Computational Materials Science 139 (2017) 285–294

Contents lists available at ScienceDirect

Computational Materials Science

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

Phase-field simulations of thermomechanical behavior of MnNi shape memory alloys using finite element method

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ARTICLE INFO

Article history:
Received 15 June 2017
Received in revised form 7 August 2017
Accepted 8 August 2017

Keywords:
Phase-field model
Shape memory alloy
Thermomechanical behavior

ABSTRACT

The thermomechanical behavior and associated microstructure evolution of MnNi shape memory alloys (SMAs) are studied via two-dimensional phase-field simulations. Simulations with complex geometries and boundary conditions are realized by using finite element method. Shear-related surface relief, determined by the combination of Bain strain and crystal rotation, was observed. In the process of pseudoelastic bending, large bending degree was realized by formation of triangular martensitic domains, and the elastic strain energy did not apparently increase. The coupling strength of a SMA pipe coupling was greatly influenced by the proceeding of the reverse transformation upon heating. It was found that large shape change of SMAs was realized by the transition between different crystal structures, this transition was driven by the free energy difference between the structures, and the stress plateau during a pseudoelastic cycle was related to the thermodynamic equilibrium state of austenite–martensite interface.

1. Introduction

Shape memory alloys (SMAs) are well-known functional materials because of their pseudoelasticity and shape memory effect [1–4], which stem from the thermoelastic structural transformation between a high-symmetry austenite phase and a low-symmetry martensite phase [5]. This transformation can be induced by temperature or stress, thus SMA shows a strong thermomechanical coupling [6]. Based on this coupling, various engineering applications have been realized, and can be divided into four categories: free recovery, constrained recovery, work production (actuators) and superelasticity [7]. The origin and mechanism of shape memory are well understood, but many of the engineering aspects are not [7]. Numerical simulation is an effective approach to investigate these issues.

Phase-field simulations have been widely applied to investigate the structural transformation of SMAs [8]. Falk [9] proposed a phenomenological model, based on Landau's theory. In this model the free energy density is a polynomial in terms of strain components, and the stress is obtained by derivative of the free energy with respect to strain. In the simulations based on this model, the evolution of strain field is governed by a time-dependent Ginzburg-Landau (TDGL) equation, and the components of the strain tensor are related to each other by the elastic compatibility relations. Jacobs et al. [10] studied the cubic-tetragonal transformation, the obtained stable and transient patterns were also observed in experiment. Ahluwalia et al. [11] simulated the hexagonal-orthorhombic transformation. They also simulated the mechanical response and microstructure evolution of FePd SMAs during dynamic strain loading [12]. Dhote et al. [13] simulated the forward and reverse cubic-tetragonal transformation. On the other hand, Wang and Khachaturyan [14] proposed a phase-field model of martensitic transformation based on the TDGL phase transition theory integrated with the Khachaturyan-Shatalov (KS) microelasticity theory. In this kind of model, the free energy is a Landau polynomial in terms of order parameters, and the transformation strain couples with order parameters by a linear or quadratic term. The TDGL equation is used to govern the evolution of order parameter. The elastic strain energy is obtained via the KS theory. This model has been widely applied to study the microstructure evolution of SMAs. Jin et al. [15] studied the cubic-trigonal transformation of AuCd alloys in polycrystals. Man et al. [16] studied the microstructure evolution of MnCu alloys under temperature field. Gao et al. [17] simulated the pattern formation during cubic-orthorhombic transformation in NiTi alloys.

For the phase-field model proposed by Wang and Khachaturyan, periodic boundary condition is required, thus the surface effect (e.g. surface relief) is not taken into account. Complex deformation process (e.g. bending of beam) could not be simulated as

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http://dx.doi.org/10.1016/j.commatsci.2017.08.010
0927-0256/

well. Furthermore, the microstructure evolution in complex-shaped materials (e.g. ring-shaped SMA coupling) is difficult to be simulated. Recently, finite element method has been applied to phase-field simulations [18–20], the elastic strain energy is obtained by solving the mechanical equilibrium equations, instead of the KS microelasticity approach in the Fourier space. Therefore, problems with complex boundary conditions can be investigated. Mamivand et al. [21] studied the formation of a surface relief induced by the tetragonal to monoclinic transformation. They also simulated the shape memory effect and pseudoelasticity behavior in zirconia [22]. She et al. [23] studied the effect of surface energy on the martensitic transformation with free boundary condition. Paranjape et al. [24] simulated the interaction between phase transformation and plasticity in SMAs. Javanbkht and Barati [25] studied the surface tension effect on the martensitic transformation, and it was found that the surface tension can suppress nucleation.

Nevertheless, phase-field simulations focusing on the thermo-mechanical behavior of SMAs can be rarely found in literature. In fact, the micromechanism of the thermomechanical behavior has not been well understood, e.g. the correspondence between microstructure evolution and stress–strain curve during superelastic bending, and the microstructure evolution of SMA pipe coupling during the application process.

In the present work, finite element simulations of phase-field model are applied to study the thermomechanical behavior and microstructure evolution of MnNi SMAs. Owing to the ability of solving problem with complex boundary condition by using finite element method, the thermomechanical response during the engineering application process is simulated and the micromechanism is discussed in this paper, which have hardly been investigated in literature. Because three-dimensional (3D) simulations with relatively large number of meshes are beyond our computational ability, only 2D simulations were performed. In 2D space, the square-to-rectangle transformation was simulated, including the thermally induced transformation, the pseudoelastic behaviors during tensile and bending tests, the shape memory effects with free and constraint recoveries, and the strain-temperature relationship under constant stress.

