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ABSTRACT

Since the phase change in SMA-based devices such as actuators is accompanied by a significant heat exchange with the surroundings, different concepts to heat/cool SMAs have been proposed in the literature. Most of these concepts require the analysis of a multilayered (e.g., "sandwich"-type) structure where the SMA layer is placed between layers with another material. In this paper we propose a mathematical model and an efficient numerical method for this analysis.

Although our approach can be applied to a wide range of different designs of multilayered actuators, the basic idea of the model construction is explained in this paper for a specific design based on the introduction of semiconductor "heat pump" modules into the device and the Peltier effect for the heat exchange. The dynamics of thermomechanical fields is studied with a coupled system of PDEs based on conservation laws. The system, supplemented by constitutive relationships in the Falk form, is reduced to a differential-algebraic (DA) model and solved with an effective DA solver developed in our previous works. Numerical results on thermomechanical behaviour of SMA components in multilayered actuators are presented.

Keywords: Multilayered SMA structures, differential-algebraic systems, coupled thermomechanical fields

1. INTRODUCTION

Smart structures are often defined as such structures which are able to perform the following three functions (a) to collect data on changes in surroundings or their own damage, (b) to process the collected data, and (c) to react through their actuators' actions.[1] In such structures, sensors, processors, and actuators are integrated at the *macroscopic* level and the concept of material appears if these components are incorporated into a classical composite material. In this type of material, smart functions are created by the assembly of the components at the *mesoscopic* level. In this paper we deal with shape-memory alloys (SMA) applications and all models and experiments discussed here are the result of the assumptions based on the Landau-Devonshire phenomenology established on the mesoscopic scale (see[2] for details).

Due to their ability to induce large deformations and due to their relatively easy integration into composites, SMAs become an important candidate for their potentially wide use in applications of embedded actuators. Until now a lot of attention has been concentrated on advanced adaptive SMA-composites where thin (with diameter below 0.2mm) SMA wires integrated in fibre-reinforced polymer composites. The results of these studies give convincing evidence to believe that the integration of SMAs in composites provides a lot of advantages compared to more traditional actuating technologies. Such advantages include high reversible strains, high damping capacity, large reversible changes of mechanical/physical characteristics, and ability to generate very high recovery stresses.[3,4] However, in order to use effectively these advantages, we have to challenge two principal difficulties in theory and applications of SMA actuators, namely (a) complex nonlinear behaviour of SMAs, and (b) the problem of cooling/heating of the SMA components. These two issues will be addressed in the present paper.

Modern (including emerging) technologies for embedding actuators into composites are typically based on piezo-electricity, magnetostriction, magnetic shape memory (MSM) effect, electrostriction, and SMAs. While piezoelectrics are thought to be most effective for high frequency applications, SMAs became quite popular in low-frequency applications and shape control. Two promising areas of research in increasing frequency of actuation for SMA-based actuators and their improved energetic efficiency are connected with

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- the development of magnetic shape memory actuators,[5,6] and

- the introduction of more efficient mechanisms of cooling.[7,8]

The reader should consult[9] for an excellent survey in up-to-date development in the field of MSM actuators. In this paper we concentrate on the second area, in particular on some mathematical and numerical modelling aspects related to the implementation of more efficient cooling mechanisms into SMA parts in adaptive structures.

Our purpose in this paper is to show how basic equations of conservation laws can be used to describe main features of the coupled thermomechanical behaviour of SMAs as a part of multilayered adaptive structures. Recall that in[10] a simplified model was used to model the thermomechanical dynamics of SMA actuators. However, the effect of coupling between mechanical and thermal fields, which lags the temperature evolution and restrains cooling of the interior material, requires further investigation. This effect impedes the response of the SMA actuator. In applications of SMAs as actuators (e.g. for shape and vibration control of structures), the response time of a SMA is controlled by a combined effect of heat transfer (to and from the device) and mechanical loading. Therefore, in order to quantify and ultimately optimise heating/cooling conditions heat transfer models alone might not be sufficient. Although many efforts have been concentrated on the development of thermal models for stress-free SMA samples,[11,12] the development of full thermoelectromechanical models and numerical methods for their solutions constitutes an important problem in theory and applications of shape memory materials.[13-15,2] In what follows, we adopt a specific form of constitutive equations derived on the premises of the Landau-Devonshire form of the free energy (see details in[15] and references therein). We emphasise that this form can be easily augmented, if necessary, and appropriate changes can be implemented into the model. With this remark in mind we do not discuss further the choice of constitutive equations for our model and the interested reader should consult[16,17,3,10] for critical discussions on existing constitutive models.

