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Patrick Joly Pekka Neittaanmäki (Eds.)

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Nonlinear Coupled Thermomechanical Waves: Modelling Shear Type Phase Transformation in Shape Memory Alloys

Linxiang Wang[1] and Roderick Melnik[1]

University of Southern Denmark, MCI, Faculty of Science and Engineering, Sonderborg, DK-6400, Denmark

Summary. Starting from a two-dimensional model approximating the dynamics of cubic-to-tetragonal and tetragonal-to-orthorhombic phase transformations in shape memory materials, it is shown that the Falk model in the one dimensional case is a special case of the formulated model. Computational experiments based on a conservative difference scheme are carried out to analyse thermomechanical wave interactions in a rod with shape memory effect.

1 Introduction

A better understanding of the dynamics of phase transitions in shape memory alloys (SMA) is an important task in many areas of applications ([1] and references therein). However, even for the one dimensional case, the analysis of this dynamics is quite involved due to a strongly nonlinear pattern of interaction between mechanical and thermal fields [9].

Martensitic phase transformations of the shear type [3] have been a subject of intensive studies, in particular in the one-dimensional case where the model for shape memory alloys is usually based on the Landau-Ginzburg free energy function. Although various approximations to the free energy function have been proposed in both one dimensional and three dimensional cases (e.g., [14] and references therein), most of the results available in the literature in the context of SMA modelling deal with one-dimensional models.

In this paper, we propose a two-dimensional model describing square-to-rectangular phase transformations in materials with shape memory. Such transformations are known to provide an approximation to cubic-to-tetragonal and tetragonal-to-orthorhombic transformations observed in the general three-dimensional case [5, 6, 7]. We reduce the formulated model to the one-dimensional case, and solve the resulting system numerically applying a conservative difference scheme.

2 Mathematical model for square-to-rectangular transformations

Based on conservation laws for linear momentum and energy, the system describing coupled thermomechanical wave interactions for the first order phase transitions in a two dimensional SMA structure can be written as follows (e.g., [14, 10])

$$\rho\frac{\partial^2 u_i}{\partial t^2} = \nabla_x \cdot \boldsymbol{\sigma} + f_i, \quad i,j = 1,2,$$
$$\rho\frac{\partial e}{\partial t} - \boldsymbol{\sigma}^T : (\nabla \mathbf{v}) + \nabla \cdot \mathbf{q} = g, \tag{1}$$

where ρ is the density of the material, $\mathbf{u} = \{u_i\}|_{i=1,2}$ is the displacement vector, $\mathbf{v}$ is the velocity, $\boldsymbol{\sigma} = \{\sigma_{ij}\}$ is the stress tensor, $\mathbf{q}$ is the heat flux, e is the internal energy, $\mathbf{f} = (f_1, f_2)^T$ and g are mechanical and thermal loadings, respectively. Let ϕ be the free energy function of a thermomechanical system described by (1). Then, stress and the internal energy function are connected with ϕ by the following relationships

$$\boldsymbol{\sigma} = \rho\frac{\partial \phi}{\partial \boldsymbol{\eta}}, \quad e = \phi - \theta\frac{\partial \phi}{\partial \theta}, \tag{2}$$

where θ is the temperature, and the Cauchy-Lagrangian strain tensor $\boldsymbol{\eta}$ is given by its components as follows (with the repeated-index convention used)

$$\eta_{ij}(\mathbf{x},t) = \left(\frac{\partial u_i(\mathbf{x},t)}{\partial x_j} + \frac{\partial u_j(\mathbf{x},t)}{\partial x_i}\right)\Big/ 2, \quad i,j = 1,2, \tag{3}$$

where $\boldsymbol{x}$ is the coordinates of a material point in the domain of interest.

