ELSEVIER

Materials Science and Engineering A 481–482 (2008) 190–193

MATERIALS SCIENCE & ENGINEERING A

www.elsevier.com/locate/msea

Modifying macroscale variant combinations in a two-dimensional structure using mechanical loadings during thermally induced transformation

L.X. Wang [a,*], R.V.N. Melnik [b]

[a] *MCI, Faculty of Science and Engineering, University of Southern Denmark, Sonderborg DK-6400, Denmark*

[b] *Mathematical Modelling & Computational Sciences, Wilfrid Laurier University, 75 University Avenue West, Waterloo, Ont., Canada N2L 3C5*

Received 17 May 2006; received in revised form 16 October 2006; accepted 7 December 2006

Abstract

It is demonstrated how the formation of macroscopic martensite variant combinations in a two-dimensional shape memory alloy structure can be modified by mechanical loadings during thermally induced phase transformations. The dynamics involving square to rectangular transformations are modelled using a modified Ginzburg–Landau theory. The macroscale dynamics of the structure is described by a set of coupled partial differential equations of nonlinear dynamic thermoelasticity. The switching and modification of martensite variant combinations during thermally induced transformations are simulated using the developed dynamic model.

Keywords: Square to rectangular transformations; Martensite variant combinations; Ginzburg–Landau theory; Nonlinear thermoelastic dynamics

1. Introduction

Shape memory alloys (SMAs) have a promising potential in many engineering applications due to their ability to change properties at different temperatures and to recover the original configurations upon heating after being permanently deformed. It is well known now that such changes of the material properties are caused by the dynamics of material phases and their combinations which can be induced by mechanical and/or thermal loadings [1].

Many early instructive investigations have been carried out towards a better understanding of microstructures and phase combinations in ferroelastic materials [2,3]. In these investigations, the material microstructure is usually associated with a global minimizer of the total energy in the considered domain, and the problem is reformulated in a variational sense. Phase combinations on microscale can be obtained by simulating the formation of domains separated by domain walls [4,5]. The difficulties in the analysis at the microscale or even at the mesoscale often lie with the implementation of realistic mechanical boundary conditions. To overcome these difficulties a number of authors used periodic boundary conditions or specified strain values on the boundaries [6,7]. Another problem that one needs to face while using such approaches is that the connection between phase combinations and macroscopic dynamics of the considered structure is far from being straightforward [7–9].

In this paper, we propose a macroscopic approach to model the formation and modification of macroscale martensite variant combinations in a two-dimensional SMA structure (patch) at low temperature with mechanical boundary conditions enforced in terms of displacements. For this purpose, the modified Ginzburg–Landau free energy (non-convex) function is employed, in a way similar to the approach mentioned above for the microstructure analysis, in order to characterize the martensite and austenite phases by local minima of this function. Instead of directly minimizing the bulk energy in the SMA sample in attempts to get the global energy minimizer in terms of chosen order parameters (strains), or applying the time-dependent Ginzburg–Landau theory for the dynamic simulation of phase nucleation and growth in terms of order parameters, we use a different approach. We construct constitutive relations for the material by using a non-convex potential function, and employ nonlinear elastic theory to obtain governing equations for the macroscopic dynamics of the considered SMA patch in terms of displacement and temperature distributions. Macroscale martensite variant combinations and their evolution in the SMA patch are characterized by the deviatoric component of strain and its evolution, which can be calculated from

* Corresponding author. Tel: +45 6550 1686; fax: +45 6550 1660.
E-mail address: wanglinxiang@mci.sdu.dk (L.X. Wang).

0921-5093/$ – see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.msea.2006.12.194

the displacement distributions. By using the constructed model, various variant combinations in a finite SMA patch are modelled; switching and modification of variant combinations in the patch are also simulated by using the dynamic model developed here.