In order to increase the rates of cooling in high frequency applications different methodologies have been proposed and compared with more traditional techniques such as free and forced convection.[7] Many such methodologies require dealing with multilayered structures which complicates the analysis and modelling of material dynamics.[18] In many cases a typical basic unit structure of the device (and the associated SMA modelling region) can be presented in the form depicted in Fig. 1, where the left (L) and right (R) layers are usually made of the material with a substantially smaller thermal conductivity. As an example, in this paper we consider sandwich-type SMA actuators with semiconductor modules. The principle of work of these devices is based on the use of thermoelectric effects and the conceptual design of such devices has been explained in.[8,7] Thermoelectric effects (namely, the Seebeck, Peltier, and Thomson effects) are widely used in thermoelectric circuits to produce useful heating/cooling and/or power generation, and the areas of applications of thermoelectricity-based devices range from refrigeration/generation tools to nuclear industry and solar energy converters. In the context of SMA applications, the choice of semiconductors for the thermoelectric cooling "cover" of the SMA module is due to the fact that as thermoelectric materials semiconductors and semiconductor alloys are often superior to metals (as evident from Table 1, the electrical resistivity of the semiconductor is much higher compared to the SMA). In our discussion we limit ourselves to semiconductor modules made of bismuth telluride (Bi_2Te_3) n- and p-type thermocouples.

The foundation for modelling thermoelectric devices was laid by the group of researchers led by Ioffe,[19] and since then various models of thermoelectricity have been proposed in the literature in the context of specific (both steady-state and transient) applications (see, for example,[20,8,7,11] and references therein). All such models are based on the fact that due to the Peltier effect (resulting from dissimilarity of materials at junctions between layers), the "heat pumping" along a temperature gradient leads to the heat absorption at the high temperature junction and the heat dissipation at the cold junction. In the context of SMA-based thermoelectric devices, it has been recently shown[14] that if we consider a sandwich-type SMA actuator consisting of SMA and semiconductor layers (similar to the schematic representation of Fig. 1) and direct the current from N (L-layer) to P (R-layer) semiconductor, then the Peltier effect leads the heat loss by the SMA at both interfaces, N-SMA and SMA-P, and these interfaces act as heat sinks for the SMA. Since the issues of energetic efficiency of multilayered SMA devices are beyond the scope of this paper, we refer the reader to the above cited paper for further insight on procedures for estimating the energy conversion efficiency of thermoelectric SMA actuators. Finally, we note that in contrast to the Joule heat the Peltier heat is linear, and since the rate at which thermal energy is transfered from the hot to the cold surface is directly proportional to the carrier current the energy removed from the surface surrounding the SMA layer can be estimated with a mathematical model. Although the analysis of mathematical models for important classes of multilayered

