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Dynamics of Multivariant Phase Transformation in Shape Memory Materials: A Microscopic Theory to Device-Scale Simulation

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ABSTRACT

Dynamics of Phase Transformation (PT) in Shape Memory Alloys (SMAs) under the combined effect of stress and temperature is one of the most complex and intriguing phenomena, which is far from completely tractable till date. Propagation of the transformation fronts as they are spontaneously formed and diffused under constraints in the macroscopic structure is one of the important aspects that influence the performance of SMAs as sensors and actuators. The initial state, the transients and the characteristics of stress and the thermal cycles play important roles in the device performance. Investigation of these aspects using crystallographic framework of the constituent materials, and subsequently, tackling the complexities in carrying out numerical simulation in the physical scales constitutes the main theme of this paper. Three-dimensional Gibbs free-energy is derived by consistent partitioning the chemical energy and the transformation energy. In order to perform the time-resolved analysis of real SMA device having truly three-dimensional geometry, a 3D nonlinear finite element model is developed and a large-scale computational scheme is proposed. The variational framework couples (1) the momentum balance (2) the heat conduction and (3) the first-order phase kinetics. Numerical validation of this newly developed microscopic model is reported using a NiAl sample.

Keywords: Shape memory alloys, Phase transformation, Martensitic variants, Thermoelasticity, Landau Theory

1. INTRODUCTION

Shape Memory Alloys (SMAs) are known to have various proven applications in transducer devices and in control of dynamical systems. However, given the availability of numerous phenomenological models, design and analysis involving new SMA structures are found to be extremely difficult task. These phenomenological models vary drastically depending on material constants, conditions at which experiments are done, effective dimension and size of the sample and the nature of thermo-mechanical loading. A deep mathematical understanding on the origin of the SMA microstructure under deformation has been developed over past few decades (see e.g. [1-7]), and computational challenges encountered while applying related theory has been reviewed recently in [8]. It has been pointed out in [8] that the sequence of minimization process over a set of austenite-martensite energy wells gives rise to the observed microstructure having precise analytical description. In macroscopic scale, these local deformations, which are equivalent to transformation of Austenite (A) to variants of Martensite (M) and the reverse transformation, give rise to the shape-memory effect. However, not much development has taken place till date in which the three-dimensional and time-dependent dynamics of the real-scale SMA devices could be studied by linking the above theoretical framework to practical engineering applications. The main difficulties encountered to achieve this is mainly numerical and in the underlying interdependence of following two aspects: (1) the sequence of energy minimization, at the end of which the global minimum is actually *not attained* under the prescribed dynamic loading and macroscopic constraints, the discrete version of this process is called *quasi-convexification* of the original non-convex minimization problem (2) the conditions required to match the spatial discretization with the evolved

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interfaces dynamically, meaning an efficient implementation of a mesh adaptation scheme within the variational framework (e.g. adaptive finite elements).

In context of resolving the phase transformation dynamics in 3D, the main challenge is as follows. Most of the available phenomenological models are applicable in macroscopic and mesoscopic scales. A macroscopic model requires the description of the 3D geometry and variational minimization of an appropriate potential involving the thermoelastic energy and the energy due to dynamic self-accommodation of the martensitic variants. Whereas a mesoscopic model, such as the Falk-Kanopka free energy model [9], requires the description of the free energy as a function of the strain invariants of a single crystal and its point group symmetry. The strain field in such model is beyond the resolution of bain strain. A more detailed description of the PT requires a microscopic model, such as the model by Levitas and Preston [10], where the invariance of the free energy with

$$G(\eta) = -\boldsymbol{\sigma} : \boldsymbol{\lambda} : \boldsymbol{\sigma} / 2 - \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_{\mathbf{t}} \varphi(\eta) + f(\theta, \eta), \tag{1}$$

where $\boldsymbol{\lambda}$ is the constant fourth-rank elastic compliance tensor, $\boldsymbol{\varepsilon}_{\mathbf{t}}$ is the transformation strain tensor at the thermodynamic equilibrium of the martensite (obtained from crystallography), $\varphi(\eta)$ is a monotonic function with $\varphi(0) = 0$ indicating stable A phase and $\varphi(1) = 1$ indicating stable M phase. $f(\theta, \eta)$ is the chemical part of the free energy with property: $f(\theta,1) - f(\theta,0) = \Delta G^{\theta}(\theta)$, where ΔG^{θ} is the difference between the thermal parts of the Gibbs free energy density of the M and A phases, which can be obtained indirectly from experiments through the relation [21]

