Modelling the essential atomistic influence in the phase transformation dynamics of shape memory materials

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ABSTRACT

A Ginzburg-Landau free energy model of multivariant phase transformation in shape memory alloy has been developed. This paper is focused on linking the developed microscopic model with the atomistic reordering process which finally give rise to self-accommodating microstructure. It is analyzed how the kinetics influences the computation of stress-temperature induced dynamics of phase transformation in microscopic and larger length-scales without attempting to solve a molecular dynamic problem in a coupled manner. A variational approach is adopted and phase transformation in Ni-Al thin film is simulated. The simulations capture a qualitative picture of the onset of microstructure formation.

Keywords: Phase transformation, kinetics, atomistic, free energy, finite element.

1. INTRODUCTION

Shape memory effects in alloys are observed due to the existence of large differences in the variants of the crystal lattice transformation strain tensors.[1] For practical engineering applications of the shape memory effects, thus the understanding of the self-accommodation of the crystallographic variants in a particular geometry under thermomechanical constraints are important and various related problems have been studied over the last three decades with great interests. There are a number of published works which cover the subject in a comprehensive manner and will not be possible to discuss here. Various related discussions can be found on the theoretical aspects (see references[1–6]), on the computational aspects (see references[5, 7–12]) and and also on the experimental aspects (see reference[13]). For micromechanical applications of the shape memory effects, it is essential to understand the evolution of microstructure. Since the process is highly nonlinear, both in terms of the transformation path as well as the geometry, variations in the spatio-temporal loading can produce altogether different microstructures. Related aspects have not been reported much in published literature except few (e.g. tent formation in thin film[14] which has been analyzed only in context of the terminal shape).

Phase transformations in crystalline solids are known to be the results of the atomic reordering. To treat this phenomenon in theory, two somewhat different approaches have been developed over the years. One is based on the physical descriptions, such as the atomic reordering, quantum-mechanical interaction and thermodynamic fluctuation. Since an atomistic simulation with few millions of atoms in a box is too insufficient to study the transformation dynamics in any reasonable scale for engineering applications, renormalization group theory based scaling approaches have been considered to study a relative large system, which extends the present computational capability to the scale of few single crystal domains for shape memory alloys where the deformation of the box itself is significant and needs to be included in the atomistic simulations.[15, 16] A deterministic version of the phase transformation in crystalline solids as a critical phenomenon is often studied by analyzing the phonon branches corresponding to the unstable modes of lattice vibration. An application of this technique to study the stability and hysteresis in shape memory alloys can be found in.[12] Again, such technique is suitable mainly for periodic lattice in single crystals and dealing with general boundary conditions appears difficult. In order to analyze a shape memory alloy sample in the form of wire or thin film, where the macroscopic scale is in the order of centimeter of larger, it appears advantageous to employ variational method where one first defines

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an appropriate energy density and then thermodynamic conservation law. In order to develop a variational method, one requires to describe the non-equilibrium thermodynamics for a particular type of alloys involving entropy changes due to phase transformation. Within the framework of plasticity, one finds such description as a phenomenology (e.g. see [2,17]), where a large number of parameters have to be adjusted considering the dynamics of the phase evolution *a priori*. On the other hand, there is another thermodynamic approach known as Ginzburg-Landau theory, which is microscopic in nature and also requires phenomenology, but with systematic guesses of material parameters. However, for problems in two or more dimensions, here also the number of unknown material parameters become very large and their experimental determinations are often impractical and requires molecular dynamic simulation. Thus, one sees that as the complexities in the model increases, which is indeed expected as one deals with various engineering aspects at the microscale, it becomes increasingly important to account for the small-scale dynamics. In this paper we discuss a Ginzburg-Landau theory and a variational method for finite element simulation of the phase transformation dynamics in Ni-Al thin film, where certain aspects of the atomic reordering process is introduced through the first-order kinetics systematically. Some of the issues related to scales are discussed. Molecular dynamic simulation need not explicitly be coupled in this approach, however scopes remain to do so in a multi-scale framework.