SMA devices (e.g., sandwich-type actuators) has been a subject of intensive research during recent years,[11,12] this analysis is typically limited to the thermal field only and, with some noticeable exception,[14] little attention has been paid to the description of the dynamics of coupled thermomechanical fields during phase transformations in these types of devices.
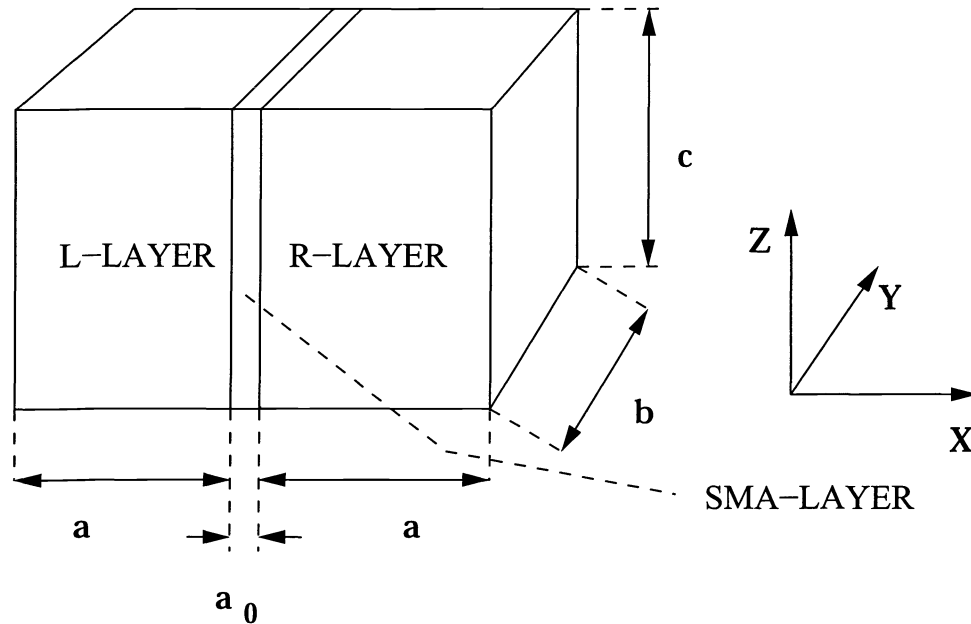

Figure 1. Schematic representation of a unit cell of multilayered SMA actuators.

2. MATHEMATICAL MODELS AND REDUCTION PROCEDURES

The dynamics of phase transitions in the shape-memory-alloy layer of multilayered SMA actuators can be adequately described with coupled thermomechanical models based on conservation laws. Such models play an increasingly important role in the design of SMA devices and structures, and the development of numerical methods for approximate solutions of resulting problems becomes an important direction of research in this field.[13-15,2] In applications of multilayered SMA-based devices this task is complicated by the need to account for the transient heat exchange not only with the surrounding environment but also with other layers of the structure. For thermoelectric sandwich-type SMA actuators many studies performed so far have been limited to the assumption of uniformity of temperature in the SMA layer[14] and the focus has been made on the analysis of thermoelectric effects without taking into account the coupling between thermal and mechanical fields.[11,12]

In this section we explain a basic procedure for the analysis of coupled thermomechanical fields in the SMA layer of a multilayered device on the example of thermoelectric SMA actuators. In order to describe the dynamics of the device we assume the existence of a functional Ψ invariant under time transformations and we choose such a functional in the form of the Helmholtz free energy

$$\Psi = e - \theta\eta, \quad \eta = -\frac{\partial\Psi}{\partial\theta}, \tag{1}$$

where e is the internal energy (per unit mass) of the system, η is the density of the entropy function, and θ is the temperature of the system. Then, we define the symmetric strain tensor $\vec{\epsilon}$ via the Cauchy relation

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad i,j = 1,2,3, \tag{2}$$

where **u** is the vector of spatial displacements. Note that although the use of the Cauchy relation in the definition of strain might be questionable in the general case (and models developed in the framework of finite deformations might be required), it is known that the relation (2) provides us with an adequate approximation for most SMA applications.[14]   The constitutive relationships that couple stresses, deformation gradients, temperature and heat fluxes can be represented in the following generic form

$$\Phi_1(\vec{\sigma}, \vec{\epsilon}) = 0, \quad \Phi_2(\mathbf{q}, \theta) = 0, \tag{3}$$

where we assume implicitly that the above relations may involve spatial and temporal derivatives of the functions. As soon as the function Ψ is specified the stress-strain relationship is defined in the form

$$\vec{\sigma} = \frac{\partial \Psi}{\partial \vec{\epsilon}}. \tag{4}$$

One possible choice for the approximation of the second dependency in (3) would be a general model for heat conduction that is based on the Cattaneo-Vernotte equation (see previous discussion in[2] and references therein). However, having regard to difficulties in modelling thermomechanical fields in multilayered SMA-based actuators, in this paper we limit ourselves by a simpler model. Recall that the Peltier effect is driven by the electric current in the multilayered system and is based on the interface condition for the energy flux. This effect influences the temperature gradients and, depending on a specific design, typically manifest itself as a heat sink/source at the SMA interface. Therefore, the standard Fourier low in this case should be modified because the thermal energy (heat) flux in the SMA layer with temperature θ depends on the current density vector $\mathbf{j} = \mathbf{j}(\mathbf{x}, t)$ accounting for the Joule heat (which is usually negligible during phase transformations)

$$\nabla \cdot \mathbf{q} = \nabla \cdot (k\nabla\theta) + \rho|\mathbf{j}|^2. \tag{5}$$