$$\Delta G^{\theta} = -\Delta s_e(\theta - \theta_e) - \Delta c\theta[\ln(\theta / \theta_e) - 1] - \Delta c\theta_e, \tag{2}$$

where Δc is the difference between the specific heat of the phases, Δs_e is the jump in the specific entropy at the equilibrium temperature (θ_e). The objective is to obtain the unknown functions φ and

4. A VARIATIONAL FRAMEWORK

We have so far described the phase transformation by the order parameters ($\eta_k, k = 1,\mathrm{K}, N$). The physical implication is that the statistical ensemble of the order variables (the state of the constituent atoms) is expressed in a spatially homogenized sense where their correlation in the atomistic length scale is approximated by ensemble average. The transformation kinetics can be written in the form of Ginzburg-Landau equation, where the coefficients in the first-order system are related to the ensemble aggregate of the atomistic reordering. Most interestingly this kinetics plays the main role in controlling the coupling between the thermodynamic conservation law and the momentum balance. In our study, we have analyzed the governing system of partial differential equations (PDEs) obtained from the present model, and these PDEs dynamically switch their characteristics at the onset of transformation spanned over a significantly smaller time-scale compared to the time scale of the SMA device dynamics. It poses one of the most challenging problems in computational mathematics. It has been suggested in [8] that one way to avoid the inherent ill-poseness of the computational version of the energy minimization problem is to relax the error-estimates. In our study, the additional difficulty is the fast time scale at which the transformation occurs. One possibility is to develop a singular perturbation scheme within the finite element framework. In the following sections we focus our discussion on developing a discrete version of the problem. Resolving the temporal events at the atomistic scale remains a future issue.

We first write the governing system of partial differential equations as follows. The transformation kinetics is represented by the Ginzburg-Landau equation

$$\frac{\partial \eta_k}{\partial t} = -\sum_{k=1}^{N} \mathbf{L}_{kp} \left[\frac{\partial G}{\partial \eta_p} + \boldsymbol{\beta}_p : \nabla\nabla \eta_p \right] + \theta_k \tag{17}$$

where $\mathbf{L}_{kp}$ 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 arising in context of non-equilibrium thermodynamics. While Eq.(17) governs the evolution process, the macroscopic energy conservation law is governed by the heat conduction

$$\frac{\partial H}{\partial t} - \nabla.(\boldsymbol{\sigma}.\frac{\partial \mathbf{u}}{\partial t} + \mathbf{q}) = h_\theta \tag{18}$$

4.1 Spatial Discretization

We interpolate the fields $u(x,y,z,t)$, $\theta(x,y,z,t)$ and $\eta_k(x,y,z,t)$, $k=1,\mathrm{K},N$ using non-conforming finite element and *h*-refinement. This is an established scheme for modeling SMA microstructure [18]. Noting that all the three governing equations have highest order of spatial derivative as two, we choose the standard Lagrangian isoparametric interpolation function $\mathbf{N}$,

$$\{u_1 \quad u_2 \quad u_3\}^T = \mathbf{N}_u \mathbf{v}^e, \qquad \theta = \mathbf{N}_\theta v^e, \qquad \eta = \mathbf{N}_\eta \mathbf{v}^e \tag{20}$$

$$\mathbf{v} = \{u_1 \quad u_2 \quad u_3 \quad \theta \quad \eta_1 \quad \Lambda \quad \eta_n\} \tag{21}$$