There are three important mathematical and computational issues for reliable numerical simulation of shape-memory alloys, which are (1) an accurate description of the free energy density, its frame-invariance and material symmetry properties,[1,3] (2) prediction of the microstructures[1,10] and their evolutions[5,18,19] and (3) prediction of the thermo-mechanical hysteresis at the macroscopic scale, which is important in the numerical simulation based design of shape-memory alloy devices.[11] A challenging task is thus to meet all of the above objectives systematically in a unified modeling, analysis and computational framework. The computational model is based on a Ginzburg-Landau free energy description, detailed analytical studies of which can be found in.[6,20–22] Various related discussions regarding the application of Landau theory to the first-order martensitic phase transition can be found in.[23] Also, numerical simulations of microstructure due to cubic to tetragonal transformation in thin films based on continuum theory of lattice have been reported,[10] where quadratic polynomials of the strain invariance have been employed to construct the free energy densities separately for the austenite and the martensites.

In order to perform numerical simulations, we have developed a variational framework and a finite element code, where general thermo-mechanical loading can be handled while studying the lattice-based kinetics of the microstructures. Here, the thermodynamic conservation law couples the mechanical deformation, temperature and the order variables. The order variables describe the type of phase (parent austenite phase or a martensitic variant) at a material point. The outline of the paper is the following. In Sec. 3, we summarize the Ginzburg-Landau free energy model, which has been implemented in the variational framework. The variational framework and the finite element formulation are discussed in Sec. 4. Computational issues are discussed in Secs. 5. Numerical results for cubic to tetragonal phase transformation in Ni-Al are reported in Sec 6.

2. ATOMISTIC SCALE INFLUENCE ON MICROSCOPIC MODEL OF PHASE TRANSFORMATION

Phase transformation in shape memory alloys is diffusion-less and first-order in nature, which means the atoms do not migrate but electrons and holes do. Atomic reordering takes place within the length of few lattices in one phase which results in new lattices corresponding to another phase. Let us us consider the molecular dynamic model[15] which accounts for both the atomic coordinate as well as the volume fluctuation of the lattice. The Hamiltonian of the atomic ensemble can be expressed as

$$H = \frac{1}{V} \int_V \left[\frac{1}{2} \sum_i m_i \dot{\boldsymbol{s}}_i^T (\boldsymbol{h}^T \boldsymbol{h}) \dot{\boldsymbol{s}}_i + \frac{1}{2} m' \mathrm{Tr}(\dot{\boldsymbol{h}}^T \dot{\boldsymbol{h}}) + \Phi(r_{ij}, \theta) + p|\boldsymbol{h}| \right] dV \; , \tag{1}$$

where $\boldsymbol{r}_i = \boldsymbol{h}\boldsymbol{s}_i$ denotes the position vector of the ith atom in the ensemble with $\boldsymbol{s}$ as the atomic coordinate with respect to the lattice and the three components of the lattice vector in the columns of $\boldsymbol{h}$. In Eq. (1), the first two terms represent the momentum, the third term represents the potential involving the electron density and

the core-core repulsion, and the last term represents the work done due to pressure. The equations of motion for the atom i can be expressed as

$$\ddot{\boldsymbol{s}}_i = -\sum_{j\neq i} m_i^{-1} \frac{1}{r_{ij}} \frac{\partial \Phi(r_{ij},\theta)}{\partial r_{ij}}(\boldsymbol{s}_i - \boldsymbol{s}_j) - (\boldsymbol{h}^T\boldsymbol{h})^{-1}\left[\frac{\partial}{\partial\tau}(\boldsymbol{h}^T\boldsymbol{h})\right]\boldsymbol{s}_i \ , \tag{2a}$$

$$\ddot{\boldsymbol{h}} = m'^{-1}(\boldsymbol{\sigma} - \boldsymbol{p})|\boldsymbol{h}|(\boldsymbol{h})^{-1} \ , \tag{2b}$$