For the square-to-rectangular transformations [5, 6], it was established earlier that the free energy function ϕ can be represented in terms of a Landau free energy functions F_L as follows

$$\phi = -c_v\theta\ln\theta + \frac{1}{2}a_1e_1^2 + \frac{1}{2}a_3e_3^2 + F_L, \quad F_L = \frac{1}{2}a_2(\theta-\theta_0)e_2^2 - \frac{1}{4}a_4e_2^4 + \frac{1}{6}a_6e_2^6, \tag{4}$$

where c_v is the specific heat constant, θ_0 is the martensite transition temperature, a_i, $i = 1,2,3,4,6$ are the material-specific coefficients, and e_1, e_2, e_3 are dilatational, deviatoric, and shear components of strain, respectively. The later are defined as follows

$$e_1 = (\eta_{11} + \eta_{22})\Big/\sqrt{2}, \quad e_2 = (\eta_{11} - \eta_{22})\Big/\sqrt{2}, \quad e_3 = (\eta_{12} + \eta_{21})/2. \tag{5}$$

By substituting the free energy function defined by (4)–(5) into model (1)–(3), the following coupled system of equations is obtained

$$\frac{\partial^2 u_1}{\partial t^2} = \frac{\sqrt{2}}{2}\frac{\partial}{\partial x}\left(a_1 e_1 + a_2(\theta-\theta_0)e_2 - a_4 e_2^3 + a_6 e_2^5\right) + \frac{\partial}{\partial y}\left(\frac{1}{2}a_3 e_3\right) + f_1,$$
$$\frac{\partial^2 u_2}{\partial t^2} = \frac{\partial}{\partial x}\left(\frac{1}{2}a_3 e_3\right) + \frac{\sqrt{2}}{2}\frac{\partial}{\partial y}\left(a_1 e_1 - a_2(\theta-\theta_0)e_2 + e_4 e_2^3 - a_6 e_2^5\right) + f_2, \quad (6)$$
$$c_v\frac{\partial \theta}{\partial t} = k\left(\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2}\right) + \frac{\sqrt{2}}{2}a_2\theta e_2\frac{\partial e_2}{\partial t} + g.$$

3 Numerical methodology

For the analysis of system (6) describing nonlinear interactions of coupled thermomechanical waves in a two-dimensional structure with shape memory effect, the development of efficient numerical tools is necessary. In what follows we assume that the deformation of the two dimensional SMA structure along x_1 direction substantially exceeds the deformation in the other direction, so that the deformation along x_2 direction can be neglected. In this case $\partial u_2/\partial x_2 = 0$, $\partial u_2/\partial x_1 = 0$, $\partial u_1/\partial x_2 = 0$, and system (6) is reduced to

$$\begin{aligned}\frac{\partial^2 u_1}{\partial t^2} &= \frac{\partial}{\partial x}\left(\frac{\sqrt{2}}{2}(a_1\epsilon + a_2(\theta-\theta_0)\epsilon - a_4\epsilon^3 + a_6\epsilon^5)\right) + f_1,\\ c_v\frac{\partial\theta}{\partial t} &= k\left(\frac{\partial^2\theta}{\partial x^2}\right) + \frac{\sqrt{2}}{2}a_2\theta\epsilon\frac{\partial\epsilon}{\partial t} + g.\end{aligned} \quad (7)$$

By setting $\theta_1 = \theta_0 - a_1/a_2$ system (7) can be re-written in the form of the Falk model

$$\begin{aligned}\rho\frac{\partial^2 u}{\partial t^2} &= \frac{\partial}{\partial x}\left(k_1(\theta-\theta_1)\frac{\partial u}{\partial x} - k_2\left(\frac{\partial u}{\partial x}\right)^3 + k_3\left(\frac{\partial u}{\partial x}\right)^5\right) + F,\\ c_v\frac{\partial\theta}{\partial t} &= k\frac{\partial^2\theta}{\partial x^2} + k_1\theta\frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + G,\end{aligned} \quad (8)$$

