ONE-DIMENSIONAL THERMOMECHANICAL PHASE TRANSITIONS WITH NON-CONVEX POTENTIALS OF GINZBURG-LANDAU TYPE

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ONE-DIMENSIONAL THERMOMECHANICAL PHASE TRANSITIONS WITH NON-CONVEX POTENTIALS OF GINZBURG-LANDAU TYPE

JÜRGEN SPREKELS*

Abstract. In this paper we study the system of partial differential equations governing the nonlinear thermomechanical processes in non-viscous, heat-conducting, one-dimensional solids. To allow for both stress- and temperature-induced solid-solid phase transitions in the material, possibly accompanied by hysteresis effects, a non-convex free energy of Ginzburg-Landau form is assumed. Results concerning the well-posedness of the problem, as well as the numerical approximation and the optimal control of the solutions, are presented in the paper, in particular in connection with the austenitic-martensitic phase transitions in the so-called "shape memory alloys".

Key words. phase transitions, non-convex potentials, Ginzburg-Landau theory, shape memory alloys, hysteresis, conservation laws.

AMS(MOS) subject classifications. 35L65, 35K60, 73U05, 73B30

1. Introduction. In this paper we consider thermomechanical processes in non-viscous, one-dimensional heat-conducting solids of constant density ρ (assumed normalized to unity) that are subjected to heating and loading. We think of metallic solids that do not only respond to a change of the strain $\epsilon = u_x$ (u stands for the displacement) by an elastic stress $\sigma = \sigma(\epsilon)$, but also react to changes of the curvature of their metallic lattices by a couple stress $\mu = \mu(\epsilon_x)$. Thus, the corresponding free energy F is assumed in Ginzburg-Landau form, i.e.,

$$F = F(\epsilon, \epsilon_x, \theta), \tag{1.1}$$

where θ is the absolute temperature. In the framework of the Landau theory of phase transitions, the strain ϵ plays the role of an "order parameter", whose actual value determines what phase is prevailing in the material (see [3]).

Since we are interested in solid-solid phase transitions, driven by loading and/or heating, which are accompanied by hysteresis effects, we do not assume that $F(\epsilon, \epsilon_x, \theta)$ is a convex function of the order parameter ϵ for all values of (ϵ_x, θ). A particularly interesting

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class of materials are the metallic alloys exhibiting the so-called "shape memory effect". Among those there are alloys like $CuZn, CuSn, AuCuZn_2, AgCd$ and, most important, $TiNi$ (so-called Nitinol). In these materials, the metallic lattice is deformed by shear, and the assumption of a constant density is justified. The relation between shear stress and shear strain ($\sigma - \epsilon$-curves) of shape memory alloys exhibit a rather spectacular temperature-dependent hysteretic behavior (see [2] for an account of the properties of shape memory alloys):

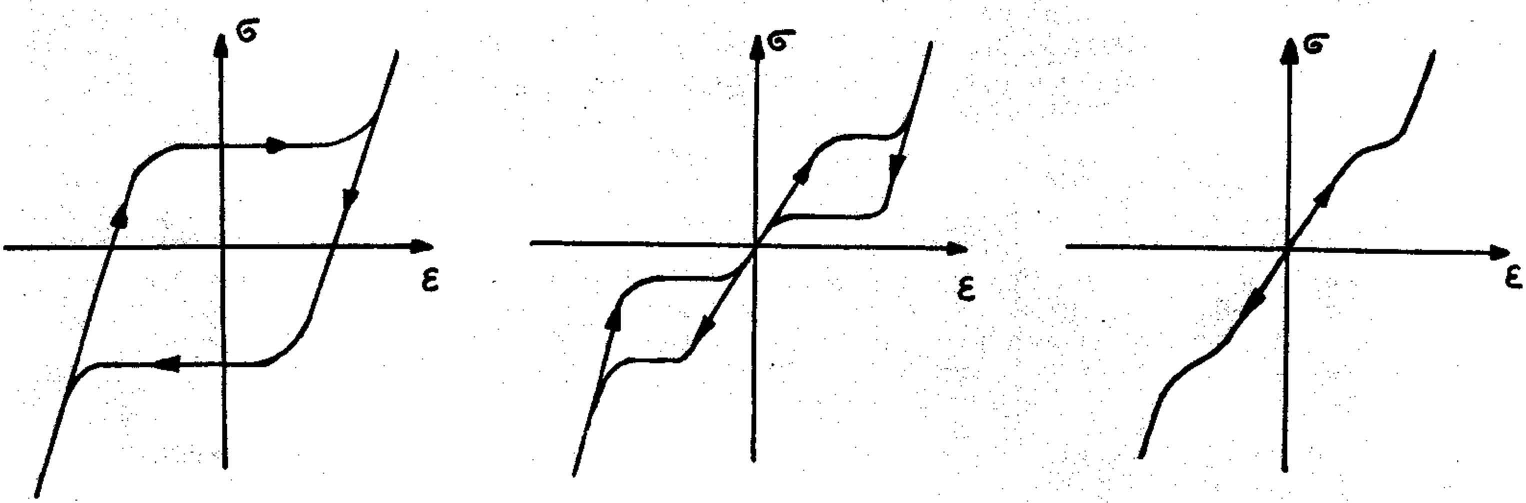

Fig 1. Typical $\sigma - \epsilon$-curves in shape memory alloys, with temperature θ increasing from a) to c).