2. Phase-field model

The phase-field model used in this study is based on the model proposed by Wang and Khachaturyan [14], and the simulation method is based on that proposed by Mamivand et al. [26]. Order parameter (η) is used to describe the microstructure field, and the temporal evolution of η is governed by the TDGL equation:

$$\frac{\partial \eta}{\partial t} = -L\frac{\delta G}{\delta \eta} \tag{1}$$

where L is the kinetic parameter. G is the total free energy of the system, which can be defined as the summation of the chemical free energy (G_{ch}), the gradient energy (G_{gr}), and the elastic strain energy (G_{el}):

$$G = G_{ch} + G_{gr} + G_{el} \tag{2}$$

For the square-to-rectangle transformation, there are two Bain variants. Actually, one order parameter is adequate to express two variants, i.e., $\eta = 0$, $\eta = 1$ and $\eta = -1$ correspond to austenite, variant-1 and variant-2, respectively. To satisfy the symmetry requirement of free energy, the Landau 2-4-6 polynomial is applied to express the chemical free energy [27]:

$$G_{ch} = \int_V \left[\frac{A}{2}\eta^2 - \frac{B}{4}\eta^4 + \frac{C}{6}\eta^6\right] dV \tag{3}$$

where the coefficients are $A = 32\Delta G^*$, $B = 4A - 12\Delta G_m$ and $C = 3A - 12\Delta G_m$. ΔG_m is the thermodynamic driving force, and ΔG^* is the energy barrier.

The gradient energy is expressed as:

$$G_{gr} = \int_V \frac{\beta}{2}(\nabla\eta)^2 dV \tag{4}$$

where β is the gradient energy coefficient, and ∇ is the differential operator. It is assumed that the interfacial energy is isotropic, thus a single and constant gradient energy coefficient is used.

The elastic strain energy can be expressed as:

$$G_{el} = \int_V \frac{1}{2} C_{ijkl}\varepsilon_{ij}^{el}\varepsilon_{kl}^{el} dV \tag{5}$$

where C_{ijkl} is the elastic coefficient tensor. The elastic strain tensor (ε_{ij}^{el}) is defined as the difference between the total strain (ε_{ij}^{t}) and the stress-free transformation strain (ε_{ij}^{0}):

$$\varepsilon_{ij}^{el} = \varepsilon_{ij}^{t} - \varepsilon_{ij}^{0} \tag{6}$$

A first order coupling between transformation strain and order parameter is assumed, based on the non-linear free energy description of SMAs [9,27], as:

$$\varepsilon_{ij}^{0} = \varepsilon_{ij}^{00}\eta \tag{7}$$

where ε_{ij}^{00} is the transformation strain corresponding to $\eta = 1$, and can be given as:

$$\varepsilon_{ij}^{00} = \begin{pmatrix} \varepsilon_3 & 0 \\ 0 & \varepsilon_1 \end{pmatrix} \tag{8}$$

where $\varepsilon_1 = (a_p - a_m)/a_m$ and $\varepsilon_3 = (c_p - a_m)/a_m$. a_m, a_p and c_p are the crystal lattice parameters of the matrix and product phases, respectively. The total strain is expressed as:

$$\varepsilon_{ij}^{t} = \frac{1}{2}\left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i}\right) \tag{9}$$

where u_i is the displacement vector. The elastic stress is evaluated using Hooke's law:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}^{el} \tag{10}$$

According to the above equations, the detailed expression of Eq. (1) is given by [26]:

$$\frac{\partial \eta}{\partial t} = -L\left(-\beta\nabla^2\eta + A\eta - B\eta^3 + C\eta^5 + \frac{\delta G_{el}}{\delta \eta}\right) \tag{11}$$

and

$$\frac{\delta G_{el}}{\delta \eta} = -\frac{1}{2}C_{ijkl}\left\{\varepsilon_{kl}^{00}\left[\frac{1}{2}(u_{i,j} + u_{j,i}) - \varepsilon_{ij}^{00}\eta\right] + \varepsilon_{ij}^{00}\left[\frac{1}{2}(u_{k,l} + u_{l,k}) - \varepsilon_{kl}^{00}\eta\right]\right\} \tag{12}$$

The displacement is obtained by solving the equation of mechanical equilibrium, as:

$$\frac{\partial \sigma_{ij}}{\partial r_j} = 0 \Rightarrow C_{ijkl}\left[\frac{1}{2}(u_{k,lj} + u_{l,kj}) - \varepsilon_{kl}^{00}\frac{\partial \eta}{\partial r_j}\right] = 0 \tag{13}$$

COMSOL Multiphysics [28] based on the finite element method is applied to solve the partial differential equations (PDEs). The dependent variables contain the order parameter (η) and the displacements (u_i). The time-dependent PDE of η (i.e. Eq. (11)) was solved by the implicit backward differentiation formulas, and the gradient term was obtained by using finite-difference approximation. Calculation of displacements, i.e. solving the stationary PDE, Eq. (13), was performed for every step of time. In order to guarantee the convergence, an adaptive time step algorithm was implemented, and the maximum time step was set to be 0.2 s. The