For the description of the dynamics of thermomechanical fields in the SMA layer we apply a general model based on conservation laws (see[15,2] for details)

$$\rho\frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla_x \cdot \vec{\sigma} + \mathbf{f}, \quad \rho\frac{\partial e}{\partial t} = \nabla \cdot \mathbf{q} + \vec{\sigma}^T : (\nabla\mathbf{v}) + g, \tag{6}$$

where ρ is the density of the SMA material, $\mathbf{v} = \frac{\partial u}{\partial t}$ is the velocity, f and g are given functions of mechanical and thermal loadings, respectively. Note that the function g in (6) models contributions of heat sources, excluding Joule heating taken into account in the model by (5). Such a representation allows us to "localise" heat contributions from other layers of the actuator in (5).

It should be emphasised that if the phase transformation is induced by heating (with or without the presence of body forces), the stress in the SMA layer is produced, and the mechanical field in this case can be adequately described with the *nonstationary* equation for the conservation of momentum (the equation of motion) as indicated by system (6). A special case of this system has been recently studied in[14] under the assumption of (a) negligible body forces and the temperature gradients in the SMA layer, and (b) the stationarity of the equation for the conservation of momentum. Our approach is different from that proposed in[14] where the analysis of thermomechanical coupling was performed in the context of the heat conduction equation only. In our approach we consider not only the thermomechanical coupling incorporated in the heat conduction equation via the definition of the heat flux, but also the thermomechanical coupling incorporated into the model via the free energy function directly. This results in a strongly nonlinear momentum equation coupled to the energy balance equation. Our method of solution is also different. The computational scheme proposed in[14] is based on a reduction of the heat conduction equation to a system of ODEs and the application of the forth-order Runge-Kutta method. Having the temperature on the new time layer, the authors of[14] used this value in an iterative procedure for determining mechanical field characteristics and the volume fraction. Note that an explicit (essentially uncoupled) scheme was used with an iterative refinement and convergence criteria for mechanical field characteristics were based on the convergence criterion for temperature. In the general case the application of such schemes for problems involving phase transitions is questionable due to stability issues.

Of course, thermal and mechanical characteristics of the actuator on the SMA boundary interfaces are not only functions of the coupled thermomechanical field in the SMA layer but also functions of the thermomechanical fields

of the neighbouring layers. By approximating mechanical and thermal boundary conditions at the SMA interfaces, it is often sufficient to restrict the solution of the problem of computing thermomechanical fields in the multilayered actuator to the SMA layer only. This approach is used in the present paper. The problem is solved in two stages.

At the first stage, we follow the idea developed in[12] and solve the coupled problem of thermal analysis for the whole multilayered structure. Using the assumptions of[14] we reduce the continuity equation for charges to the simple relationship $\nabla \cdot \mathbf{j} = 0$, $\mathbf{j} = J(t)\mathbf{n}_x$, and then we derive an approximation for thermal boundary conditions at the interfaces of SMA with semiconductor layers applying the methodology described in details in[11,12] (assuming that a_0/a is small). Recall that in the one-dimensional case, the system for approximating the temperature in the P semiconductor layer has the form:

$$
\begin{cases}
C_v^P \dfrac{\partial T_P}{\partial t} = k_P \dfrac{\partial^2 T_P}{\partial x^2} + \rho_P J^2 - h\dfrac{P}{A}(T_P - T_0), & a_0/2 < x < a_0/2 + a, \\[2mm]
T_P(x,0) = T_0, \quad T_P(a_0/2 + a, t) = T_0, & \\[2mm]
2k_P \dfrac{\partial T_P}{\partial x} + \rho_S a_0 J^2 - a_0 h\dfrac{P}{A}(T_P - T_0) = -2T_P \alpha_P J + C_v a_0 \dfrac{\partial T_P}{\partial t}, & x = a_0/2,
\end{cases}
\tag{7}
$$