Here, the superscript 'e' indicates element nodal quantities. Introducing admissible weights ($\overline{u}_i$, $\overline{\theta}$, $\overline{\eta}_k$) chosen from the linear span of $\mathbf{v}^e$, a variational statement can be posed as

$$\delta\prod = \delta\prod_{PT} + \delta\prod_\theta + \delta\prod_u + \delta V = 0, \qquad t \in [0,+\infty] \tag{22}$$

where

$$\delta\prod_{PT} = \int_\Omega \sum_{k=1}^N \delta\overline{\eta}_k \left[\frac{\partial \eta_k}{\partial t} - \theta_k\right] \mathrm{d}\mathbf{x} + \int_\Omega \sum_{k=1}^N \sum_{p=1}^N \delta\overline{\eta}_k \left[\mathbf{L}_{kp}\left(\frac{\partial G}{\partial \eta_p} + \boldsymbol{\beta}_p : \nabla\nabla\eta_p\right)\right] \mathrm{d}\Omega \tag{23}$$

$$\delta\prod_\theta = \int_\Omega \delta\overline{\theta}\left[\frac{\partial H}{\partial t} - \nabla.(\boldsymbol{\sigma}.\frac{\partial \mathbf{u}}{\partial t} + \mathbf{q}) - h_\theta\right] \mathrm{d}\Omega \tag{24}$$

$$\delta\prod_u = \int_\Omega \delta\overline{\mathbf{u}}.\left[\rho\frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla.\boldsymbol{\sigma} - \mathbf{p}\right] \mathrm{d}\Omega \tag{25}$$

and *V* stands for the external work done plus the boundary integral terms. Integrating Eqs.(31) by parts and applying divergence theorem, we construct our discrete version of the finite element model.

4.2 Computational Scheme

We implement the finite element model with the associated Dirichlet boundary conditions and the initial conditions in a general three-dimensional finite element code. For the present problem we use 8-node, 7 d.o.f/node hexahedral element with tri-linear isoparametric interpolation and reduced Gauss-quadrature integration for shear terms. A second order time integration scheme has been employed. We use additional controlling parameter which reduces the integration rule for parabolic part of the governing PDEs to explicit scheme. Ensuring numerical stability for such a strongly coupled problem is not clearly understood at present and further investigation is needed. In context of viscoplasticity, the stability issues while using a generalized mid-point rule (first-order accurate) has been discused in [23]. Extension of such analysis with higher-order scheme for the present problem may be needed, since the solid-state transformation process is spontaneous in nature and the associated rates varies over wide range which makes the problem far more complex than continuum elasto-plasticity.

A major complexity arises in nonlinear iteration. Note that the energy minimization process can take a different and unphysical path unless the phase transformation conditions are enforced in a consistent manner in the incremental algorithm. Following steps have been adopted:

Step 1: With the known matrices and vectors obtained from the time step $t = t_i$, compute the stress and and transformation barrier.

Step 2: Check the loss of stability $\mathrm{A} \to \mathrm{M_k}$ for all *k*. Obtain the increment $\Delta\eta_k$ by satisfying consistency condition in the neighborhood of the transformation surface (similar to the return mapping algorithm for elasto-plasticity [23]).

Step 3: Compute the consistent tangent matrix $[K]_t$. Here the effective internal force vector has three parts:

$$\{\mathbf{b}\} = \left\{\{\mathbf{f}\}_u^T \quad \{\mathbf{f}\}_\theta^T \quad \{\mathbf{f}\}_\eta^T\right\}^T$$

$$f_{uj} = \frac{\partial\prod_u}{\partial u_j}, \quad f_{\theta j} = \frac{\partial\prod_\theta}{\partial\theta}, \qquad f_{\eta k} = \frac{\partial\prod_{PT}}{\partial\eta_k}$$

The incremental update at *n*th iteration is obtained as

$$\{\Delta \mathbf{v}\}_{n+1}^{e} = -[\mathbf{K}]_{t}^{-1}\left(\{\mathbf{b}\}_{n+1}^{\text{int}} - \{\mathbf{b}\}_{n+1}^{ext}\right) \tag{26}$$

Eq.(26) is then solved by Newton iteration until a specified convergence is achieved.

Step 4: Compute the updated vectors, velocity and acceleration and move to next time step $t_{i+1} = t_i + \Delta t$.

