A Dynamic Model for Phase Transformations in 3D Samples of Shape Memory Alloys

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Abstract. Despite recent progress in modelling the shape memory alloy (SMA) behaviour, many difficulties remain due to various limitations of the existing free energy models and strong nonlinearity of these nonlinear materials. Phase kinetics of SMA coupled with thermoelastodynamics is still not fully tractable, and one needs to deal with complicated multiscale character of SMA materials requiring a linkage between their microstructure and macroscopic properties. In this paper we develop a new dynamic model of 3D SMA which employs an improved version of the microscopic Landau theory. Essential properties of the single and multivariant martensitic phase transformations are recovered using consistent steps, which eliminates the problem of non-uniqueness of energy partitioning and relaxes the over-sensitivity of the free energy due to many unknown material constants in previously reported models. We exemplify our results on a model for cubic to tetragonal transformations in a rectangular SMA bar by showing key algorithmic steps which can be extended to more complex cases.

1 Introduction

Modelling of dynamics of phase transformations (PT) in Shape Memory Alloys (SMAs) under the combined effect of stress and temperature is one of the most challenging problems in computational science and engineering. Our better understanding of such dynamics can be achieved with multi-physics multiscale models which assist the researchers in designing new materials and devices by harnessing the shape memory effect. Phenomenological framework based on Landau theory of martensitic transformations (e.g., [1]) has become a convenient choice for basic building blocks in the computational models. However, most of the phenomenological models are applicable at macroscopic and mesoscopic scales as discussed in [2], and the strain field in such model is often beyond the resolution of bain strain. Also it may be noted that a majority of the works (see e.g.[3, 4]) in this direction is based on selectively chosen strain gradient plasticity models that require extensive parameter fitting from experimental data. Also, in such framework, the true nature of nonlinearity and coupling is not fully tractable. For a more detail description of the PT, one requires a microscopic model, such as [5, 6], where the invariance of the free energy with respect to the crystallographic point group symmetry is preserved but the discontinuous

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nature of the deformation across the individual habit planes is introduced. This provides the most essential information to describe the morphology of the microstructural evolution, whereas the process of reshuffling of the atoms, which actually causes the reconstructive PT, remains beyond such a microstructural scale. The latter process requires the description of chemical interaction energy between atoms [7] and spin stabilized Hamiltonian [8]. Coupling such an atomistic process with the microstructural phenomenology means coupling a molecular dynamic model [9, 10] with a microscopic free energy model [6, 11, 12] through the thermal fluctuation term, strain and the motion of the domain walls.

In the present paper we focus our attention on linking SMA microstructure and macroscopic behaviour by developing the microscopic free energy and the associated coupled field model to simulate the dynamics of 3D macroscopic sample of NiAl undergoing cubic to tetragonal PT. First, we observe that the free energy is highly sensitive to many interdependent constants which are to be obtained experimentally [11]. As a result of this sensitivity and due to a fairly complex polynomial representation of the 3D Landau-Ginzburg free energy function, there may be situations where multidimensional simulations produce unphysical spurious oscillations. In the new model developed in the present paper, the above set of interdependent constants, that need to be determined from experimental data, is reduced to uniquely identifiable set of constants for each transformation surface among the austenitic phase and a particular martensitic variant.

Note that earlier, a new low-dimensional model for the time-dependent dynamics of SMA was derived in [2] and a class of such reduced models was rigorously analyzed in [13]. Computational results presented in [2, 13] confirmed robustness of our modelling approach for a number of practically important cases. The main results of the present paper are pertinent to *the general three-dimensional case*. There are several recent studies where the time-dependent Ginzburg-Landau (TDGL) (Langevin) equation with the correct microscopic description of the Falk-Konopka type free energy function has been analyzed (e.g. [14, 12]). We are not aware of any dynamic model of 3D SMA samples that bases its consideration on the correct Ginzburg-Landau free energy representation in the microscopic scale and the momentum balance and heat conduction in the macroscopic scale. The Ginzburg-Landau free energy function derived in the first part of this paper is incorporated in the coupled dynamic field model. This model is exemplified for cubic to tetragonal PT with single martensitic variant along the axis of a bar with rectangular cross-section under axial stress and heat flux.

2 3D Landau Theory of Martensitic Phase Transformation

It has been demonstrated by Levitas and Preston [6, 12] that the polynomial structures 2-3-4 and 2-4-6 of the Gibbs free energy in order parameter η in Cartesian coordinate can eliminate the problem of unphysical minima and re-

tain all the necessary properties of the Ginzburg-Landau free energy function with respect to point group symmetry of the crystals. Such polynomial structure can be constructed in such a way that the stability of the austenitic phase (A) and martensitic variants (M_j), non-extremal diffusion barrier and nucleation can be described in stress-temperature space. Furthermore, while using such polynomial structure the interfaces (domain walls) $M_j - M_i$ between the martensitic variants (i, j) can be interpreted by using a newly introduced barrierless A nucleation mechanism, i.e. by splitting the original into two simultaneously present interfaces $M_j - A$ and $A - M_i$. In this section a 2-3-4 polynomial structure is constructed by improving upon the model of Levitas and Preston [6, 11].