where $A = bc$ and $P = 2(b+c)$ are the area and perimeter of the cross section of the device, ρ_S and ρ_P are electrical resistivities of the SMA and semiconductor layer, respectively, h is the heat convection coefficient (the variable and coefficients with sub/superscripts N and P are reserved for the N and P semiconductor layers, respectively). In[12] it was proposed to approximate the dependency between T_P and $\dfrac{\partial T_P}{\partial x}$ at $x = a_0/2$ via an "independent" integro-differential equation. In the general case such approximations of interface boundary conditions will involve the coupling between thermal and mechanical fields (see the definition of parameter μ in[14]) and the simultaneous solution of this equation with the coupled system (6) is required. A simple way to circumvent this difficulty would be to determine an approximate law of the heat exchange at the boundary interface by assuming (a) that in the vicinity of this interface variations in C_v can be neglected (if needed, the dependency of C_v on $J(t)$ can be incorporated via an appropriate interpolation procedure), and (b) that the first equation in (7) is satisfied at the boundary. These assumptions allow us to express $\dfrac{dT}{dt}(a_0/2, t)$ from the first equation equation of (7) and substitute it into the interface boundary condition. Within the small variation in thermal spatial gradients at the boundary interface (in the semiconductor layer) we come the following approximation of the boundary interface condition

$$
2k_P \frac{\partial T_P}{\partial x} = (T_P - T_0)\left[a_0 h\frac{P}{A} - a_0 \frac{C_v}{C_v^P} h\frac{P}{A}\right] - 2T_P \alpha_P J - J^2 a_0 \left[\rho_S - \rho_P \frac{C_v}{C_v^P}\right].
\tag{8}
$$

With the specified mechanical boundary conditions at the interface of the SMA layer ("pinned ends" or the given stress), this approximation (that can be easily represented in the form of Robin's type boundary condition as $\dfrac{\partial \theta}{\partial x} = -\dfrac{\beta}{k}(\theta - T_0)$) completes the formulation of an approximate model for the description of coupled thermomechanical fields in the SMA layer of the multilayered actuator.

3. NUMERICAL APPROXIMATIONS AND COMPUTATIONAL EXPERIMENTS

Using the approximate model described in the previous section we performed a series of computational experiments in the 1D case. The coupling phenomenon was modelled with the middle term in the following expression for the free energy function

$$
\Psi(\theta, \epsilon) = \psi_0(\theta) + \psi_1(\theta)\psi_2(\epsilon) + \psi_3(\epsilon),
\tag{9}
$$

where specific forms for the thermal (ψ_0), mechanical (ψ_3) and coupled thermomechanical ($\psi_1\psi_2$) contributions were taken in the Falk form as in[15]

$$
\psi_0(\theta) = \alpha_0 - \alpha_1 \theta \ln \theta, \quad \psi_1(\theta) = \frac{1}{2}\alpha_2 \theta, \quad \psi_2(\epsilon) = \epsilon^2,
$$

$$
\psi_3(\epsilon) = -\frac{1}{2}\alpha_2 \theta_1 \epsilon^2 - \frac{1}{4}\alpha_4 \epsilon^4 + \frac{1}{6}\alpha_6 \epsilon^6,
\tag{10}
$$