In addition, for sufficiently small shear stresses σ another hysteresis occurs in the $\epsilon - \theta$-diagrams:

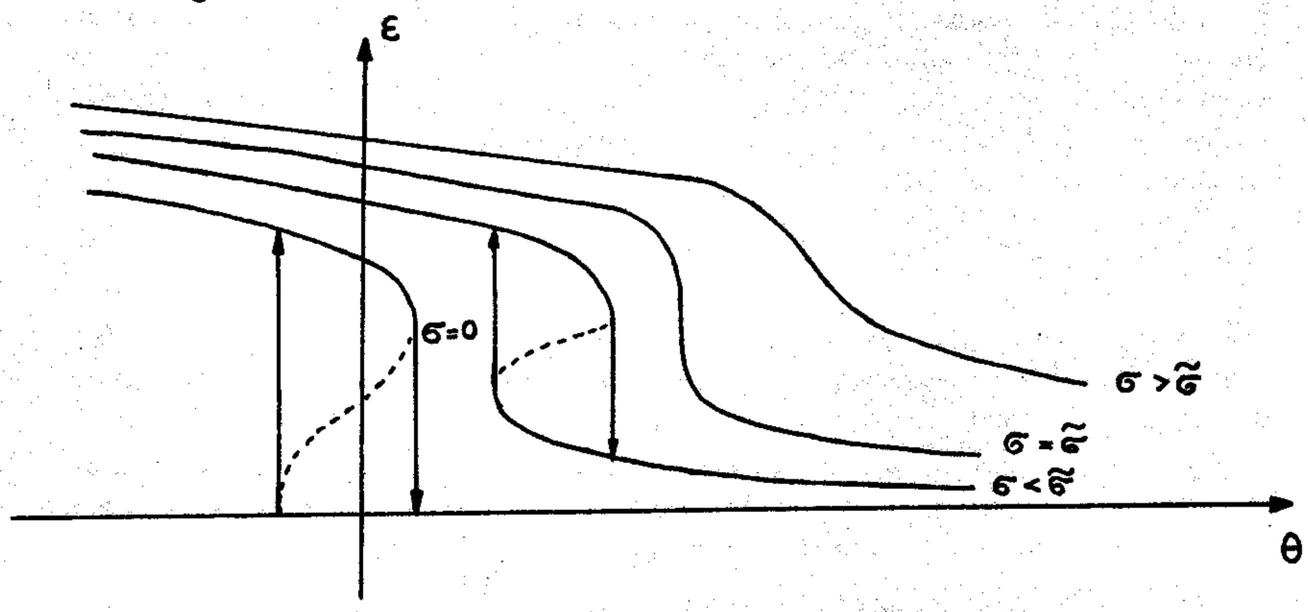

Fig 2. $\epsilon - \theta$ curves in shape memory alloys for different values of σ.

On the microscopic scale, this hysteretic behaviour is ascribed to first-order stress-induced (fig. 1a,b) or temperature-induced (fig. 2) phase transitions between different configurations of the metallic lattice, namely the symmetric high-temperature phase "austenite" (taken as reference configuration) and its two oppositively oriented sheared versions termed "martensitic twins", which prevail at low temperatures (cf., [6], [7]).

The simplest form for the free energy F which matches the experimental evidence given by figs. 1,2 quite well and takes interfacial energies into account is given by (cf., [4], [5])

$$F(\epsilon, \epsilon_x, \theta) = -C_V\theta\log(\theta/\theta_2) + C_V\theta + \widetilde{C} + \kappa_1(\theta-\theta_1)\epsilon^2 - \kappa_2\epsilon^4 + \kappa_3\epsilon^6 + \frac{\gamma}{2}\,\epsilon_x^2\,, \tag{1.2}$$

where C_V denotes the specific heat, $\widetilde{C}$ is some constant, θ_1 and θ_2 are (positive) temperatures and $\kappa_1, \kappa_2, \kappa_3, \gamma$ are positive constants. A complete set of data for the alloy $AuCuZn_2$ is given in [5]. Note that within the range of interesting temperatures, for $\theta \to \theta_1$, F is not convex as function of ϵ.

In the sequel, we assume F in the somewhat more general form (with positive $\kappa_1, \kappa_2, \gamma$)

$$F(\epsilon, \epsilon_x, \theta) = -C_V\theta\log(\theta/\theta_2) + C_V\theta + \widetilde{C} + \kappa_1\theta F_1(\epsilon) + \kappa_2 F_2(\epsilon) + \frac{\gamma}{2}\,\epsilon_x^2\,, \tag{1.3}$$

where F_1 and F_2 satisfy the hypothesis:

(H1) $F_1, F_2 \in C^4(\mathbf{R})$; $F_2(\epsilon) \geq \bar{c}_1|\epsilon| - \bar{c}_2$, $\forall \epsilon \in \mathbf{R}$, with positive constants $\bar{c}_1, \bar{c}_2$.

The dynamics of thermomechanical processes in a solid are governed by the conservation laws of linear momentum, energy and mass. The latter may be ignored since ρ is constant for the materials under consideration (we assume $\rho \equiv 1$). The two others read

$$u_{tt} - \sigma_x + \mu_{xx} = f\,, \tag{1.4a}$$

$$e_t + q_x - \sigma\epsilon_t - \mu\epsilon_{xt} = g\,. \tag{1.4b}$$

Here the involved quantities have their usual meanings, namely: σ-elastic stress, μ-couple stress, u-displacement, f - density of loads, e - density of internal energy, q - heat flux, g -density of heat sources or sinks.

We have the constitutive relations

$$\sigma = \frac{\partial F}{\partial \epsilon}\,, \quad \mu = \frac{\partial F}{\partial \epsilon_x}\,, \quad e = F - \theta\,\frac{\partial F}{\partial \theta}\,, \tag{1.5}$$

and we assume the heat flux in the Fourier-form

$$q = -\kappa\theta_x\,, \quad \text{where } \kappa > 0 \text{ is the heat conductivity.} \tag{1.6}$$

Notice that (1.6) implies that the second principle of thermodynamics in form of the Clausius-Duhem inequality is automatically satisfied.

Inserting (1.3), (1.5), (1.6) in the balance laws and assuming a one-dimensional sample of unit length, we obtain the system

$$u_{tt} - \left(\kappa_1 \theta F_1'(\epsilon) + \kappa_2 F_2'(\epsilon)\right)_x + \gamma u_{xxxx} = f\,, \tag{1.7a}$$

$$C_V \theta_t - \kappa_1 \theta F_1'(\epsilon)\epsilon_t - \kappa \theta_{xx} = g, \tag{1.7b}$$

$$\epsilon = u_x\,, \tag{1.7c}$$

to be satisfied in the space-time cylinder Ω_T, where $T > 0$, $\Omega = (0,1)$, and, for $t > 0$, $\Omega_t := \Omega \times (0,t)$.