where $\boldsymbol{\sigma}$ is the stress tensor, θ is the temperature and τ denotes time in the atomistic scale dynamics. Integrating Eq. (2a) over the characteristic time τ_0 and with the help of Eq. (2b), we obtain the equation for kinetics where the contribution of the free surfaces and domain walls are not included. It can be stated that the phase transition occurs within the time interval τ_0 and the atomic coordinate relative to the lattice changes from $\boldsymbol{s}(0)$ to $\boldsymbol{s}(b\tau_0)$, $b > 1$. $\boldsymbol{s}(0)$ can be expressed in terms of the lattice constants of the parent phase (austenite phase) and $\boldsymbol{s}(b\tau_0)$ can be expressed in terms of the lattice constants of one of the transformed phase (martensite phase). Intermediate or diffused phase may exist which are unstable and may lead to deffects and dislocations. We now consider a control volume $\bar{V} = V^q$, $q \leq 1$ and define the vector $\eta(t)$, $t = b\tau$, $b > 1$ of the order variables such that

$$\dot{\boldsymbol{\eta}} = \left\langle \frac{1}{b\tau_0}\int_t^{t+b\tau_0} \dot{\boldsymbol{s}}_i d\tau \right\rangle_{\bar{V}} \ , \tag{3}$$

where the Poisson bracket indicates ensemble average of the quantity within the control volume $\bar{V}$. We use the vector $\boldsymbol{\eta}$ of order variables to introduce phase transition in our free energy model.

3. GINZBURG-LANDAU FREE ENERGY MODEL

We denote the order variables $\eta_k \in [0,1]$, where $k = 1,\cdots,N$ indicates the number of martensitic variants, $\eta_k = 0$, $\forall k$ defines the austenite and $\eta_k = 1$, $\eta_j = 0$, $k \neq j$ defines the kth martensitic variant at a material point. According to the point group of crystallographic symmetry, only one variant of martensite is allowed to exist at a material point. Denoting the vector of the order variables as $\boldsymbol{\eta} = \{\eta_1,\cdots,\eta_N\}^T$, the Gibbs free energy density is defined as $G(\boldsymbol{\sigma},\theta,\boldsymbol{\eta})$. Here $\boldsymbol{\sigma}$ is the stress tensor, θ is the temperature. The finite strain tensor $\boldsymbol{\varepsilon}$ is decomposed into the elastic part and the transformation-induced part as

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_{\text{el}} + \sum_{k=1}^{N} \boldsymbol{\varepsilon}_k^t \varphi(\eta_k) \ , \tag{4}$$

where $\varphi(\eta_k)$ is a polynomial in η_k and $\boldsymbol{\varepsilon}_k^t$, $k = 1,\cdots,N$ are the transformation strain tensors[1] obtained by experiments. The structure of the initially unknown polynomial $\varphi(\eta_k)$ is such that it satisfies the following two conditions.

$$\varphi(0) = 0 \ , \quad \varphi(1) = 1 \ . \tag{5}$$

The frame-invariance property of the free energy density is imposed by the polynomial structure in η_k such that interchanges between two indices produce identical structure of the free energy, i.e.,

$$G(\boldsymbol{\sigma},\theta,\eta_i,\eta_j) = G(\boldsymbol{\sigma},\theta,\eta_j,\eta_i) \ . \tag{6}$$

Material symmetry under proper rotation of the lattice vector is preserved due to the decomposition in Eq. (4), which can be easily proved for isotropic and homogeneous crystals. Gibbs free energy density then takes the following form.

$$G(\boldsymbol{\sigma},\theta,\boldsymbol{\eta}) = -\frac{1}{2}\boldsymbol{\sigma} : \left[\boldsymbol{\lambda}_0 + \sum_{k=1}^{N}(\boldsymbol{\lambda}_k - \boldsymbol{\lambda}_0)\varphi(\eta_k)\right] : \boldsymbol{\sigma} - \boldsymbol{\sigma} : \sum_{k=1}^{N}\boldsymbol{\varepsilon}_k^t\varphi(\eta_k)$$

$$-\boldsymbol{\sigma} : \left[\boldsymbol{\varepsilon}_{\theta 0} + \sum_{k=1}^{N}(\boldsymbol{\varepsilon}_k^\theta - \boldsymbol{\varepsilon}_0^\theta)\varphi(\eta_k)\right] + \sum_{k=1}^{N}f(\theta,\eta_k) + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}F_{ij}(\eta_i,\eta_j) \ , \tag{7}$$