and all α_i and θ_1 are positive constants. Now, using (4) it is straightforward to deduce an approximate model for the first constitutive relation in (3) (i.e. the stress-strain dependency). A schematic representation of this model is presented in Fig. 2 for the alloy $Au_{23}Cu_{30}Zn_{47}$, with different values of temperature indicated in the plot. This representation is a consequence of the form (10) for the free energy function where the central minimum of this function represents the austenite, while the symmetric minima correspond to the martensitic twins M^+ and M^-. As seen from Fig. 3, the free energy function (10) can mimic effectively a complete loop of transformations of the material from elastoplastic behaviour to quasiplastic, pseudoelastic, and finally to almost-elastic.
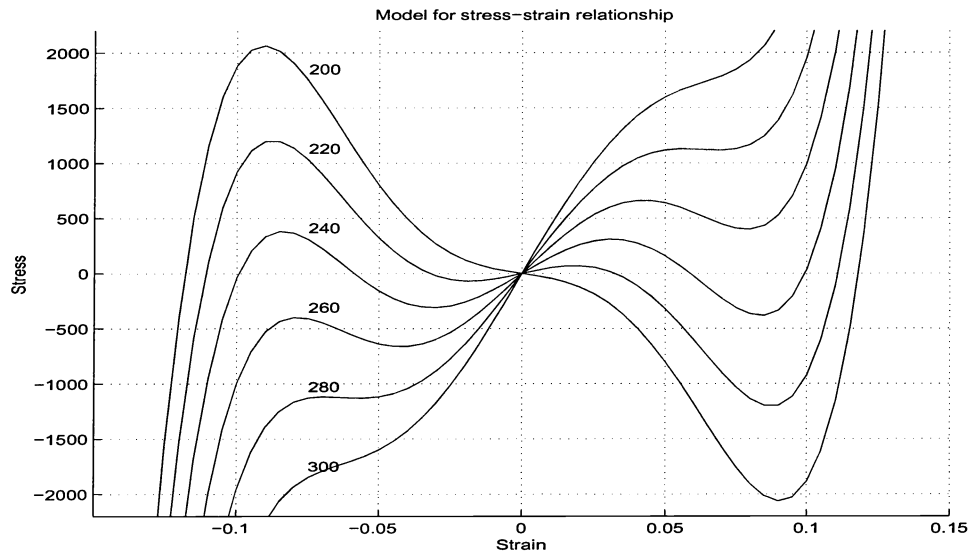

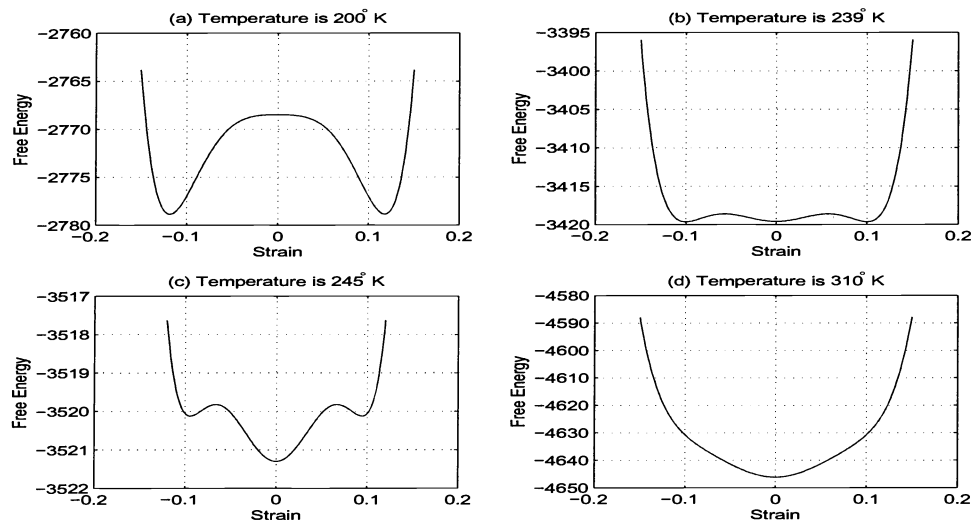**Figure 2.** Models for stress-strain relationship for different values of temperature.

Figure 3. Free energy curves for different values of temperature.

Coefficient	SMA	Semiconductor (P)
Seebeck coefficient $(\mathrm{cm}^2\mathrm{g}/\mathrm{ms}^3\mathrm{AK})$	1.2×10^{-7}	2.15×10^{-6}
Thermal conductivity $(\mathrm{cmg}/\mathrm{ms}^3 K)$	1.9×10^{-2}	1.63×10^{-4}
Heat capacity $(\mathrm{g}/(\mathrm{ms}^3\mathrm{cm}K)$	2.12×10^{-2}	4.35×10^{-2}
Electrical resistivity $(\mathrm{cm}^3\mathrm{g}/\mathrm{ms}^3 A^2)$	6.32×10^{-7}	1.15×10^{-5}