In addition, we prescribe the initial and boundary conditions

$$u(x,0) = u_0(x), u_t(x,0) = u_1(x),\ \theta(x,0) = \theta_0(x), x \in \overline{\Omega}, \tag{1.7d}$$

$$u(0,t) = u_{xx}(0,t) = u(1,t) = u_{xx}(1,t) = 0,\ t \in [0,T], \tag{1.7e}$$

$$\theta_x(0,t) = 0,\quad -\kappa\theta_x(1,t) = \beta\big(\theta(1,t) - \theta_\Gamma(t)\big),\ t \in [0,T], \tag{1.7f}$$

where $\beta > 0$ is a heat exchange coefficient, and θ_Γ stands for the outside temperature at $x = 1$.

In the following sections we state some results concerning the well-posedness of the system (1.7a–f), including a convergent numerical algorithm for its approximate solution. To abbreviate the exposition, all constants in (1.7a–f) are assumed to equal unity; this will have no bearing on the mathematical analysis.

2. Well-posedness. We consider (1.7a–f). In addition to (H1), we generally assume:

(H2) $u_0 \in \widetilde{H}^4(\Omega) = \{u \in H^4(\Omega) | u(0) = u(1) = 0 = u''(0) = u''(1)\}$;
$u_1 \in \overset{\circ}{H}{}^1(\Omega) \cap H^2(\Omega)$; $\theta_0 \in H^2(\Omega)$, $\theta_0(x) > 0$, $\forall\, x \in \overline{\Omega}$.

(H3) $\theta_0'(0) = 0$, $\theta_\Gamma(0) = \theta_0(1) + \frac{\kappa}{\beta}\, \theta_0'(1) > 0$ (compatibility).

(H4) $f, g \in H^1(0,T;H^1(\Omega))$, $\theta_\Gamma \in H^1(0,T)$, where $g(x,t) \geq 0$ on Ω_T and $\theta_\Gamma(t) > 0$ on $[0,T]$.

We have the result:

THEOREM 2.1. *Suppose (H1)–(H4) hold. Then (1.7a–f) has a unique solution (u,θ) which satisfies*

$$u \in W^{2,\infty}(0,T;L^2(\Omega)) \cap W^{1,\infty}(0,T;\overset{\circ}{H}{}^1(\Omega) \cap H^2(\Omega)) \cap L^\infty(0,T;\widetilde{H}^4(\Omega)), \tag{2.1a}$$

$$\theta \in H^1(0,T;H^1(\Omega)) \cap L^2(0,T;H^3(\Omega)), \tag{2.1b}$$

$$\theta(x,t) > 0, \quad \textit{on} \quad \overline{\Omega}_T. \tag{2.1c}$$

Moreover, the operator $(f, g, \theta_\Gamma) \longmapsto (u, \theta)$ *maps bounded subsets of* $H^1(0,T;H^1(\Omega)) \times H^1(0,T;H^1(\Omega)) \times \mathcal{M}$ *into bounded subsets of* $X \times Y$, *where* $\mathcal{M} := \{z \in |H^1(0,T)| \; z(t) > 0$ *on* $[0,T]$, $z(0) = \theta_0(1) + \theta_0'(1)\}$, $X := W^{2,\infty}(0,T;L^2(\Omega)) \cap W^{1,\infty}(0,T;\overset{\circ}{H}{}^1(\Omega) \cap H^2(\Omega)) \cap L^\infty(0,T;\widetilde{H}^4(\Omega))$ *and* $Y := H^1(0,T;H^1(\Omega)) \cap L^2(0,T;H^3(\Omega))$, *respectively.*

Proof. The existence result is easily obtained by combining the Galerkin approximation employed in the proof of Theorem 2.1 in [9] with the a priori estimates derived in the proof of Theorem 2.1 in [12]; the uniqueness is a direct consequence of the subsequent Theorem 2.3. Finally, the boundedness of the mapping $(f, g, \theta_\Gamma) \longmapsto (u, \theta)$ follows from the abovementioned a priori estimates. □

A sharper existence result, with regards to the smoothness properties of the solution (u, θ), has been established in [12]:

THEOREM 2.2. *Suppose that, in addition to (H1)-(H4), the following assumptions on the data of (1.7a–f) are satisfied:*

$$
\begin{aligned}
&u_0 \in H^5(\Omega), \;\; u_1 \in H^3(\Omega), \; \theta_0 \in H^4(\Omega), \\
&f_{tt} \in L^2(\Omega_T), \; g \in L^2(0,T;H^2(\Omega)), \;\; \theta_\Gamma \in H^2(0,T) \, .
\end{aligned}
\tag{2.2}
$$

Furthermore, suppose that θ_0 *satisfies compatibility conditions of sufficiently high order. Then (1.7a–f) has a unique classical solution* (u, θ), *and all the partial derivatives appearing in (1.7a–c) belong to the Hölder class* $C^{\alpha,\alpha/2}(\overline{\Omega}_T)$, *for some* $\alpha \in (0,1)$.

Proof. See Theorem 2.1 in [12]. □

We now derive a stability result with respect to the data (f, g, θ_Γ) which guarantees the uniqueness of the solution (u, θ).

THEOREM 2.3. *Suppose the general hypotheses (H1), (H2) and* $\theta_0'(0) = 0$ *are satisfied. We consider the variational problem*

(2.3a)
$$\int_\Omega u_t(x,t)\varphi(x,t)\,dx - \int_\Omega u_1(x)\varphi(x,0)\,dx - \int_0^t\int_\Omega u_t\varphi_t dx\,d\tau$$
$$+\int_0^t\int_\Omega \left[\frac{\partial F}{\partial \epsilon}\,(u_x,\theta)\varphi_x + u_{xx}\varphi_{xx} - f\varphi\right]\,dx\,d\tau = 0,$$
$$\forall \varphi \in H^1(0,T;\overset{\circ}{H}{}^1(\Omega)) \cap L^2(0,T;H^2(\Omega))\ ,\quad 0 \le t \le T,$$

(2.3b)
$$\int_0^t\int_\Omega [\theta_t\eta - g\eta - \theta u_x u_{xt}\eta + \theta_x\eta_x]dx\,d\tau$$
$$+\int_0^t (\theta(1,\tau) - \theta_\Gamma(\tau))\eta(1,\tau)d\tau = 0\ ,\quad \forall\, \eta \in L^2(0,T;H^1(\Omega)),\quad 0 \le t \le T\ ,$$

(2.3c)
$$\theta(x,0) = \theta_0(x)\ ,\quad u(x,0) = u_0(x),\quad x \in \overline{\Omega}.$$