where $\boldsymbol{\lambda}_k$ is the second-order forth-rank compliance tensor for the kth martensitic variant (M_k phase), $\boldsymbol{\lambda}_0$ is for austenite phase (A phase), $\boldsymbol{\varepsilon}_0^\theta = \boldsymbol{\alpha}_0(\theta - \theta_e)$, $\boldsymbol{\varepsilon}_k^\theta = \boldsymbol{\alpha}_k(\theta - \theta_e)$. θ_e is the temperature at which the stress-free martensite losses stability. $\boldsymbol{\alpha}_0$ and $\boldsymbol{\alpha}_k$ are the thermal expansion tensors for A and M_k phases, respectively. $f(\theta, \eta_k)$ is the chemical part of the free energy of the M_k phases and assumed in the form of a polynomial which is to be determined. F_{ij} is an interaction potential required to preserve the frame-invariance of G with respect to the point group of symmetry and uniqueness of the multivariant phase transformation at a given material point. The description of the order variables can now be generalized with three sets of order parameters: $\bar{0} = \{0, \eta_k = 0, 0\}$ for A phase, $\bar{1} = \{0, \eta_k = 1, 0\}$ for M_k phase and $\bar{\eta}_k = \{0, \eta_k, 0\}$, $\eta_k \in (0, 1)$ for diffused $A - M_k$ interface. The role of the first-order kinetics in the order variables is to assist in reaching the bottom of the energy well, i.e.,

$$\frac{\partial G}{\partial \eta_k} = 0 , \quad \boldsymbol{\eta} = \bar{0}, \bar{1} , \tag{8}$$

$$\frac{\partial^2 G}{\partial \eta_k^2} \le 0 , \quad \boldsymbol{\eta} = \bar{0} \quad (A \to M_k) \tag{9}$$

$$\frac{\partial^2 G}{\partial \eta_k^2} \le 0 , \quad \boldsymbol{\eta} = \bar{1} \quad (M_k \to A) \tag{10}$$

The transformation energy associated with $A \leftrightarrow M_k$ transformation is

$$G(\boldsymbol{\sigma}, \theta, \bar{0}) - G(\boldsymbol{\sigma}, \theta, \bar{1}) = \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_k^t - \Delta G^\theta , \tag{11}$$

where ΔG^θ is the jump in the free energy due to to phase transformation. With the help of Eqs. (5)-(11), we determine $\varphi(\eta_k)$ and $f(\theta, \eta_k)$ (see[21] for the details). According to Landau theory, for example, a quadratic polynomial in strain components can be adequate to describe the free energy for cubic to tetragonal transformation. Therefore, following Eq. (4) one finds that for cubic to tetragonal transformation, the interaction potential can have the following form (see[20] for the details)

$$F_{ij} = \eta_i \eta_j (1 - \eta_i - \eta_j) \left[B \left\{ (\eta_i - \eta_j)^2 - \eta_i - \eta_j \right\} + D\eta_i \eta_j \right] + \eta_i^2 \eta_j^2 (\eta_i Z_{ij} + \eta_j Z_{ji}) \tag{12}$$

where the material constants B and D are obtained by experiments or numerical estimation. The matrix elements Z_{ij} are obtained as functions of the constants B and D and an energy scale factor in $f(\theta, \eta_k)$.

3.1. Thermodynamic conservation

Note that a jump in the free energy ΔG^θ has been introduced in Eq. (11). The consequence of this jump, as well as the jump in the total strain across the $A - M_j$ interface, is the thermodynamic forcing as a source of dissipation. The forcing term would eventually be balanced by the kinetic force. Therefore, one has to establish a link between the evolution of the phases and the non-negativity of the thermodynamic potential (Helmholtz free energy). This is unlike the notion in plasticity-based framework (see e.g.[2]), where the nonnegativity of the rate of phase fraction is directly enforced.

