Computer Physics Communications 192 (2015) 48–53

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Shape memory alloy nanostructures with coupled dynamic thermo-mechanical effects

R.P. Dhote [a,*], H. Gomez [c], R.N.V. Melnik [b], J. Zu [a]

[a] Mechanical and Industrial Engineering, University of Toronto, 5 King's College Road, Toronto, ON, M5S3G8, Canada

[b] The MS2Discovery Interdisciplinary Research Institute, M^2 NeT Laboratory, Wilfrid Laurier University, Waterloo, ON, N2L3C5, Canada

[c] Department of Applied Mathematics, University of A Coruña Campus de Elvina, s/n. 15192 A Coruña, Spain

ARTICLE INFO

Article history:
Received 15 July 2014
Received in revised form
2 February 2015
Accepted 20 February 2015
Available online 27 February 2015

Keywords:
Phase-field model
Ginzburg–Landau theory
Nonlinear thermo-elasticity

ABSTRACT

Employing the Ginzburg–Landau phase-field theory, a new coupled dynamic thermo-mechanical 3D model has been proposed for modeling the cubic-to-tetragonal martensitic transformations in shape memory alloy (SMA) nanostructures. The stress-induced phase transformations and thermo-mechanical behavior of nanostructured SMAs have been investigated. The mechanical and thermal hysteresis phenomena, local non-uniform phase transformations and corresponding non-uniform temperatures and deformations' distributions are captured successfully using the developed model. The predicted microstructure evolution qualitatively matches with the experimental observations. The developed coupled dynamic model has provided a better understanding of underlying martensitic transformation mechanisms in SMAs, as well as their effect on the thermo-mechanical behavior of nanostructures.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Shape memory alloys (SMAs) exhibit a remarkable hysteresis behavior that arises from an interplay between microstructures in two phases, a high temperature higher symmetric austenite and low temperature lower symmetric martensite phases. The phase transformations between two phases, called martensitic transformations (MTs), reveal non-uniform and temperature dependent microstructure morphology. The microstructure morphology manifests itself through a domain pattern [1] and surface relief [2] due to elastic deformations (or strains) under temperature or stress induced loadings. The ability to control deformations in different geometries and loading conditions can lead to tailoring of mechanical structures [3] for better SMA-based actuators and sensors in NEMS, MEMS and biomedical applications [4–9]. The ability to control deformations in SMAs as well as in other functional materials and semiconductor devices [10,11] can be better understood by physics-based modeling approaches. The physics-based models facilitate the study of 3D complex martensitic twin microstructures and properties of SMAs.

Recently, MTs have been studied by using atomistic simulations [12]. Simulating larger domains at submicron scales requires enormous computational power which limits their use. In order to overcome this limitation, continuum descriptions at the submicron length scale have become an effective tool to model experimentally observed phenomena. One of the continuum based methods is the phase-field (PF) approach that has been widely used to investigate qualitatively microstructures and underlying mechanisms in nanoferroic systems [13,14]. Particularly, in the ferroelastic systems, the PF model has been implemented successfully to understand martensitic transformations in SMA nanostructures under isothermal [15] or athermal conditions [16]. The dynamics of phase transformation in martensites and solids have been studied in [17–19, 15,20–23]. Especially, under the dynamic loading conditions, the effect of temperature evolution is important as the phase transformation causes the temperature evolution due to self-heating or cooling of the system, consequently affecting their mechanical behavior, due to insufficient time for heat transfer to dissipate in the environment as observed experimentally [24,25]. Therefore, a theoretical framework that couples dynamically the mechanical behavior with temperature evolution is imperative to describe the MTs and their behavior in SMA nanostructures for critical application developments.

2. Mathematical model

For the first time, we develop and apply a fully coupled dynamic thermo-mechanical 3D PF model to the investigation of the

* Corresponding author. Tel.: +1 4169463709; fax: +1 4169787753.
E-mail address: rakesh.dhote@mail.utoronto.ca (R.P. Dhote).

http://dx.doi.org/10.1016/j.cpc.2015.02.019
0010-4655/© 2015 Elsevier B.V. All rights reserved.