2. Mathematical model of ferroelastic dynamics

To model the dynamics of the SMA sample at macroscale accounting for phase transformations, we start from conservation laws for mass and momentum, which will give us governing equations for the mechanical field. Due to the coupling between mechanical and thermal fields during phase transformations, the governing equation for temperature evolution of the considered sample should also be added. This can be done on the basis of the conservation law for the internal energy. The entire model is then constructed on the basis of the same potential energy function at the mesoscale.

In order to characterize both, austenite at high temperature and martensite at low temperature, by using a generic expression, the potential energy is constructed on the basis of the modified Ginzburg–Landau free energy function as follows [6,10]:

$$\mathcal{F}(\theta,\varepsilon)=\frac{a_1}{2}e_1^2+\frac{a_3}{2}e_3^2+\mathcal{F}_1(\theta,\varepsilon)+\mathcal{F}_g(\nabla e_2),$$
$$\mathcal{F}_1(\theta,\varepsilon)=\frac{a_2}{2}(\theta-\theta_0)e_2^2-\frac{a_4}{4}e_2^4+\frac{a_6}{6}e_2^6,$$
$$\mathcal{F}_g(\nabla e_2)=\frac{k_g}{2}\left[\left(\frac{\partial e_2}{\partial x}\right)^2+\left(\frac{\partial e_2}{\partial y}\right)^2\right], \tag{1}$$

where e_1, e_2, and e_3 are dilatational, deviatoric, and shear components of strains, respectively, defined as $e_1=(\eta_{11}+\eta_{22})/\sqrt{2}$, $e_2=(\eta_{11}-\eta_{22})/\sqrt{2}$, $e_3=(\eta_{12}+\eta_{21})/2$, in which the Cauchy–Lagrangian strain tensor $\boldsymbol{\eta}$ is defined by its components as $\eta_{ij}=[(\partial u_j/\partial x_i)+(\partial u_i/\partial x_j)]/2$ (with the repeated-index convention used); u_i, $i=1,2$ are displacements along the x and y directions, respectively; θ is the material temperature, while θ_0 is the reference transformation temperature, which is a material-specific constant, and a_i, $i=1,\ldots,6$ and k_g are also material-specific constants.

In the above potential energy, the deviatoric strain e_2 is chosen as the only *order parameter* to characterize different phases. By associating its local minima to different phases, it has been shown that, thanks to its non-convexity, the above potential energy function is capable to characterize different phases, with different temperatures. It has two symmetrical local minima at low temperature, which can be associated with the two martensite variants (rectangles), while at high temperature it has only one minimum which is associated with the austenite (square). With intermediate temperatures, the potential energy has three local minima, with the central one associated with austenite and with the two symmetrical ones associated with martensite variants. It corresponds to the well-known fact that austenite and martensite can co-exist in this case [6,7].

Governing equations for the mechanical field can be obtained by minimizing the total energy in the considered patch. To do so, the Lagrangian of the material system under consideration can be constructed as:

$$\mathcal{L}(u_1,u_2,\theta)=\frac{\rho}{2}((\dot{u}_1)^2+(\dot{u}_2)^2)-\mathcal{F}(\theta,\varepsilon). \tag{2}$$

The first two terms on the right hand side represent kinetic energy along the x and y directions, respectively. The Hamilton principle implies that the first variation of the total energy in the considered domain is zero, given that the displacement u_1 and u_2 give the solution to the problem:

$$\mathcal{H}=\int_0^T\int_\Omega(\mathcal{L}(u_1,u_2,\theta)-f_xu_1-f_yu_2)\,\mathrm{d}t\,\mathrm{d}\Omega,$$
$$\frac{\delta\mathcal{H}}{\delta u_1}=0,\quad \frac{\delta\mathcal{H}}{\delta u_2}=0, \tag{3}$$

where f_x and f_y are mechanical loadings in the x and y directions, respectively; Ω is the domain occupied by the SMA patch, and $[0,T]$ is the considered time span.