Suppose the data $(f^{(i)}, g^{(i)}, \theta_\Gamma^{(i)}), i = 1,2$, *satisfy (H3) and (H4), and suppose that* $(u^{(i)}, \theta^{(i)})$ *are solutions to (2.3a–c) corresponding to the data* $(f^{(i)}, g^{(i)}, \theta_\Gamma^{(i)})$, $i = 1,2$, *such that* $u^{(i)} \in W^{1,\infty}(0,T;\overset{\circ}{H}{}^1(\Omega)) \cap L^\infty(0,T;H^3(\Omega))$, $\theta^{(i)} \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega))$, $i = 1,2$. *Then there is some* $C > 0$ *such that*

(2.4)
$$\sup_{t\in(0,T)} \left(\|u_t(t)\|^2 + \|u_{xx}(t)\|^2 + \|\theta(t)\|^2\right) + \int_0^T\int_\Omega \theta_x^2 dx\,dt$$
$$+\int_0^T \theta^2(1,t)\,dt \le C(\|\theta_\Gamma\|^2_{L^2(0,T)} + \|g\|^2_{L^2(\Omega_T)} + \|f\|^2_{L^2(\Omega_T)}),$$

where $\theta = \theta^{(1)} - \theta^{(2)}, u = u^{(1)} - u^{(2)}, \theta_\Gamma = \theta_\Gamma^{(1)} - \theta_\Gamma^{(2)}, f = f^{(1)} - f^{(2)}, g = g^{(1)} - g^{(2)}$.

REMARKS.

1. Here (and throughout) we have omitted the arguments of the involved functions if no confusion may arise.
2. $\|\,.\,\|$ denotes always the $L^2(\Omega)$-norm.
3. Obviously, any solution (u,θ) of (1.7a–f) with (2.1a,b) solves (2.3a–c); consequently, the solution of (1.7a–f) is unique.
4. From the upcoming proof it will become evident that a corresponding stability result holds with respect to the initial data u_0, u_1, θ_0; we restrict ourselves to the

data (f, g, θ_Γ) as they are the natural candidates to serve as control variables if the system is to be controlled from the outside.

Proof. Let $\epsilon^{(i)} = u_x^{(i)}$, $i = 1,2$, and $\epsilon = \epsilon^{(1)} - \epsilon^{(2)}$. In terms of the variables (u, θ) introduced in the assertion, (2.3–c) can be rewritten as

$$\text{(2.5a)}\qquad \int_\Omega u_t(x,t)\varphi(x,t)dx - \int_0^t\int_\Omega u_t\varphi_t\, dx\, d\tau + \int_0^t\int_\Omega (u_{xx}\varphi_{xx} - f\varphi)dxd\tau$$

$$+ \int_0^t\int_\Omega \left(\frac{\partial F}{\partial \epsilon}\,(\epsilon^{(1)},\theta^{(1)}) - \frac{\partial F}{\partial \epsilon}\,(\epsilon^{(2)},\theta^{(2)})\right)\varphi_x\, dx\, d\tau = 0,$$

$$\forall\, \varphi \in H^1(0,T;\overset{\circ}{H}{}^1(\Omega)) \cap L^2(0,T;H^2(\Omega)),\quad 0 \le t \le T,$$

$$\text{(2.5b)}\qquad \int_0^t\int_\Omega [\theta_t\eta - g\eta + \theta_x\eta_x]\, dx\, dt + \int_0^t (\theta(1,\tau) - \theta_\Gamma(\tau))\eta(1,\tau)d\tau$$

$$+ \int_0^t\int_\Omega [\theta^{(2)}\epsilon^{(2)}\epsilon_t^{(2)} - \theta^{(1)}\epsilon^{(1)}\epsilon_t^{(1)}]\eta\, dxd\tau = 0,\quad \forall\, \eta \in L^2(0,T;H^1(\Omega)\ 0 \le t \le T,$$

$$\text{(2.5c)}\qquad \theta(x,0) = u(x,0) = 0\ ,\quad x \in \overline{\Omega}.$$

Next observe that, owing to our assumptions, $u_x^{(i)}, u_{xx}^{(i)}$ and $\theta^{(i)}$ belong to $C(\overline{\Omega}_T), i = 1,2$. Thus, due to (H1), expressions of the form $\frac{\partial^k}{\partial \epsilon^k}\, F_j(\epsilon^{(i)}),\ 1 \le k \le 4, j = 1,2, i = 1,2,$ are bounded. Moreover $u_t^{(i)} \in L^\infty(\Omega_T), i = 1,2$. In the sequel, $C_i, i \in \mathbb{N}$, always denote positive generic constants. We proceed in two steps:

STEP 1: Let $\delta > 0$ be given (to be specified later). We insert $\varphi = u_t$ in (2.5a), integrate by parts and use Young's inequality to arrive at the estimate

$$\text{(2.6)}\qquad \frac{1}{2}\,\|u_t(t)\|^2 + \frac{1}{2}\,\|u_{xx}(t)\|^2 \le \frac{1}{2}\,\|f\|^2_{L^2(\Omega_T)} + C_1\int_0^t \|u_t(\tau)\|^2 d\tau$$

$$+\,\delta\int_0^t\int_\Omega \left|\left(\frac{\partial F}{\partial \epsilon}\,(\epsilon^{(1)},\theta^{(1)}) - \frac{\partial F}{\partial \epsilon}\,(\epsilon^{(2)},\theta^{(2)})\right)_x\right|^2 dxd\tau.$$

Now

$$\text{(2.7)}\qquad \frac{\partial}{\partial x}\,\left(\frac{\partial F}{\partial \epsilon}\,(\epsilon^{(1)},\theta^{(1)}) - \frac{\partial F}{\partial \epsilon}\,(\epsilon^{(2)},\theta^{(2)})\right) = \theta_x F_1'(\epsilon^{(1)})$$

$$+\,\theta_x^{(2)}(F_1'(\epsilon^{(1)}) - F_1'(\epsilon^{(2)})) + F_2''(\epsilon^{(1)})u_{xx}$$

$$+\,u_{xx}^{(2)}(F_2''(\epsilon^{(1)}) - F_2''(\epsilon^{(2)})) + \theta F_1''(\epsilon^{(1)})u_{xx}^{(1)}$$

$$+\,u_{xx}^{(1)}\theta^{(2)}(F_1''(\epsilon^{(1)}) - F_1''(\epsilon^{(2)})) + \theta^{(2)}F_1''(\epsilon^{(2)})u_{xx}.$$