stress-induced phase transformations and behavior in SMA nanostructures. The cubic-to-tetragonal PT is described by deviatoric strains defined in terms of symmetry adapted combinations of the components of the strain tensor. The model is developed based on the Ginzburg–Landau theory. We call $\boldsymbol{\epsilon}$ the Cauchy–Lagrange infinitesimal strain tensor that can be defined in components as $\epsilon_{ij} = \left(u_{i,j} + u_{j,i}\right)/2$, where the u_i's represent the displacements and an inferior comma denotes partial differentiation. We will make use of the following strain measures for the cubic-to-tetragonal phase transformation; $e_1 = 1/\sqrt{3}(\epsilon_{11}+\epsilon_{22}+\epsilon_{33})$, $e_2 = 1/\sqrt{2}(\epsilon_{11}-\epsilon_{22})$, $e_3 = 1/\sqrt{6}(\epsilon_{11}+\epsilon_{22}-2\epsilon_{33})$, $e_4 = \epsilon_{23}$, $e_5 = \epsilon_{13}$, $e_6 = \epsilon_{12}$. Here, e_1 is the hydrostatic strain, e_2, e_3 are the deviatoric strains, and e_4, e_5 and e_6 are the shear strains. We use the symmetric strain-based free energy functional, for cubic-to-tetragonal phase transformations, initially proposed by Barsch et al. [26] and later modified by Ahluwalia et al. [15] to study the martensitic transformations in SMA nanostructures. The free energy functional $\mathscr{F}$ with anharmonic components of OPs and harmonic components of non-OP components is expressed as

$$\mathscr{F}[\boldsymbol{u}] = \int_{\Omega} \left[F_0(e_i, \tau) + \frac{k_g}{2}\left(|\nabla e_2|^2 + |\nabla e_3|^2\right)\right] \mathrm{d}\Omega, \tag{1}$$

where $|\cdot|$ denotes the norm of a vector, and F_0 is the function

$$F_0(e_i, \tau) = \frac{a_1}{2}e_1^2 + \frac{a_2}{2}\left(e_4^2 + e_5^2 + e_6^2\right) + a_3\tau\left(e_2^2 + e_3^2\right) + a_4 e_3\left(e_3^2 - 3e_2^2\right) + a_5(e_2^2 + e_3^2)^2. \tag{2}$$

Here, the a_i's and k_g are material parameters, τ is the dimensionless temperature coefficient defined as $\tau = (\theta - \theta_m)/(\theta_0 - \theta_m)$, where θ_0 and θ_m are the material properties specifying the transformation start and end temperatures. The kinetic energy $\mathscr{K}$, the energy associated to body forces $\mathscr{B}$, and the Raleigh dissipation $\mathscr{R}$ are defined as $\mathscr{K}[\dot{\boldsymbol{u}}] = \int_{\Omega} \frac{\rho}{2}|\dot{\boldsymbol{u}}|^2 \mathrm{d}\Omega$, $\mathscr{B}[\boldsymbol{u}] = -\int_{\Omega} \boldsymbol{f}\cdot\boldsymbol{u}\mathrm{d}\Omega$, $\mathscr{R}[\dot{\boldsymbol{u}}] = \int_{\Omega} \frac{\eta}{2}|\dot{\boldsymbol{e}}|^2 \mathrm{d}\Omega$, where a dot over a function denotes partial differentiation with respect to time, ρ is the density, $\boldsymbol{f}$ is the body load vector, η is the dissipation coefficient, and $\boldsymbol{e}$ is a vector collecting the e_i's. The potential energy of the system $\mathscr{U}$ is defined as $\mathscr{U}[\boldsymbol{u}] = \mathscr{F}[\boldsymbol{u}] + \mathscr{B}[\boldsymbol{u}]$, while the Lagrangian takes on the form $\mathscr{L}[\boldsymbol{u}, \dot{\boldsymbol{u}}] = \mathscr{K}[\dot{\boldsymbol{u}}] - \mathscr{U}[\boldsymbol{u}]$. We define the Hamiltonian as $\mathscr{H}[\boldsymbol{u}, \dot{\boldsymbol{u}}] = \int_0^t \mathscr{L}[\boldsymbol{u}, \dot{\boldsymbol{u}}]\mathrm{d}t$. Following a variational approach, the governing equation of motion has the form

$$\frac{\partial}{\partial t}\left(\frac{\delta \mathscr{L}}{\delta \dot{u}_i}\right) - \frac{\delta \mathscr{L}}{\delta u_i} = -\frac{\delta \mathscr{R}}{\delta \dot{u}_i}, \tag{3}$$

where the operator $\delta(\cdot)/\delta(\cdot)$ denotes a variational derivative. Defining

$$\sigma_{ij} = \frac{\partial \mathscr{F}}{\partial u_{i,j}}, \qquad \mu_{ij,kk} = -\left(\frac{\partial \mathscr{F}}{\partial u_{i,jk}}\right)_{,k}, \qquad \sigma'_{ij} = \frac{1}{\eta}\frac{\partial \mathscr{R}}{\partial \dot{u}_{i,j}}, \tag{4}$$

Eq. (3) may be rewritten as

$$\rho\ddot{u}_i = \sigma_{ij,j} + \eta\sigma'_{ij,j} + \mu_{ij,kkj} + f_i. \tag{5}$$