where k_1, k_2,k_3, c_v and k are re-normalised material-specific constants, and F and G are distributed mechanical and thermal loadings. Since system (8) has been already studied numerically (e.g., [3, 13, 10, 11]), we have chosen this model as the basis for the analysis of nonlinear thermomechanical wave interactions. In [8] a fully conservative scheme for the models describing SMA material dynamics has been proposed and justified theoretically. No computational results has been reported so far with that scheme. In what follows, we apply the scheme constructed in [8] to the solution of (8). For this purpose it is convenient to introduce two new variables, and re-write system (8) as follows:

$$\frac{\partial \epsilon}{\partial t} = \frac{\partial v}{\partial x}, \quad \rho \frac{\partial v}{\partial t} = \frac{\partial s}{\partial x} + F,$$
$$s = k_1 \left(\theta - \theta_1\right) \epsilon - k_2 \epsilon^3 + k_3 \epsilon^5, \quad c_v \frac{\partial \theta}{\partial t} = k \frac{\partial^2 \theta}{\partial x^2} + k_1 \theta \epsilon \frac{\partial v}{\partial x} + G, \tag{9}$$

where ϵ is strain and s is stress. While spatial discretisations of (9) have been carried out in a way analogous to that proposed in [8], we have used an idea of [12] in reducing (9) to a system of differential-algebraic equations. Then, the backward differentiation formula methodology is applied to get the numerical solution of the problem [4]. We note that to deal with a strong (cubic and quintic) nonlinearities, a smoothing procedure similar to that proposed in [13] has been employed. In particular, we have used the following expansions

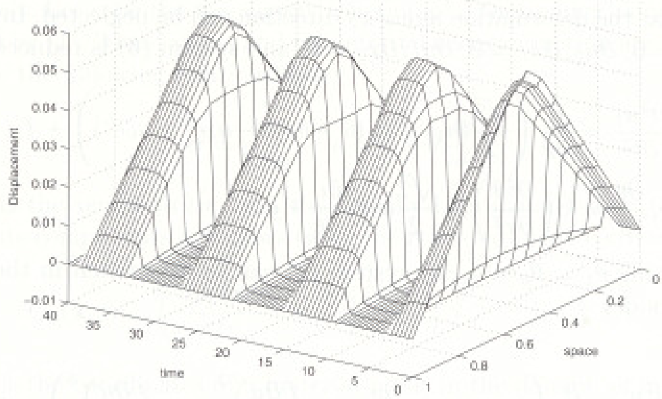

Fig. 1. Displacements in a SMA rod in the temperature-driven phase transition experiment

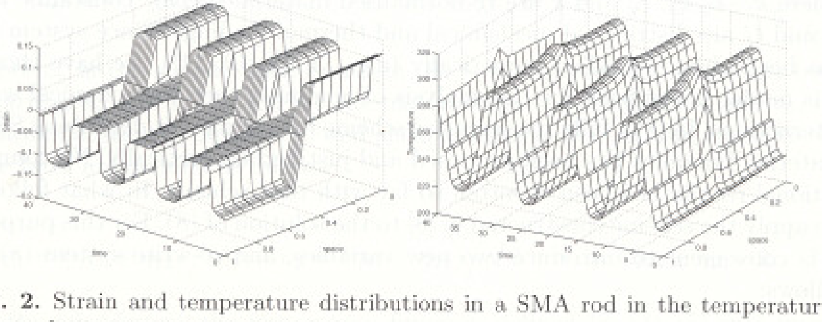

Fig. 2. Strain and temperature distributions in a SMA rod in the temperature-driven phase transition experiment

$$\epsilon^3 = \frac{1}{4}\sum_{i=0}^{3}\epsilon^i\epsilon_r^{3-i}; \quad \epsilon^5 = \frac{1}{6}\sum_{i=0}^{5}\epsilon^i\epsilon_r^{6-i}, \tag{10}$$

where ϵ_r is the strain on time level $n-1$ if the current time level is n.