Consequently, invoking the mean value theorem,

$$\int_0^t \int_\Omega \left| \left(\frac{\partial F}{\partial \epsilon} (\epsilon^{(1)}, \theta^{(1)}) - \frac{\partial F}{\partial \epsilon} (\epsilon^{(2)}, \theta^{(2)}) \right)_x \right|^2 dx\, d\tau \tag{2.8}$$

$$\leq C_2 \int_0^t \int_\Omega (\theta_x^2 + |\theta_x^{(2)}|^2 \epsilon^2 + u_{xx}^2 + \theta^2 + \epsilon^2) dx\, d\tau.$$

But

$$\int_0^t \int_\Omega |\theta_x^{(2)}|^2 \epsilon^2 dx dt \leq \int_0^t \|\epsilon(\tau)\|^2_{L^\infty(\Omega)} \|\theta_x^{(2)}(\tau)\|^2 d\tau \tag{2.9}$$

$$\leq C_3 \int_0^t \|\epsilon(\tau)\|^2_{L^\infty(\Omega)}\, d\tau,$$

since $\theta^{(2)} \in L^\infty(0,T;H^1(\Omega))$. Now observe that $u(0,t) = 0 = u(1,t)$. Hence, to any $t \in [0,T]$ there is some $x_0(t) \in (0,1)$ such that $u_x(x_0(t),t) = 0$. Thus,

$$|\epsilon(x,\tau)| \leq \|u_{xx}(\tau)\|\,, \quad 0 \leq \tau \leq t, \;\; x \in \overline{\Omega}. \tag{2.10}$$

Summarizing, we have shown the estimate

$$\|u_t(t)\|^2 + \|u_{xx}(t)\|^2 \leq C_4\, \|f\|^2_{L^2(\Omega_T)} + C_5 \int_0^t \|u_t(\tau)\|^2 dt \tag{2.11}$$

$$+ C_6 \cdot \delta \cdot \int_0^t (\|\theta_x(\tau)\|^2 + \|\theta(\tau)\|^2 + \|u_{xx}(\tau)\|^2) d\tau.$$

STEP 2: Next we substitute $\eta = \theta$ into (2.5b) to obtain via Young's inequality:

$$\frac{1}{2}\, \|\theta(t)\|^2 + \int_0^t \|\theta_x(\tau)\|^2 d\tau + \frac{1}{2} \int_0^t \theta^2(1,\tau)\, d\tau \tag{2.12}$$

$$\leq \frac{1}{2} \int_0^t \|\theta(\tau)\|^2 d\tau + \frac{1}{2}\, \|g\|^2_{L^2(\Omega_T)} + \frac{1}{2}\, \|\theta_\Gamma\|^2_{L^2(0,T)} + A,$$

where

$$A = \int_0^t \int_\Omega \theta(\theta^{(1)}\epsilon^{(1)}\epsilon_t^{(1)} - \theta^{(2)}\epsilon^{(2)}\epsilon_t^{(2)})dx\, d\tau \tag{2.13}$$

$$= \int_0^t \int_\Omega \frac{d}{dx} [\theta(\theta^{(1)}\epsilon^{(1)}u_t^{(1)} - \theta^{(2)}\epsilon^{(2)}u_t^{(2)})]dxd\tau$$

$$- \int_0^t \int_\Omega \theta_x(\theta^{(1)}\epsilon^{(1)}u_t^{(1)} - \theta^{(2)}\epsilon^{(2)}u_t^{(2)})dxd\tau$$

$$- \int_0^t \int_\Omega \theta(\theta_x^{(1)}\epsilon^{(1)}u_t^{(1)} + \theta^{(1)}u_{xx}^{(1)}u_t^{(1)}$$

$$- \theta_x^{(2)}\epsilon^{(2)}u_t^{(2)} - \theta^{(2)}u_{xx}^{(2)}u_t^{(2)})dxd\tau.$$

Since $u_{t|x=0,1} = 0$, the first integral vanishes; the other terms have to be treated individually.

a) We have, since $\theta^{(i)}, \epsilon^{(i)}, u_t^{(i)} \in L^\infty(\Omega_T),\ i = 1,2,$

$$I_1 := |\int_0^t \int_\Omega \theta_x(\theta^{(1)}\epsilon^{(1)}u_t^{(1)} - \theta^{(2)}\epsilon^{(2)}u_t^{(2)})dxd\tau| \tag{2.14}$$

$$= |\int_0^t \int_\Omega \theta_x[\theta\epsilon^{(1)}u_t^{(1)} + \theta^{(2)}\epsilon u_t^{(1)} + \theta^{(2)}\epsilon^{(2)}u_t]dx\, d\tau|$$

$$\le \delta \int_0^t \int_\Omega \theta_x^2 dxd\tau + C_7 \int_0^t \int_\Omega (\theta^2 + \epsilon^2 + u_t^2)dx\, d\tau.$$

b) Next we estimate

$$|I_2| := |\int_0^t \int_\Omega \theta(\theta_x^{(1)}\epsilon^{(1)}u_t^{(1)} - \theta_x^{(2)}\epsilon^{(2)}u_t^{(2)})dxd\tau| \tag{2.15}$$

$$|\int_0^t \int_\Omega \theta[\theta_x\epsilon^{(1)}u_t^{(1)} + \theta_x^{(2)}\epsilon u_t^{(1)} + \theta_x^{(2)}\epsilon^{(2)}u_t]dxd\tau|$$

$$\le \delta \int_0^t \int_\Omega \theta_x^2 dxd\tau + C_8 \int_0^t \int_\Omega (\theta^2 + \epsilon^2 + u_t^2)dxd\tau$$

$$+ C_9 \int_0^t \int_\Omega |\theta_x^{(2)}|^2\theta^2 dx\, d\tau.$$

Recalling Nirenberg's inequality in one space dimension (cf., [1]), we have with suitable $\alpha_1 > 0, \alpha_2 > 0$:

$$\begin{aligned} \|\theta(\tau)\|^2_{L^\infty(\Omega)} &\le \alpha_1 \|\theta_x(\tau)\| \; \|\theta(\tau)\| + \alpha_2 \|\theta(\tau)\|^2 \\ &\le \delta \|\theta_x(\tau)\|^2 + C_{10} \|\theta(\tau)\|^2. \end{aligned} \tag{2.16}$$