For the present problem, the kinetic equation is derived by balancing the thermodynamic force with the kinetic force as

$$C\frac{\partial \eta_k}{\partial t} + \frac{\partial G'}{\partial \eta_k} = 0 , \tag{13}$$

where C is a constant and $G' = G + \tilde{G}(\nabla \boldsymbol{\eta})$ describes the modified Gibbs free energy including the gradient terms to account for the non-local nature of the interface energy. By rearranging Eq. (13) and expanding the forcing terms, we get the Ginzburg-Landau equation for phase kinetics, which is given by

$$\frac{\partial \eta_k}{\partial t} = -\sum_{p=1}^{N} L_{kp} \left[\frac{\partial G}{\partial \eta_p} + \boldsymbol{\beta}_p : \nabla \nabla \eta_p \right] + \theta_k , \tag{14}$$

where L_{kp} are positive definite kinetic coefficients, $\boldsymbol{\beta}_p$ are positive definite second rank tensor. θ_k is the thermal fluctuation satisfying the dissipation-fluctuation theorem. From the time integrated form of Eq. (2a), one finds that

$$L_{kp} \approx \tau_0 \sum_{i \neq j} \frac{|\boldsymbol{s}_i^0 - \boldsymbol{s}_j^0|}{m_i r_{ij} |\boldsymbol{h}|} \ . \tag{15}$$

Eq. (14) is complemented by the macroscopic conservation law

$$\frac{\partial}{\partial t} \left[\mathcal{W} - \theta \frac{\partial \mathcal{W}}{\partial \theta} \right] - \boldsymbol{\nabla} \cdot (\boldsymbol{\sigma} \cdot \dot{\boldsymbol{u}} - \boldsymbol{q}) = h_\theta \ , \tag{16}$$

and the momentum balance equation

$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} + \boldsymbol{p} \ , \tag{17}$$

where $\mathcal{W}$ is the Helmholtz free energy given by

$$\mathcal{W} = G + c_v \theta + \frac{1}{2} \boldsymbol{\sigma} : \left[\boldsymbol{\lambda}_0 + \sum_{k=1}^{N} (\boldsymbol{\lambda}_k - \boldsymbol{\lambda}_0) \varphi(\eta_k) \right] : \boldsymbol{\sigma} + \boldsymbol{\sigma} : \left[\boldsymbol{\varepsilon}_{\theta 0} + \sum_{k=1}^{N} (\boldsymbol{\varepsilon}_{\theta k} - \boldsymbol{\varepsilon}_{\theta 0}) \varphi(\eta_k) \right] \ , \tag{18}$$

$\boldsymbol{q}$ is the heat flux, h_θ is the heat source and $\boldsymbol{p}$ is the body force.

4. VARIATIONAL FRAMEWORK AND FINITE ELEMENT DISCRETIZATION

We relate the elastic part of displacements to the elastic strain $\boldsymbol{\varepsilon}_{\text{el}}$ via the linear strain-displacement relation, i.e. $\boldsymbol{\varepsilon}_{\text{el}} = ((\nabla \boldsymbol{u}) + (\nabla \boldsymbol{u})^T)/2$. It is now obvious that the order variables $\eta_k, k = 1, \cdots, N$ are to be treated as internal variables in the variational formulation. We want to interpolate the fields $\boldsymbol{u}(x, y, z, t)$, $\theta(x, y, z, t)$ and $\eta_k(x, y, z, t)$ over the domain $\Omega(x, y, z) \subset R^3$ with Lipschitz continuous boundary $\partial \Omega$ such that the control volume $\bar{V}$ of interest in context of the ensemble averaging in Eq. (6) satisfy the relation diam.$(\Omega)^3 = \bar{V}$. We are interested in fixed-order finite elements with h-refinement. We consider the Lagrangian isoparametric interpolation function $\boldsymbol{N}$,

$$\{u_1 \ u_2 \ u_3\}^T = \boldsymbol{N}_u \boldsymbol{v}^e \ , \quad \theta = \boldsymbol{N}_\theta \boldsymbol{v}^e \ , \quad \eta = \boldsymbol{N}_\eta \boldsymbol{v}^e \ , \tag{19}$$

$$\boldsymbol{v} = \{u_1 \ u_2 \ u_3 \ \theta \ \eta_1 \ , \cdots , \eta_n\}^T \ . \tag{20}$$