By substituting all the contributions of the potential energy into (3), it is easy to get the following two equations, for the displacement components u_1 and u_2:

$$\rho\frac{\partial^2u_1}{\partial t^2}=\frac{\partial\sigma_{11}}{\partial x}+\frac{\partial\sigma_{12}}{\partial y}+f_x,\quad \rho\frac{\partial^2u_2}{\partial t^2}=\frac{\partial\sigma_{12}}{\partial x}+\frac{\partial\sigma_{22}}{\partial y}+f_y,$$
$$\sigma_{11}=\frac{\sqrt{2}}{2}(a_1e_1+a_2(\theta-\theta_0)e_2-a_4e_2^3+a_6e_2^5+k_g\nabla_x^2e_2),$$
$$\sigma_{22}=\frac{\sqrt{2}}{2}(a_1e_1-a_2(\theta-\theta_0)e_2+a_4e_2^3-a_6e_2^5+k_g\nabla_y^2e_2),$$
$$\sigma_{12}=\frac{1}{2}a_3e_3=\sigma_{21}, \tag{4}$$

where ρ is the density of the material. This is a nonlinear dynamic problem of elasticity, but with thermo-mechanical coupling. Now, boundary conditions for the mechanical field can also be taken into account. Because they are problem-specific, they will be given in the simulation section along with the specified problems.

To describe the dynamics of thermal field, the governing equation can be obtained by using the conservation law for the internal energy e:

$$\rho\frac{\partial e}{\partial t}-\boldsymbol{\sigma}^{\mathrm{T}}:\nabla\boldsymbol{v}+\nabla\cdot\boldsymbol{q}=g, \tag{5}$$

where $\boldsymbol{q}=-k\nabla\theta$ is the (Fourier) heat flux vector and k the heat conductance coefficient of the material, g is the thermal loading. The internal energy is connected with the potential energy constructed above via the Helmholtz free energy:

$$e=\psi(\theta,\varepsilon)-\theta\frac{\partial\psi(\theta,\varepsilon)}{\partial\theta},\quad \psi(\theta,\varepsilon)=\mathcal{L}-c_v\theta\ln\theta, \tag{6}$$

where c_v is the specific heat capacitance. By substituting the above relationship into the Eq. (5), the governing equation for the thermal field can be formulated as:

$$c_v\frac{\partial\theta}{\partial t}=k\left(\frac{\partial^2\theta}{\partial x^2}+\frac{\partial^2\theta}{\partial y^2}\right)+\frac{\sqrt{2}}{2}a_2\theta e_2\frac{\partial e_2}{\partial t}+g. \tag{7}$$

It has been shown in Refs. [12,6,10] that the mathematical model defined by Eqs. (4) and (7) is capable to capture the first

order square-to-rectangular phase transformations. In this case, the thermal and mechanical fields are intrinsically coupled due to the fact that governing equations for the mechanical and thermal fields are based on the same potential energy function which is a function of strain and temperature. The macroscale dynamics of the considered two-dimentional structure under thermal and mechanical loadings can be modelled using these equations, supplemented by suitable boundary and initial conditions [6,10]. Due to strong nonlinearity and coupling between the mechanical and thermal fields, numerical simulations based on this model are far from trivial. Numerical schemes should be designed to deal efficiently with nonlinearities, including hysteresis induced by phase transformations. This is especially true in cases where the dimension of the problem is higher than one [10].

3. Simulation of phase combinations

At low temperature, only combinations between martensite variants occur, because only martensite is stable in this case. When mechanical loadings are employed, it is expected that the SMA patch will have martensite variant combinations which are able to accommodate themselves in the confined domain with mechanical constraints. variant combinations can be switched by employing mechanical loadings directly, but the loadings required to do so should be sufficiently strong, so that transformations between martensite variants can be induced mechanically. In this section, we take another approach to switch martensite variant combinations. The idea is to heat the SMA patch up, so that the material will be transformed from martensite into austenite; then cool it down to the original temperature, so that it will be transformed back into martensite. If, during the austenite to martensite transformation, there is a small mechanical loading employed, the combination between martensite variants at low temperature will be formed in a way favored by the applied mechanical loading.