Since $\theta_x^{(2)} \in L^\infty(0,T;L^2(\Omega))$, this implies that

$$\begin{aligned} \int_0^t \int_\Omega |\theta_x^{(2)}|^2 \theta^2 \, dx d\tau &\le \int_0^t \|\theta(\tau)\|^2_{L^\infty(\Omega)} \|\theta_x^{(2)}(\tau)\|^2 d\tau \\ &\le C_{10}\delta \int_0^t \int_\Omega \theta_x^2 \, dx d\tau + C_{11} \int_0^t \int_\Omega \theta^2 \, dx dt, \end{aligned} \tag{2.17}$$

whence

$$\begin{aligned} |I_2| \le & C_{11}\delta \int_0^t \|\theta_x(\tau)\|^2 d\tau \\ & + C_{12} \int_0^t (\|\theta(\tau)\|^2 + \|u_{xx}(\tau)\|^2 + \|u_t(\tau)\|^2) d\tau. \end{aligned} \tag{2.18}$$

c) Finally we have

$$\begin{aligned} |I_3| := & \left| \int_0^t \int_\Omega \theta[\theta^{(1)} u_{xx}^{(1)} u_t^{(1)} - \theta^{(2)} u_{xx}^{(2)} u_t^{(2)}] dx d\tau \right| \\ = & \left| \int_0^t \int_\Omega \theta[\theta u_{xx}^{(1)} u_t^{(1)} + \theta^{(2)} u_{xx} u_t^{(1)} + \theta^{(2)} u_{xx}^{(2)} u_t] dx d\tau \right. \\ \le & C_{13} \int_0^t (\|\theta(\tau)\|^2 + \|u_{xx}(\tau)\|^2 + \|u_t(\tau)\|^2) dx d\tau. \end{aligned} \tag{2.19}$$

Summarizing the inequalities (2.12), (2.14), (2.18) and (2.19), we have shown that

$$\begin{aligned} & \frac{1}{2} \|\theta(t)\|^2 + \int_0^t \|\theta_x(\tau)\|^2 d\tau + \frac{1}{2} \int_0^t \theta^2(1,\tau) d\tau \\ & \le C_{14} \cdot \delta \int_0^t \|\theta_x(\tau)\|^2 d\tau + \frac{1}{2} \|g\|^2_{L^2(\Omega_T)} + \frac{1}{2} \|\theta_\Gamma\|^2_{L^2(0,T)} \\ & + C_{15} \int_0^t (\|\theta(\tau)\|^2 + \|u_{xx}(\tau)\|^2 + \|u_t(t)\|^2) d\tau. \end{aligned} \tag{2.20}$$

Adding (2.11) and (2.20), adjusting $\delta > 0$ sufficiently small, and invoking Gronwall's lemma, we have finally proved the assertion. □

3. Optimal Control. We now turn our interest to optimal control problems associated with the system (1.7a–f). It is of considerable interest in the technological application of shape memory alloys to control the evolution of the austenitic-martensitic phase transitions in the material; in this connection, a typical object is to influence the system via the natural control variables f, g, θ_Γ in such a way, that a desired distribution of the phases in the material is produced. Since the phase transitions are characterized by the order parameter ϵ, it is natural to use ϵ as the main variable in the cost functional. We consider the following control problem:

(CP)

$$\text{Minimize } J(u,\theta;f,g,\theta_\Gamma) = \int_0^T \int_\Omega L_1\big(x,t,u_x(x,t),\theta(x,t),f(x,t),g(x,t)\big)\,dx\,dt$$

$$+ \int_0^T L_2\big(t,\theta_\Gamma(t)\big)\,dt + \int_\Omega L_3\big(x,u_x(x,T),\theta(x,T)\big)\,dx,$$

subject to (1.7a–f) and the side condition $(f,g,\theta_\Gamma) \in \mathcal{K}$, where $\mathcal{K}$ denotes some nonempty, bounded, closed and convex subset of $H^1(0,T;H^1(\Omega)) \times \{g \in H^1(0,T;H^1(\Omega)) | g(x,t) \geq 0$ on $\overline{\Omega}_T\} \times \mathcal{M}$.

For $L_1 : \mathbf{R}^6 \to \mathbf{R}, L_2 : \mathbf{R}^2 \to \mathbf{R}, L_3 : \mathbf{R}^3 \to \mathbf{R}$, we assume:

(H5) (i) L_1, L_2, L_3 are measurable with respect to the variables (x,t), resp. t, resp. x, and continuous with respect to the other variables.

(ii) L_1 is convex with respect to f and g.

(iii) L_2 is convex with respect to θ_Γ.

These assumptions are natural in the framework of optimal control; a typical form for J would be

$$\begin{aligned}(3.1)\qquad J(u,\theta;f,g,\theta_\Gamma) &= \beta_1\|u_x - \overline{u}_x\|^2_{L^2(\Omega_T)} + \beta_2\|\theta - \overline{\theta}\|^2_{L^2(\Omega_T)} \\ &+ \beta_3\|u_x(\cdot,T) - \tilde{u}\|^2 + \beta_4\|\theta(\cdot,T) - \widetilde{\theta}\|^2 \\ &+ \beta_5\|f\|^2_{L^2(\Omega_T)} + \beta_6\|g\|^2_{L^2(\Omega_T)} + \beta_7\|\theta_\Gamma\|^2_{L^2(0,T)},\end{aligned}$$

with $\beta_i \geq 0$, but not all zero, and functions $\overline{u}_x, \overline{\theta} \in L^2(\Omega_T), \tilde{u}, \widetilde{\theta} \in L^2(\Omega)$, representing the desired strain and temperature distributions during the evolution and at $t = T$.