For analytical clarity we first consider a single variant of martensite and single order parameter $\eta \in [0, 1]$. First we define the Gibbs free energy density in stress-temperature space $(\boldsymbol{\sigma}, \theta)$ as

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

where $\boldsymbol{\lambda}$ is the constant fourth-rank elastic compliance tensor, $\boldsymbol{\varepsilon}_t$ 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 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 [15] The objective now is to obtain the functions φ and f by satisfying their properties mentioned above and the conditions of extremum of the energy for existence of equilibrium of A and M phases: $\partial G/\partial \eta = 0$ at $\eta = 0, 1$.

The new model derived below is based on the assumption that G can be uniquely represented by a polynomial structure in η with the extremum only at $\eta = 0, 1$ and out of these two extremum only one is minimum and the other is maximum for phase transformation (PT) to happen. At equilibrium, we have

$$\frac{\partial G}{\partial \eta} = -\boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t \frac{\partial \varphi(\eta)}{\partial \eta} + \frac{\partial f(\theta, \eta)}{\partial \eta} = 0 \ , \quad \eta = 0, 1. \tag{2}$$

The total strain tensor ($\boldsymbol{\varepsilon} = -\partial G/\partial \boldsymbol{\sigma}$) is the sum of the elastic strain tensor ($\boldsymbol{\lambda} : \boldsymbol{\sigma}$) and the transformation strain tensor ($\boldsymbol{\varepsilon}_t \varphi(\eta)$). Hence, for reconstructive PT through vanishing misfit strain, the condition

$$\boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t \frac{\partial \varphi(\eta)}{\partial \boldsymbol{\sigma}} - \frac{f(\theta, \eta)}{\partial \boldsymbol{\sigma}} = 0 \quad \forall (\boldsymbol{\sigma}, \eta) \tag{3}$$

must be satisfied. It is observed in the reported results [6] that the transformation barrier is dependent on stress. In the context of interface barrier, Levitas and Preston [12] have treated the associated η to be dependent on $\boldsymbol{\sigma}$. In the present paper, we propose an alternate approach by considering stress-dependent barrier height because the stress $\boldsymbol{\sigma}$ is the only driving factor for PT under isothermal condition. The polynomial structure which satisfies the extremum properties can be expressed as

$$\partial G/\partial \eta = \eta(\eta - 1)(\eta - \eta_b) \ , \tag{4}$$

so that its roots $\eta = 0, 1$ satisfy Eq. (2) and the root $\eta = \eta_b(\boldsymbol{\sigma}, \theta)$ represents the $A \leftrightarrow M$ PT barrier. Integrating Eq. (4) and imposing the combined properties of $\varphi(\eta)$ and $f(\theta, \eta)$ stated earlier as

$$G(\boldsymbol{\sigma}, \theta, 0) - G(\boldsymbol{\sigma}, \theta, 1) = \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t - \Delta G^{\theta} \ , \tag{5}$$

we get that $\eta_b = -6\boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t + 6\Delta G^{\theta} + 1/2$. Using Eq. (1) in Eq. (4) and by differentiating with respect to $\boldsymbol{\sigma}$, one has

$$-\boldsymbol{\varepsilon}_t \frac{\partial \varphi(\eta)}{\partial \eta} - \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t \frac{\partial^2 \varphi(\eta)}{\partial \boldsymbol{\sigma} \partial \eta} + \frac{\partial^2 f(\theta, \eta)}{\partial \boldsymbol{\sigma} \partial \eta} = \frac{\partial}{\partial \boldsymbol{\sigma}} \left[\eta_b \eta - (\eta_b + 1)\eta^2 + \eta^3 \right] \ . \tag{6}$$

The term involving f can be eliminated from Eq. (6) with the help of Eq. (3), and can be expressed as

$$\boldsymbol{\varepsilon}_t \frac{\partial \varphi(\eta)}{\partial \eta} = \eta(\eta - 1) \frac{\partial \eta_b}{\partial \boldsymbol{\sigma}} = \eta(\eta - 1)(-6\boldsymbol{\varepsilon}_t) \ . \tag{7}$$

Integrating Eq. (7) and following the properties of the transformation strain, i.e. $\varphi(0) = 0$ and $\varphi(1) = 1$, we have $\varphi(\eta) = 3\eta^2 - 2\eta^3$, $\quad 0 \leq \eta \leq 1$. Substituting this form in Eq. (3) and integrating with respect to η, the chemical part of the free energy density is obtained as

$$f(\theta, \eta) = \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t (3\eta^2 - 2\eta^3) + \frac{1}{2}\eta_b \eta^2 - \frac{1}{3}(\eta_b + 1)\eta^3 + \frac{1}{4}\eta^4 \ . \tag{8}$$

For $A \rightarrow M$ PT, the criteria for the loss of stability of A phase is $\partial^2 G / \partial \eta^2 \leq 0$ at $\eta = 0$, which gives the stress driven condition:

$$\boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t \geq \Delta G^{\theta} + \frac{1}{12} \ . \tag{9}$$

Similarly, for $M \rightarrow A$ PT, the criteria for the loss of stability is $\partial^2 G / \partial \eta^2 \leq 0$ at $\eta = 1$, which gives the stress driven condition:

$$\boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t \leq \Delta G^{\theta} - \frac{1}{12} \ . \tag{10}$$

$M_j \leftrightarrow M_i$ PT or diffused interface can evolve for stresses outside the range obtained by Eqs. (9) and (10). Note that no parameter fitting is required in the present model as opposed to the earlier model [6]. Eqs. (9) and (10) indicate a nonlinear dependence of the transformation surface on the temperature, which can be compared with the experimental data.