Here, the superscript e indicates element nodal quantities. Introducing admissible weights $\{\bar{u}_i, \bar{\theta}, \bar{\eta}_k\}$ chosen from the linear span of $\boldsymbol{v}^e$, the variational formulation of the problem can be stated as follows

$$\delta \Pi = \delta \Pi_{\text{PT}} + \delta \Pi_\theta + \delta \Pi_u + \delta W = 0 \ , \quad t \in [0, +\infty] \tag{21}$$

where

$$\delta \Pi_{\text{PT}} = \int_\Omega \sum_{k=1}^{N} \delta \bar{\eta}_k \left[\frac{\partial \eta_k}{\partial t} - \theta_k \right] \mathrm{d}\mathbf{x} + \int_\Omega \sum_{k=1}^{N} \sum_{p=1}^{N} \delta \bar{\eta}_k \left[L_{kp} \left(\frac{\partial G}{\partial \eta_p} + \boldsymbol{\beta}_p : \boldsymbol{\nabla} \boldsymbol{\nabla} \eta_p \right) \right] \mathrm{d}\mathbf{x}$$

$$- \int_{\partial \Omega} \sum_{k=1}^{N} \sum_{p=1}^{N} \delta \bar{\eta}_k L_{kp} \frac{\partial G}{\partial \eta_k} \mathrm{d}s(\mathbf{x}) \ , \tag{22}$$

$$\delta \Pi_\theta = \int_\Omega \delta \bar{\theta} \left[\frac{\partial}{\partial t} \left(\mathcal{W} - \theta \frac{\partial \mathcal{W}}{\partial \theta} \right) - \boldsymbol{\nabla} \cdot (\boldsymbol{\sigma} \cdot \frac{\partial \boldsymbol{u}}{\partial t}) \right] \mathrm{d}\mathbf{x}$$

$$+ \int_\Omega \delta \bar{\theta} \left[\boldsymbol{\nabla} \cdot \left(-\kappa \boldsymbol{\nabla} \theta - \alpha' \kappa \boldsymbol{\nabla} \frac{\partial \theta}{\partial t} \right) \right] \mathrm{d}\mathbf{x} - \int_{\partial \Omega} \delta \bar{\theta} \boldsymbol{q}_\perp \mathrm{d}s(\mathbf{x}) \ , \tag{23}$$

$$\delta \Pi_u = \int_\Omega \delta \bar{\boldsymbol{u}}^T \left[\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} \right] \mathrm{d}\mathbf{x} - \int_{\partial \Omega} \delta \bar{\boldsymbol{u}}^T \boldsymbol{\sigma}_\perp \mathrm{d}s(\mathbf{x}) \ , \tag{24}$$

and W is the external work done over the sample. Integrating Eq. (21) by parts we obtain the finite element approximation

$$M\frac{\partial^2 v}{\partial t^2} + D(v)\frac{\partial v}{\partial t} + K(v)v = f \; , \tag{25}$$

with initial state and microstructure

$$v(t) = v(0) \; , \quad \frac{\partial}{\partial t}v(t) = 0 \; . \tag{26}$$

We solve the time discretized version of the nonlinear system of equations in Eq. (25) by Newton iteration along with the stability conditions in Eqs. (9)-(10).