There holds

THEOREM 3.1. *Suppose (H1)–(H5) are true, then (CP) has a solution $(\overline{u},\overline{\theta};\overline{f},\overline{g},\overline{\theta}_\Gamma)$.*

Proof. Let $\{(f_n,g_n,\theta_{\Gamma,n})\}\subset\mathcal{K}$ denote a minimizing sequence, and let (u_n,θ_n) denote the solution of (1.7a–f) associated with $(f_n,g_n,\theta_{\Gamma,n}), n\in\mathbb{N}$. Since $\mathcal{K}$ is bounded, we may assume that

$$(3.2)\qquad \begin{aligned} f_n &\to \overline{f}, && \text{weakly in } H^1(0,T;H^1(\Omega)),\\ g_n &\to \overline{g}, && \text{weakly in } H^1(0,T;H^1(\Omega)),\\ \theta_{\Gamma,n} &\to \overline{\theta}_\Gamma, && \text{weakly in } H^1(0,T). \end{aligned}$$

Due to the weak closedness of the convex and closed set $\mathcal{K}, (\overline{f},\overline{g},\overline{\theta}_\Gamma)\in\mathcal{K}$. Let $(\overline{u},\overline{\theta})$ denote the associated solution of (1.7a–f). Now, owing to the boundedness of $\mathcal{K}$ and Theorem 2.1, $\{(u_n,\theta_n)\}_{n\in\mathbb{N}}$ is a bounded subset of $X\times Y$. Therefore, we may assume that for some $(u,\theta)\in X\times Y$ there holds

$$(3.3a)\qquad \begin{aligned} u_{n,x} &\to u_x,\\ \theta_n &\to \theta, \end{aligned} \qquad \text{uniformly on } \overline{\Omega}_T,$$

$$(3.3b)\qquad \begin{aligned} u_{n,tt} &\to u_{tt},\\ u_{n,xx} &\to u_{xx},\\ u_{n,xt} &\to u_{xt},\\ u_{n,xxxx} &\to u_{xxxx}, \end{aligned} \qquad \text{weakly in } L^2(\Omega_T),$$

as well as

$$(3.3c)\qquad \begin{aligned} \theta_{n,x} &\to \theta_x,\\ \theta_{n,t} &\to \theta_t,\\ \theta_{n,xx} &\to \theta_{xx}, \end{aligned} \qquad \text{weakly in } L^2(\Omega_T).$$

Passing to the limit as $n\to\infty$ in the equations (1.7a–f) shows that (u,θ) solves (1.7a–f) for the data $(\overline{f},\overline{g},\overline{\theta}_\Gamma)$, i.e., $u=\overline{u},\theta=\overline{\theta}$. Hence, $(\overline{u},\overline{\theta};\overline{f},\overline{g},\overline{\theta}_\Gamma)$ is admissible, and, in view of (H5),

$$(3.4)\qquad J(\overline{u},\overline{\theta};\overline{f},\overline{g},\overline{\theta}_\Gamma)\le \lim_{n\to\infty}\inf\ J(u_n,\theta_n;f_n,g_n,\theta_{\Gamma,n}).$$

Thus $(\overline{u},\overline{\theta};\overline{f},\overline{g},\overline{\theta}_\Gamma)$ is a solution of (CP). □

REMARKS.

5. The above way of arguing follows the lines of [10] where a related result was derived for a much more restricted free energy F.
6. It is natural to look for necessary conditions of optimality for the optimal controls of (CP). A corresponding result has not yet been derived.
7. The problem of the automatic self-regulation of the system via a fixed feedback control regulating the boundary temperature θ_Γ has been considered in [11].

4. Numerical Approximation. In this section we follow the lines of [8]. We assume the free energy in the special form (see (1.2))

$$F(\epsilon,\epsilon_x,\theta) = -\theta\log\theta + \theta + \frac{1}{2}\,\theta\epsilon^2 - \frac{1}{4}\,\epsilon^4 + \frac{1}{6}\,\epsilon^6 + \frac{1}{2}\,\epsilon_x^2. \tag{4.1}$$

Let

$$F_0(\epsilon,\theta) = \frac{1}{2}\,\theta\epsilon^2 - \frac{1}{4}\,\epsilon^4 + \frac{1}{6}\,\epsilon^6. \tag{4.2}$$

Then, for $\epsilon_1 \neq \epsilon_2$,

$$\frac{F_0(\epsilon_1,\theta) - F_0(\epsilon_2,\theta)}{\epsilon_1 - \epsilon_2} = \frac{1}{2}\,\theta(\epsilon_1+\epsilon_2) + \Psi(\epsilon_1,\epsilon_2), \tag{4.3}$$

where $\Psi(\epsilon_1,\epsilon_2)$ is a polynomial of degree 5 in ϵ_1,ϵ_2.

We are going to construct a numerical scheme for the approximate solution of (1.7a–f). To this end, we assume that (H1)–(H4) and (2.2) hold, so that Theorem 2.2 applies.

Now let $K,N,M \in \mathbb{N}$ be chosen. We put $h = \frac{T}{M}$, $t_m^{(M)} = mh$, $0 \le m \le M$, and $x_i^{(N)} = \frac{i}{N}$,$0 \le i \le N$.

Define

$$Y_N = \{\text{linear splines on } [0,1] \text{ corresponding to the partition } \{x_i^{(N)}\}_{i=0}^N \text{ of } [0,1]\}, \tag{4.4}$$

and let

$$Z_K = \operatorname{span}\{z_1,\ldots,z_K\}, \tag{4.5}$$

where z_j denotes the j-th eigenfunction of the eigenvalue problem

$$z'''' = \lambda z \ , \ \text{in } (0,1), z(0) = z''(0) = 0 = z''(1) = z(1). \tag{4.6}$$

We introduce the projection operators

$$\begin{aligned} P_K &= H^4(0,1) - \text{orthogonal projection onto } Z_K,\\ Q_K &= H^2(0,1) - \text{orthogonal projection onto } Z_K,\\ R_N &= H^1(0,1) - \text{orthogonal projection onto } Y_N, \end{aligned} \tag{4.7}$$

and the averages

$$f_M^m(x) = \frac{1}{h}\int_{(m-1)h}^{mh} f(x,t)dt \ , \quad g_M^m(x) = \frac{1}{h}\int_{(m-1)h}^{mh} g(x,t)dt, \tag{4.8}$$

$$\theta_{\Gamma,M}^m = \frac{1}{h}\int_{(m-1)h}^{mh} \theta_\Gamma(t)\,dt.$$

We then consider the discrete problem

$\underline{(D_{M,N,K})}$ Find $u^m = \sum_{k=1}^K \alpha_k^m z_k, \theta^m = \sum_{k=0}^N \beta_k^m y_k^{(N)}$,