Table 1. Material parameters of SMA and semiconductor layers

Taking into account (1), system (6) was reduced to the following form

$$
\begin{cases}
C_v \dfrac{\partial \theta}{\partial t} - k_1 \theta \dfrac{\partial u}{\partial x} \dfrac{\partial^2 u}{\partial t \partial x} - \dfrac{\partial}{\partial x}\left(k \dfrac{\partial \theta}{\partial x}\right) = g, \\[2mm]
\rho \dfrac{\partial^2 u}{\partial t^2} - \dfrac{\partial}{\partial x}\left[k_1 \dfrac{\partial u}{\partial x}(\theta - \theta_1) - k_2 \left(\dfrac{\partial u}{\partial x}\right)^3 + k_3 \left(\dfrac{\partial u}{\partial x}\right)^5\right] = f,
\end{cases}
\tag{11}
$$

where ρ, k_i, $i = 1, 2, 3$ are given constants for the alloy $\mathrm{Au}_{23}\mathrm{Cu}_{30}\mathrm{Zn}_{47}$, taken from.[15] Results reported below were obtained for $b = c = 0.5$cm, $h = 2.5 \times 10^{-5}\mathrm{g}/\mathrm{ms}^3 K$, $a_0 = 1$cm, $a = 2$cm, and $J = -2\mathrm{A}/\mathrm{mm}^2$. We provide all the remaining parameters in Table 1 (note that the Seebeck coefficients, denoted in (7) as α_P, rather the Peltier coefficients, are given in the table[19,20]). Finally, it should be mentioned that with the specified values of the material parameters, the coefficient β in the reduced thermal boundary conditions (see the last paragraph in Section 2) is small indeed. Of course, for other materials and values of the electric current it may not be the case and improved approximations (8) should be sought.

All computations were performed via the reduction of model (11) to a system of differential-algebraic equations and the application of an effective DAE solver developed in our previous works.[15,2] Recall that in[15] we showed how a combined boundary stress and thermal control can be used to "guide" the phase transformation in the case when a mechanical loading alone is not sufficient for this purpose. In the first experiment reported in this paper we assume the "pinned ends" boundary conditions $(u(0, t) = u(1, t) = 0)$ and uniform forcing $f = 500 \text{ g}/(\mathrm{ms}^2\mathrm{cm}^2)$. We start this experiment in the low temperature range by using the following initial condition for temperature

$$
\theta(x, 0) = 200,
\tag{12}
$$

where, as it is seen from Fig. 2, the martensitic phase is stable. A specific form of the martensitic twins is chosen via the mechanical initial condition

$$
u(x, 0) = 0.11809 \min(x, 1 - x), \quad 0 \le x \le 1.
\tag{13}
$$

With the heating conditions changing in accord to the rule

$$
g = -175\pi \left(\frac{|g_0|}{g_0}\right)^3, \quad g_0 = \frac{1}{6}\pi t - 3,
\tag{14}
$$

in Fig. 4 we demonstrate a typical behaviour of shape memory alloy in thermally induced phase transitions. Upon heating, martensitic twins are transformed into an austenite, as demonstrated in Fig. 4 by the region of zero strain and displacements (with superposed elastic vibrations). As it is expected, this transformation is accompanied by a slight decrease in temperature. After the peak of temperature is reached the cooling process starts and it leads to the reverse transformation of the austenite into two martensitic twins. This reverse transformation is accompanied by a slight increase in temperature, and in this case the effect of phase transformation slows down the cooling processes of the thermoelectric SMA device.