5. KINETICS AND MULTIPLE SCALES

The problem of simulating the microstructure in shape memory alloys is well discussed in literature. While simulating the macrosopic deformation under dynamic loading, resolving the sharp interfaces and the dendritic microstructure with multiscale features are some of the computational difficulties that need to addressed. The approach presented in this paper, which accounts for the atomic reordering in its ensemble average form is one way to resolve the fine-scale dynamics and obtain the sharp interfaces at a microscopic scale. At the microscopic scale, a smoothed version of the transformation conditions in Eqs. (8)-(10) leads to the time-dependent Ginzburg-Landau phase kinetics, where the fast time scale has to be controlled depending on the global time stepping (in slow time scale) in the finite element time integration. Note that η_k represents the reordering of the atomic ensemble in a box. Choice of the length-scale for defining this box can be arrived at by applying a finite-difference scheme to the phase kinetic equation. Thus, it becomes eventually clear that the chosen time scale for the kinetics dictates the limit to the coarse graining of η_k. This in turn restricts the order of interpolation for a given size of the finite element. Since the elastic part of the strain is defined in the lattice coordinate for the current phase, special care is necessary to ensure continuity of elastic strain and hence displacement within that phase. For example, if linear interpolation is used for displacement and there exist a number of elements having same phase connected to a finite element node, then we average out the displacement for that particular node. For higher-order interpolation, this is not necessary, except when additional intermediate nodes are used in an element for interpolation of η_k.

6. NUMERICAL SIMULATIONS

For numerical simulation, we consider an effectively two-dimensional domain of rectangular shape. Ni-Al which undergoes cubic to tetragonal transformation is considered. There are three tetragonal martensitic variants in this case and $N = 3$. The transformation strain tensors for these three variants are, respectively,

$$\varepsilon_1^t = \begin{pmatrix} \gamma & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix} \; , \quad \varepsilon_2^t = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \gamma & 0 \\ 0 & 0 & \alpha \end{pmatrix} \; , \quad \varepsilon_3^t = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \gamma \end{pmatrix} \; , \tag{27}$$

where the transformation stretches are given by

$$\alpha = \frac{a}{a_0} \; , \quad \gamma = \frac{c}{a_0} \; , \tag{28}$$

with a_0 as the lattice constant for the high temperature austenite phase and a, c are the lattice constants for the low temperature martensite phases. By solving a differential algebraic problem, the free energy is obtained with the following polynomial structure in η_k.

$$\phi(\eta_k) = 3\eta_k^2 - 2\eta_k^3 \; . \tag{29}$$

The chemical part of the free energy then takes the following form

$$f(\theta, \eta_k) = \left(\Delta G^\theta + \frac{G_0}{12}\right)\phi(\eta_k) + G_0\left(\frac{1}{4}\eta_k^4 - \frac{1}{3}\eta_k^3\right) \; , \tag{30}$$

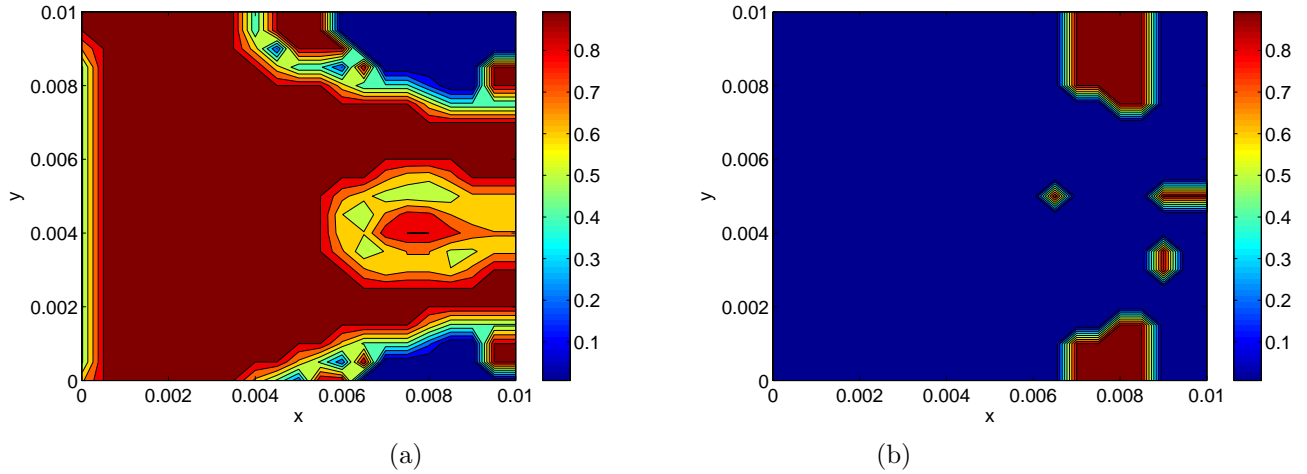**Figure 1.** Contours of the martensitic variants (a) η_1 and (b) η_2 during nucleation from the right edge at the first one-fourth of the loading cycle ($t = 25ms$).