Finally, the internal energy is $\iota = \Psi(\theta, \boldsymbol{u}) - \theta\frac{\partial \Psi(\theta,\boldsymbol{u})}{\partial \theta}$ with $\Psi(\theta, \boldsymbol{u}) = \mathscr{L}[\boldsymbol{u}, \dot{\boldsymbol{u}}] - C_v\theta\ln(\theta)$. Stating an energy balance equation, and using Fourier's law, the following equation for the temperature evolution may be derived as

$$C_v\dot{\theta} = \kappa\theta_{,ii} + \Xi\theta\left(u_{i,i}\dot{u}_{j,j} - 3u_{i,j}\dot{u}_{i,i}\right) + g. \tag{6}$$

Here, C_v, κ, and Ξ are positive constants that represent, respectively, specific heat, thermal conductance coefficient, and strength of the thermo-mechanical coupling, while g is a thermal load. We remark that Eq. (6) is derived under an assumption of no effects of viscosity and higher-order stresses on the temperature evolution.

The simulations were performed for homogeneous single crystal FePd nanowire. The material properties used during the simulations are [13,27]: $a_1 = 192.3$ GPa, $a_2 = 280$ GPa, $a_3 = 19.7$ GPa, $a_4 = 2.59 \times 10^3$ GPa, $a_5 = 8.52 \times 10^4$ GPa, $k_g = 3.15 \times 10^{-8}$ N, $\theta_m = 270$ K, $\theta_0 = 295$ K, $C_v = 350$ J kg^{-1} K^{-1}, $\kappa = 78$ W m^{-1} K^{-1}, and $\rho = 10\,000$ kg m^{-3}.

The governing Eqs. (5)–(6) are strongly thermo-mechanically coupled in a non-linear manner, with the fourth-order differential terms. These complex equations are not amenable to a closed form solution. They pose great challenges to numerical approaches. We have developed an isogeometric analysis (IGA) [28] framework that allows the straightforward solution to the developed model. It also allows the use of coarser meshes, larger time steps along with geometrical flexibility and accuracy [29].

3. Numerical simulations

To elucidate the capabilities of the developed model from physics point of view, the simulations have been conducted on a rectangular prism nanowire of dimension 160 × 40 × 40 nm (meshed with 162 × 42 × 42 uniform quadratic $\mathscr{C}^1$-continuous B-spline basis functions) to investigate its thermo-mechanical behavior subjected to dynamic stress-induced loadings. Simulations to examine the pseudoelastic (PE) and shape memory effect (SME) behavior of SMAs, as a function of microstructures, have been performed.

To study the PE behavior, the SMA nanowire is quenched to the dimensionless temperature corresponding to $\tau = 1.12$ and allowed to evolve starting from random initial displacements and periodic boundary conditions. The nanowire has been evolved till the microstructure and free energy are stabilized. The nanowire remains in the austenite phase. The evolved microstructures are then axially loaded by mechanically constraining one end of the specimen $\boldsymbol{u} = \boldsymbol{0}$, and loading the opposite end using a ramp based displacement equivalent to the strain rate 3×10^7/s as shown in Fig. 1(j). Fig. 1(a)–(g) shows different time snapshots of microstructure evolution during loading (a)–(f) and the end of unloading cycle (g). The austenite (yellow) is converted into the favorable M_1martensite (red) with the formation and migration of habit plane in the nanowire. At the end of unloading, the nanowire returns to the austenite phase (refer to Fig. 1(g)). The mechanical hysteresis, the average σ_{11}–ϵ_{11} (blue color), forms a full loop with zero remnant strain at the end of unloading in Fig. 1(h). The temperature hysteresis, the average τ–ϵ_{11} (red color), indicates a global increase in the temperature during loading and a decrease during unloading as a result of exothermic and endothermic processes.

The phase transformation is a local phenomenon that leads to non-uniform deformation and temperature fields in the domain. The local variation of the non-dimensional temperature τ is presented as an arc-length extrusion plot along the central axis of the nanowire during loading and unloading in Fig. 1(i). The non-uniform strain and deformation are apparent during phase transformations. The local increase in temperature, as observed in Fig. 1(i) serves as a signature of formation or movement of habit planes as indicated in the inset. As the loading progresses, the heat produced is conducted in the domain causing self-heating thus increasing the global temperature. As the domain is small, the heat is conducted quickly causing small local peaks as compared to the experiments where large temperature peaks were observed in big macro specimens [30].

To study the SME behavior, the SMA nanowire is quenched to the temperature corresponding to $\tau = -1.2$ and allowing the microstructures and energy to stabilize. The nanowire domain is evolved into the accommodated twinned martensites with all three variants present in approximately equal proportions as

Download English Version:

https://daneshyari.com/en/article/6919996

Download Persian Version:

https://daneshyari.com/article/6919996

Daneshyari.com