$1 \leq m \leq M$, such that

$$\int_\Omega \Big[\frac{u^m - 2u^{m-1} + u^{m-2}}{h^2}\,\xi + \frac{1}{2}\,\theta^{m-1}(u_x^m + u_x^{m-1})\xi_x \tag{4.9a}$$

$$+ \Psi(u_x^m, u_x^{m-1})\xi_x + u_{xx}^m \xi_{xx} - f_M^m \xi\Big] dx = 0, \quad \forall\, \xi \in Z_K,$$

$$\int_\Omega \Big[\frac{\theta^m - \theta^{m-1}}{h}\,\eta - \frac{1}{2}\,\theta^{m-1} \cdot \frac{(u_x^m)^2 - (u_x^{m-1})^2}{h}\,\eta \tag{4.9b}$$

$$+ \theta_x^m \eta_x - g_M^m \eta\Big] dx + (\theta^m(1) - \theta_{\Gamma,M}^m)\eta(1) = 0, \quad \forall\, \eta \in Y_N,$$

$$u^0 = P_K(u^0), \frac{u^0 - u^{-1}}{h} = Q_K(u_1), \quad \theta^0 = R_N(\theta_0). \tag{4.9c}$$

The following result has been shown in [8]:

THEOREM 4.1. *Suppose (H1)–(H4) and (2.2) are true, and let N be sufficiently large. Then there exist constants $\widehat{C}_1 > 0, \widehat{C}_2 > 0$, which do not depend on M, N, K, such that for $\frac{1}{3N^2} < \frac{1}{M} \leq \widehat{C}_1$ the discrete problem $(D_{M,N,K})$ has a solution which satisfies*

$$\theta^m(x) \geq 0, \quad \forall\, x \in \overline{\Omega}, \quad 0 \leq m \leq M, \tag{4.10a}$$

$$\max_{0 \leq m \leq M} \left\{ \left\| \frac{u^m - u^{m-1}}{h} \right\| + \left\| \frac{u_x^m - u_x^{m-1}}{h} \right\|^2 + \left\| u_{xxx}^m \right\|^2 \right\} \leq \widehat{C}_2, \tag{4.10b}$$

$$\max_{0 \leq m \leq M} \{ \|\theta_x^m\|^2 + |\theta^m(1)|^2 \} + \sum_{m=1}^M h \left\| \frac{\theta^m - \theta^{m-1}}{h} \right\|^2 \leq \widehat{C}_2. \tag{4.10c}$$

Proof. See Theorem 2.1 in [8]. □

It now easy to derive convergent approximate solutions. To this end, let $\varphi : \mathbf{N} \to \mathbf{N}$ denote some strictly increasing function. We put $N = \varphi(K)$ and $M = 2N^2$ $\left(\text{which implies } \frac{1}{3N^2} < \frac{1}{M}\right)$ and take $K \in \mathbf{N}$ large enough. Let $\{(u_K^m, \theta_K^m)\}_{m=1}^M$ denote corresponding solutions of $(D_{M,N,K})$ with the above choice of N and M.

We define the linear interpolations

$$\begin{aligned} u_K(x,t) &= (Mt - m + 1)u_K^m(x) + (m - Mt)u_K^{m-1}(x), \\ \theta_K(x,t) &= (Mt - m + 1)\theta_K^m(x) + (m - Mt)\theta_K^{m-1}(x), \\ 0 \leq x \leq 1, &\quad \frac{m-1}{M} \leq t \leq \frac{m}{M}, \ m = 1, \ldots, M. \end{aligned} \tag{4.11}$$

Then (4.10b,c) imply that, for any sufficiently large $K \in \mathbb{N}$,

$$\|u_K\|_{W^{1,\infty}\left(0,T;\overset{\circ}{H}^1(\Omega)\right)\cap L^\infty\left(0,T;H^3(\Omega)\right)} \le \widehat{C}_2, \tag{4.12a}$$

$$\|\theta_K\|_{H^1\left(0,T;L^2(\Omega)\right)\cap L^\infty\left(0,T;H^1(\Omega)\right)} \le \widehat{C}_2. \tag{4.12b}$$

From standard compactness arguments we conclude the existence of some $(\tilde{u}, \widetilde{\theta})$ such that, for some subsequence,

$$u_{K_n} \to \tilde{u}, \quad \text{weakly} -* \text{ in } W^{1,\infty}(0,T;\overset{\circ}{H}^1(\Omega)) \text{ and} \\ \text{weakly} -* \text{ in } L^\infty(0,T;H^3(\Omega)), \tag{4.13a}$$

$$\theta_{K_n} \to \widetilde{\theta}, \quad \text{weakly in } H^1(0,T;L^2(\Omega)) \text{ and} \\ \text{weakly} -* \text{ in } L^\infty(0,T;H^1(\Omega)), \tag{4.13b}$$

$$\frac{\partial}{\partial x} u_{K_n} \to \frac{\partial}{\partial x} \tilde{u}, \quad \text{uniformly on } \overline{\Omega}_T, \\ \theta_{K_n} \to \widetilde{\theta}, \quad \text{uniformly on } \overline{\Omega}_T. \tag{4.13c}$$

It is easy to see that the limit point $(\tilde{u}, \widetilde{\theta})$ is a solution of the variational problem (2.3a–c). By virtue of Theorem 2.3, $\tilde{u} = u, \widetilde{\theta} = \theta$, where (u, θ) is the (unique) solution of (1.7a–f). It follows that the whole sequence (u_K, θ_K) converges to (u, θ) in the sense of (4.13a-c).

THEOREM 4.2. *Suppose (H1)–(H4) and (2.2) are true, and assume that to $K \in \mathbb{N}$ we define $N = \varphi(K)$ and $M = 2N^2$, where $\varphi : \mathbb{N} \to \mathbb{N}$ is any strictly increasing function. For sufficiently large $K \in \mathbb{N}$, let (u_K, θ_K) be defined by (4.11). Then (u_K, θ_K) converges in the sense of (4.13a–c) to the solution (u, θ) of (1.7a–f).*

REMARK.

8. Results concerning the order of convergence have not yet been established.

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