where

$$\Delta G^\theta \approx (-\Delta s^e + \Delta c)(\theta - \theta^e) \,, \tag{31}$$

$$G_0 = A_0 \Delta s^e (\theta^e - \theta^c) \,, \quad A_0 \leq -12 \left(\frac{\Delta c}{-\Delta s^e} + 1 \right) \,, \tag{32}$$

where $\Delta G^\theta(\theta_e) = 0$, θ_e is the equilibrium temperature, $\theta^c > \theta_e$ is the critical temperature for transformation under the applied thermo-mechanical loading, Δc is jump in the specific heat capacity during transformation, $-\Delta s^e > 0$ is the jump in the specific entropy at equilibrium temperature. The value of the constant A_0 is to be estimated from experimental hysteresis curve and it is likely to depend on the loading rates and various additional inelastic effects which are inherent in a single crystal and more significantly in polycrystal sample. For the following numerical simulations, the material properties are taken from reference.[20] The film is subjected to $5Hz$ sinusoidal stress applied in longitudinal direction throughout one of its edge. The opposite edge is fully restrained. The stress distribution over the edge has triangular shape. The other two parallel edges of the film are kept free. Constant temperature of $300K$ with cubic phase (austenite) is assumed to be the initial state. Fig. 1(a) and (b) respectively shows the nucleated tetragonal phases η_1 and η_2 near the stressed right edge of the film. The results shown here provides a qualitative picture of the phase transformation and onset of microstructure formation. Further studies with refined finite element meshes are required to capture various small-scale features in the dynamics. From Fig. 2 it can be seen that the transformation front (sharp peaks in the strain) moves toward the right edge first and then moves backward as the edge is unloaded. The snap at $t = 25ms$ in Fig. 1(a) indicates $\eta_1 \to 1$ near the fully restrained left edge, and $\eta_2 \to 1$ near the free corners near the y-parallel edges.

7. CONCLUSIONS

An approach to couple the atomistic scale dynamics with the microscopic kinetics based model of phase transformation in shape memory alloys is reported in this paper. A Ginzburg-Landau free energy description is employed in a variational framework to simulate cubic to tetragonal phase transformation in thin film under mechanical loading. Several issues related to characterization of multivariant phase transformation under dynamic loading remain open. However, the computational model reported here is one step forward to combine numerical simulation with experiments to characterize various properties of multivariant phase transformation. The results shown here provides a qualitative picture of the phase transformation and onset of microstructure formation. Further studies with refined finite element meshes are required to capture various small-scale features in the dynamics.
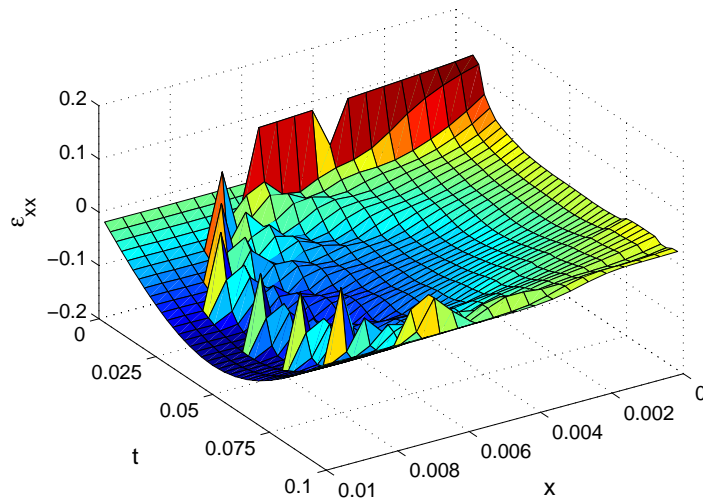
Figure 2. Time histrory of longitudinal strain ε_{xx} along the line $y = 0$.

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