Finally, we investigate the influence of the Ginzburg term γu_{xxxx} on the dynamics of phase transitions in shape memory alloys (see details in[2] and references therein). From a mathematical point of view, the Landau-Devonshire-Ginzburg model is somewhat easier to deal with, because the Ginzburg term (omitted in the first experiment) allows
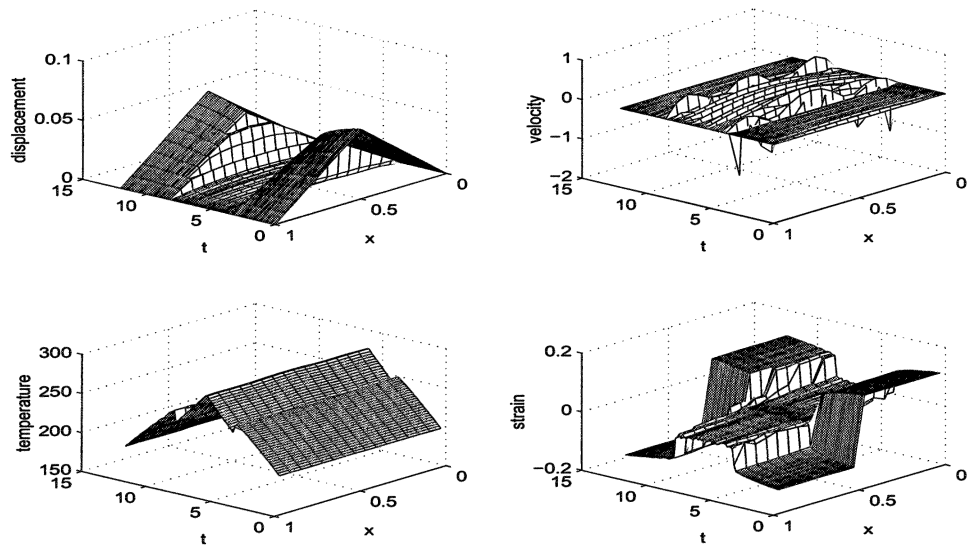
Figure 4. Thermally induced phase transition with the Landau-Devonshire model.

one to obtain a bound on the deformation gradient using a standard technique. It appears that for the model considered here the influence of this term becomes appreciable only when $\gamma \sim 1$, i.e. for the values much larger compared to the values of this coefficient reported in the literature. Typical results of computations for $\gamma = 2.5$ are presented in Fig. 5 where it is demonstrated how (upon cooling) the contribution of interfacial energies prevents the formation of stable twin martensites during the phase transformation reversal.
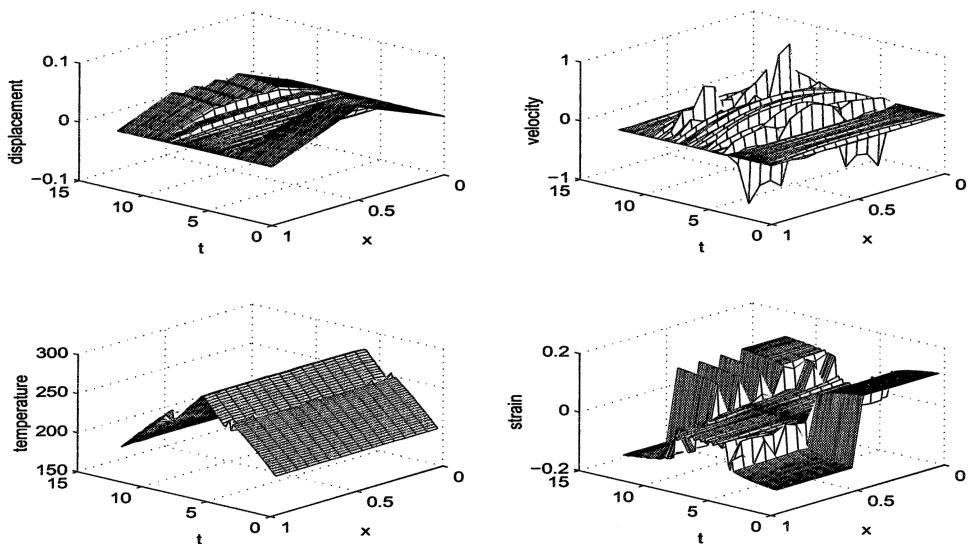

Figure 5. The effect of the Ginzburg term in the dynamics of thermally induced phase transformations.

4. CONCLUSIONS

In this paper we considered an approximate model for the description of the dynamics of thermomechanical fields in the SMA layer of multilayered actuators. The model was based on a coupled system of PDEs with the constitutive

equations derived from the Falk representation of the free energy function. On the example of thermoelectric sandwich-type actuators we demonstrated the main steps of the approximation procedure and presented typical results of numerical simulations for thermally induced phase transitions in shape memory alloys. The contribution of the interfacial energies on the dynamics of thermomechanical fields was investigated numerically via the introduction of the Ginzburg correction term into the model. A detailed analysis of this contribution should be a subject of future research.

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