5. NUMERICAL SIMULATION

Here we consider stress-induced cubic to tetragonal transformation in NiAl under longitudinal harmonic stress of amplitude 160MPa and frequency 5Hz applied at one edge of a $100\text{mm} \times 50\text{mm} \times 100\ \mu\text{m}$ film. The film is assumed to be restrained at the edge ($x = 0$). The surfaces are assumed to be in ambient environment ($\theta = 298K$), $\theta_e = 215K$. Three martensitic variants are possible during cubic to tetragonal transformation. In the present example, the film domain is such that the formation of single variants along the span of the film is interest.

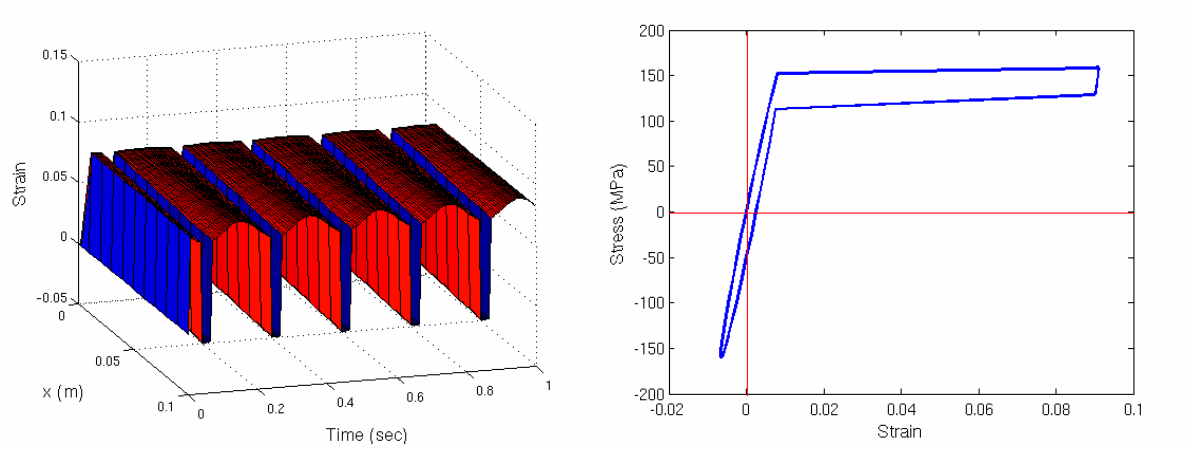

Fig. 1. (a) Strain history over the length of the film (b) dynamic stress-strain curve at the loaded edge of the film.

Fig. 1(a) shows the time history of longitudinal strain ε_{xx} over the length of the film. The transformation induced large strains around the tensile peaks of the loading can be seen, which is with same period as the applied loading. Austenitic wells are formed periodically during stress reversal. Fig. 1(b) shows the stress-strain hysteresis cycle which is recovered from our stress-space energy representation. A recoverable strain of nearly 8% can be seen which is consistent with the experimental observation in NiAl.

6. CONCLUSIONS

A Landau-Ginzburg free energy model and a computational framework to analyze the multivariant martenstic phase transformation is developed. The free energy is described in such a way that the transformation surfaces can be characterized with minimum number of material constants from experiments or molecular dynamic simulations. We arrive at the precise mathematical description of the austenite-martensite transformation energy barrier. The model is a general one and can be applied to various types of shape memory alloys. In this model the first-order diffusion kinetics below the scale of microstructue actually controls the nonlinear thermoelasticity at the macroscopic scale. In context of solving a discrete version of the energy minimization problem, the main advantage here is that the finite element mesh need not be adapted by tracking the A-M_k or M_k-M_j interfaces, instead the order parameters (η_k) can be updated from the equivalent deformation gradient for compatible microstructure in a point-wise sense. Based on the proposed model and computational scheme, several possibilities in complex design optimization of SMA actuator can be explored which is an open areas of research.

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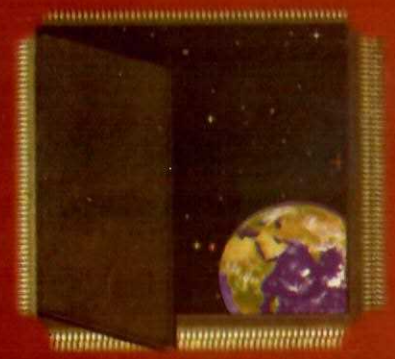

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