Finally, we demonstrate the application of the developed methodology to the analysis of phase transformations in a $Au_{23}Cu_{30}Zn_{47}$ rod of length $L = 1$cm. For this specific SMA, all necessary parameters are taken the same as in [3, 11].

As initial conditions for model (9) we took two symmetric martensites ($\epsilon^0 = \pm 0.11869$ for $0 \le x \le 0.5$ and $0.5 \le x \le 1$, respectively), $v^0 = 0$, and $\theta^0 = 220$. The distributed mechanical loading was assumed constant as $F =$ 500g/(ms^{3}cm), and the distributed thermal loading is assumed as $G = 375\pi$ $\sin^3(\pi t/6)$g/(ms^{3}cm). The boundary conditions for this experiment have been taken as pinned-end mechanically and insulated thermally. A staggered grid system was used for this simulation, there were 17 nodes used for ϵ, θ and s in the computational domain (16 nodes were used for v approximated at flux points). Time span of the simulation was [0,40] and time stepsize was set to 0.0005. Displacement, strain and temperature distributions in the SMA rod are presented in Figs. 1 and 2. The temperature-driven phase transformation between martensites and austenite are in quantitative agreement with the results reported in [11].

References

1. V. Birman, Review of mechanics of shape memory alloys structures, *Appl. Mech. Rev.* **50** (1997) 629–645.
2. N. Bunber, Landau-Ginzburg model for a deformation-driven experiment on shape memory alloys, *Continuum Mech. Thermodyn.* **8** (1996) 293–308.
3. F. Falk, Model free energy, mechanics, and thermomechanics of shpae memory alloys, *Acta Metallurgica*, **28**, (1980), 1773–1780.
4. E. Hairer, S.P. Norsett, and G. Wanner, *Solving ordinary differential equations II-stiff and differential algebraic problems*, Springer-Verlag, Berlin, 1996.
5. T. Ichitsubo, K. Tanaka, M. Koiva, and Y. Yamazaki, Kinetics of cubic to tetragonal transformation under external field by the time-dependent Ginzburg-Landau approach, *Phys. Rev. B* **62(9)** (2000) 5435–5441.
6. A.E. Jacobs, Landau theory of structures in tetragonal-orthorhombic ferroelastics, *Phys. Rev. B* **61(10)** (2000) 6587–6595.
7. T. Lookman, T.O. Williams, A. Saxena, Effect of solid-solid phase transformation on elastic constitutive relations. *J. Phys. IV France*, **11**, (2001),Pr8-11-15.
8. P. Matus, R.V.N. Melnik, I.V. Rybak, Fully Conservative Difference Schemes for Nonlinear Models Describing Dynamics of Materials with Shape Memory, *Dokl. of the Academy of Sciences of Belarus*, **47**, 2003, to appear.
9. G.A. Maugin, *Nonlinear Waves in Elastic Crystals*, Oxford University Press, Oxford, N.Y., 1999.

10. R.V.N. Melnik, A.J. Roberts, and K.A. Thomas, Computing dynamics of copper-based SMA via center manifold reduction of 3D models, *Computational Material Science*, **18**, (2000) 255–268.
11. R.V.N. Melnik, A.J. Roberts, and K.A. Thomas, Coupled thermomechanical dynamics of phase transitions in shape memory alloys and related hysteresis phenomena, *Mechanics Research Communications*, **28(6)**, (2001) 637–651.
12. R.V.N. Melnik, A.J. Roberts, and K.A. Thomas, Phase transitions in shape memory alloys with hyperbolic heat conduction and differential algebraic models, *Computational Mechanics*, **29(1)**, (2002) 16–26.
13. M. Niezgodka, J. Sprekels, Convergent numerical approximations of the thermomechanical phase transitions in shape memory alloys, *Numerische Mathematik*, **58**, (1991) 759–778.
14. I. Pawlow, Three-dimensional model of thermomechanical evolution of shape memory materials, *Control and Cybernetics*, **29**, (2000) 759–778.