To demonstrate the capability of the developed model, in what follows, we report a representative numerical experiment that targets the switching of variant combinations. The simulation has been carried out for a $Au_{23}Cu_{30}Zn_{47}$ (at %) sample with size 2 cm × 2 cm. For this specific material, physical parameters are taken the same as in Ref. [12]. For the 2D model, we take the values $a_1 = 2a_2$, $a_3 = a_2$, as suggested in Ref. [7,11]. We choose the coefficient for the Ginzburg term as $k_g = a_2 \times 10^{-4}$. Boundary conditions for the current numerical experiment are as follows:

$$\frac{\partial u_1}{\partial y} = 0, \quad u_2 = 0, \quad \frac{\partial \theta}{\partial y} = 0, \quad \text{at } y = \pm 1,$$

$$\frac{\partial u_2}{\partial x} = 0, \quad u_1 = 0, \quad \frac{\partial \theta}{\partial x} = 0. \quad \text{at } x = \pm 1.$$

The initial variant combination in the SMA patch is characterized by the distribution of the deviatoric strain e_2, as sketched in Fig. 1. It is calculated from the initial displacements u_1^0 and u_2^0, which is obtained as the steady state output of the model at

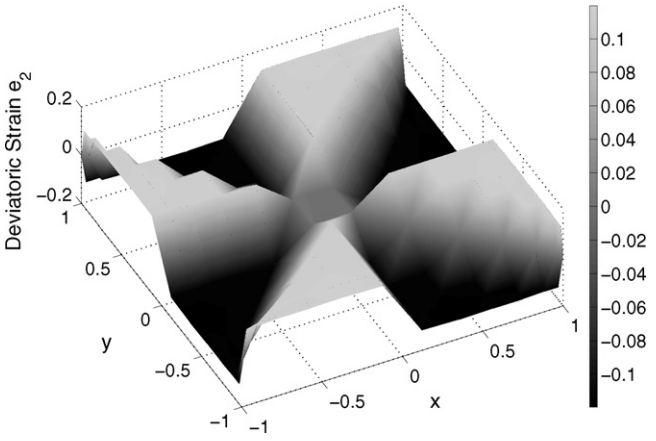

Fig. 1. Initial martensite variant combination in a SMA patch sketched by e_2 distribution.

$\theta = 210$ K with the following mechanical loadings [13]:

$$f_x\,(\mathrm{g/m\,s^2\,cm^2}) = 4000 \times \mathrm{sign}(y),$$

$$f_y\,(\mathrm{g/m\,s^2\,cm^2}) = 4000 \times \mathrm{sign}(x),$$

where $\mathrm{sign}(p) = 1$ if $p > 0$ and $\mathrm{sign}(p) = -1$ if $p < 0$ (with p being either x or y).

To show the switching of martensite variant combinations during the thermally induced phase transformation, Eqs. (4) and (7) are numerically solved simultaneously with the given boundary conditions. The initial conditions are set as

$$u_1 = u_1^0, \quad u_2 = u_2^0, \quad v_1 = v_2 = 0, \quad \theta = 210\,\mathrm{K}, \tag{8}$$

so the initial variant combination is the same as that in Fig. 1. To modify the formation of martensite variant combinations, the following mechanical and thermal loadings are employed:

$$f_x\,(\mathrm{g/m\,s^2\,cm^2}) = 400, \quad f_y\,(\mathrm{g/m\ s^2\,cm^2}) = 400,$$

$$g\,(\mathrm{g/m\,s^3\,cm}) = 1000 \times \sin\left(\frac{\pi t}{6}\right)$$

with the simulation time span [0,12] ms, which is the entire period of thermal loading.

The simulated distribution of the deviatoric strain e_2 at $t = 12$ ms is sketched in Fig. 2. The variant combination in this case is totally different from the initial one, which is the one favored by the mechanical loading and allowed by the mechanical constraints. As indicated, the mechanical loading required for the variant combination switch is very small because of the effect of the thermally induced transformation.

