$$f(\boldsymbol{\varepsilon}, \boldsymbol{\varphi}, \nabla\boldsymbol{\varphi}) = W(\boldsymbol{\varepsilon}, \boldsymbol{\varphi}) + g(\boldsymbol{\varphi}) + h(\nabla\boldsymbol{\varphi}), \tag{57}$$

where the three terms on the right-hand side denote the strain energy, the exchange energy and the gradient energy. A standard exchange energy for system constrained by $(54)_2$ is

$$g(\boldsymbol{\varphi}) = \frac{1}{2}\nu \prod_{a=1}^{A} (1-\varphi_a)^2, \quad \nu > 0. \tag{58}$$

A standard isotropic version of gradient energy is

$$h(\nabla\boldsymbol{\varphi}) = \frac{1}{2}\varkappa|\nabla\boldsymbol{\varphi}|^2, \tag{59}$$

where $\varkappa$ is a positive coefficient. A relevant expression for the strain energy is

$$W(\boldsymbol{\varepsilon},\boldsymbol{\varphi}) = \sum_{a=1}^{A} \varphi_a W_a(\boldsymbol{\varepsilon}), \tag{60}$$

where $W_a(\boldsymbol{\varepsilon})$ stands for the individual energy of phase a, given by

$$W_a(\boldsymbol{\varepsilon}) = w_a + \frac{1}{2}(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_a) : (\boldsymbol{A}_a(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_a)). \tag{61}$$

Here $\boldsymbol{\varepsilon}_a$ denotes the natural strain of phase a, $\boldsymbol{A}_a$ — the elasticity tensor of phase a, and $w_a = W_a(\varepsilon_a)$ — the minimal energy value.

We quote also an alternate example of strain energy, originally proposed by Libman and Roitburd (1987) for ordering transitions:

$$W(\boldsymbol{\varepsilon},\boldsymbol{\varphi}) = w(\boldsymbol{\varphi}) + \frac{1}{2}(\boldsymbol{\varepsilon}-\bar{\boldsymbol{\varepsilon}}(\boldsymbol{\varphi})) : (\boldsymbol{A}(\boldsymbol{\varphi})(\boldsymbol{\varepsilon}-\bar{\boldsymbol{\varepsilon}}(\boldsymbol{\varphi}))), \tag{62}$$

where $\bar{\boldsymbol{\varepsilon}}(\boldsymbol{\varphi})$ is the natural strain corresponding to the order parameter $\boldsymbol{\varphi}$, and $w(\boldsymbol{\varphi})$ is the energy of homogeneous stress free phase.

We present now the field equations corresponding to the free energy defined by (57)–(61) in case of two-component order parameter. Setting $\varphi = \varphi_2 = 1-\varphi_1$, that is, identifying phase 1 with $\varphi = 0$ and phase 2 with $\varphi = 1$, we have

$$\begin{aligned} &\boldsymbol{u}_{tt} - \nabla\cdot(1-\varphi)\boldsymbol{A}_1(\boldsymbol{\varepsilon}(\boldsymbol{u})-\boldsymbol{\varepsilon}_1) + \varphi\boldsymbol{A}_2(\boldsymbol{\varepsilon}(\boldsymbol{u})-\boldsymbol{\varepsilon}_2)) = \boldsymbol{b}, \\ &\beta(\boldsymbol{\varepsilon}(\boldsymbol{u}),\varphi,\nabla\varphi,\varphi_t)\varphi_t - 2\varkappa\Delta\varphi + g_{,\varphi}(\varphi) + W_2(\boldsymbol{\varepsilon}(\boldsymbol{u})) - W_1(\boldsymbol{\varepsilon}(\boldsymbol{u})) = \gamma, \end{aligned} \tag{63}$$

where W_i, $i = 1,2$, are given by (61), and

$$\begin{aligned} &\boldsymbol{A}_i\boldsymbol{\varepsilon}(\boldsymbol{u}) = \lambda_i(\nabla\cdot\boldsymbol{u})\boldsymbol{I} + 2\mu_i\boldsymbol{\varepsilon}(\boldsymbol{u}), \\ &g(\varphi) = \frac{1}{2}\nu\varphi^2(1-\varphi)^2. \end{aligned} \tag{64}$$

According to our knowledge the well-posedness of systems directly related to the Fried-Gurtin model has not been studied mathematically.

A specific one-dimensional version of the model with strain energy of the type (62) has been studied in Sikora, Cusumano and Jester (1998) from the point of view of numerical simulation and the analysis of equilibrium solutions. The free energy has been assumed there in the form:

$$f(\varepsilon, \varphi, \nabla\varphi) = W(\varepsilon, \varphi) + g(\varphi) + \frac{1}{2}\varkappa|\nabla\varphi|^2, \tag{65}$$

with $g(\varphi)$ as in $(64)_2$, and

$$W(\varepsilon, \varphi) = \frac{1}{2}\mu(\varepsilon - k\varphi)^2,$$

where $\varkappa, \nu, \mu$ are positive material parameters, and $k = 1/\sqrt{2}$ is a constant. In such a case the field equations read ($b = 0,\ \gamma = 0$):

$$\begin{aligned} &u_{tt} - \mu(u_x - k\varphi)_x = 0, \\ &\beta\varphi_t - \varkappa\varphi_{xx} + \nu g_{,\varphi}(\varphi) - \mu k(u_x - k\varphi) = 0, \end{aligned} \tag{66}$$

where β is a positive constant, and $g_{,\varphi}(\varphi) = \nu\varphi(1-\varphi)(1-2\varphi)$.

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