It is known that martensite variant combinations should be formed between the two rectangular martensitic variants, satisfying at the same time the mechanical constraints. These two variants are characterized by the two minima of the Landau free energy function $\mathcal{F}_l$, which could be calculated as

$$\frac{\partial \mathcal{F}_l}{\partial e_2} = 0, \quad e_2 = \pm\sqrt{\frac{a_4 + \sqrt{a_4^2 - 4a_2a_6(\theta - \theta_0)}}{2a_6}} \tag{9}$$

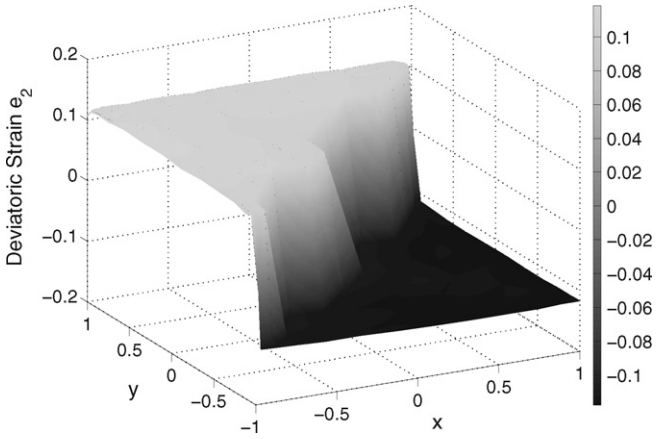

Fig. 2. Final martensite variant combination modified by a mechanical loading during thermally induced phase transformation, sketched by e_2 distribution.

with the given initial temperature of $\theta = 210\,\mathrm{K}$. One can easily deduce that the local minimum of the Landau free energy function is at $e_2 = \pm 0.1148$.

In the simulated initial and final variant combinations, it is demonstrated clearly that the entire SMA patch is divided into several sub-domains, in which e_2 takes value of either 0.11 or -0.11 (approximately). This shows that the variant combinations obtained here are the ones to minimize the free energy, while satisfying all the mechanical constraints. The numerical experiments demonstrate that the constructed model is capable to simulate the martensite variant combinations in SMA patches with square-to-rectangular phase transformations. The variant combination can be modified by very small mechanical loadings during the process of thermally induced phase transformations.

4. Conclusion

In this paper, we modelled the dynamics of a SMA patch on the basis of the modified Ginzburg–Landau theory. The dynamics involved thermo-mechanical interactions and square to rectangular phase transformations. The martensite variant combination was modified by employing appropriate mechanical loadings during the process of austenite to martensite phase transformations. It was shown that a very small mechanical loading can switch one macroscopic martensite variant combination to another via thermally induced phase transformations.

References

[1] V. Birman, Appl. Mech. Rev. 50 (1997) 629–645.
[2] J.L. Ericksen, J. Solids Struct. 22 (1986) 951–964.
[3] R. Ball, M. James, Arch. Rat. Mech. Anal. 100 (1988) 13–52.
[4] M. Luskin, Acta Numer. 5 (1996) 191–256.
[5] S. Muller, Lecture Notes in Mathematics 1713, 1999, pp. 85–210.
[6] T. Lookman, S. Shenoy, D. Rasmussen, A. Saxena, A. Bishop, Phys. Rev. B 67 (2003) 024114.
[7] A. Jacobs, Phys. Rev. B 61 (2000) 6587–6595.
[8] T. Ichitsubo, K. Tanaka, M. Koiva, Y. Yamazaki, Phys. Rev. B 62 (2000) 5435–5441.
[9] A. Saxena, A. Bishop, S. Shenoy, T. Lookman, Comput. Mater. Sci. 10 (1998) 16–21.
[10] L.X. Wang, R.V.N. Melnik, Mater. Sci. Eng. A 378 (2004) 470–474.
[11] S.H. Curnoe, A.E. Jacobs, Phys. Rev. B 64 (2001) 064101.
[12] F. Falk, Acta Metall. 28 (1980) 1773–1780.
[13] L.X. Wang, R.V.N. Melnik, Mater. Sci. Eng. A. 438–440 (2006) 427–430.