2.1 Cubic to Tetragonal Transformation Characteristics

We now consider the cubic to tetragonal PT for single variant martensitic case in absence of the elastic part of the stress. After reducing the stress and strain tensors in 1D, the equilibrium stress-transformation curve is obtained as

$$\eta = \eta_b \Rightarrow \sigma = \frac{1}{\varepsilon_t} \left[\Delta G^{\theta} + \frac{1 - 2\eta}{12} \right] \ . \tag{11}$$

Note that the increase in η causes decrease in σ which is consistent. The stress hysteresis (H) is obtained as

$$H = \sigma_{(\eta=0)} - \sigma_{(\eta=1)} = \frac{1}{6\varepsilon_t} \,, \tag{12}$$

which is independent of the temperature. Eq. (11) also shows nonzero tangent moduli where A and M lose their stability. These observations coincide with the results from the earlier model [6] (Figs.1, 2 and 5).

3 Multivariant Phase Transformation

In order to model realistic situations and macroscopic sample of SMA it is essential to incorporate the effects of (1) martensitic variants (M_k) (2) thermal strain (3) unequal compliances across the interfaces and the resulting inhomogeneity. For cubic to tetragonal transformation there are three variants of martensite according to the point group of crystallographic symmetry. The Gibbs free energy density thus should poses the associated invariance properties. In the mathematical model, this can be cross-checked by interchanging the variant indices (k). In this paper we consider the same order of variation in the compliance tensor and the thermal expansion tensor as in $\varphi(\eta)$ derived in Sec. 2. The Gibbs free energy density for cubic-tetragonal transformation having three variants $k = 1, 2, 3$ is expressed as

$$G = -\boldsymbol{\sigma} : \left[\boldsymbol{\lambda}_0 + \sum_{k=1}^{3} (\boldsymbol{\lambda}_k - \boldsymbol{\lambda}_0)\varphi(\eta_k)\right] : \boldsymbol{\sigma}/2 - \boldsymbol{\sigma} : \sum_{k=1}^{3} \boldsymbol{\varepsilon}_{tk}\varphi(\eta_k)$$

$$-\boldsymbol{\sigma} : \left[\boldsymbol{\varepsilon}_{\theta 0} + \sum_{k=1}^{3} (\boldsymbol{\varepsilon}_{\theta k} - \boldsymbol{\varepsilon}_{\theta 0})\varphi(\eta_k)\right] + \sum_{k=1}^{3} f(\theta, \eta_k) + \sum_{i=1}^{2} \sum_{j=i+1}^{3} F_{ij}(\eta_i, \eta_j) \,, \tag{13}$$

where $\boldsymbol{\lambda}$ is the second-order forth-rank compliance tensor ($\boldsymbol{\lambda}_0$ is for A phase), $\boldsymbol{\varepsilon}_{\theta 0} = \boldsymbol{\alpha}_0(\theta - \theta_e)$, $\boldsymbol{\varepsilon}_{\theta k} = \boldsymbol{\alpha}_k(\theta - \theta_e)$, $\boldsymbol{\alpha}_0$ and $\boldsymbol{\alpha}_k$ are the thermal expansion tensor of A and M_k. F_{ij} is an interaction potential required to preserve the invariance of G with respect to the point group of symmetry and uniqueness of the multivariant PT at a given material point. The description of PT can now be generalized with three sets of order parameters: $\bar{0} = \{0, \eta_k = 0, 0\}$, $\bar{1} = \{0, \eta_k = 1, 0\}$ and $\bar{\eta}_k = \{0, \eta_k, 0\}$. The extremum property of the free energy density requires

$$\frac{\partial G}{\partial \eta_k} = \eta_k(\eta_k - 1)(\eta_k - \eta_{bk}) = 0 \,, \quad \eta_k = \bar{0}, \bar{1} \,, \tag{14}$$

$$\frac{\partial^2 G}{\partial \eta_k^2} \leq 0 \,, \quad \eta_k = \bar{0} \quad (A \to M_k); \quad \frac{\partial^2 G}{\partial \eta_k^2} \leq 0 \,, \quad \eta_k = \bar{1} \quad (M_k \to A). \tag{15}$$

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

$$G(\boldsymbol{\sigma}, \theta, \bar{0}) - G(\boldsymbol{\sigma}, \theta, \bar{1}) = \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_{tk} - \Delta G^{\theta} \,. \tag{16}$$

Combining Eqs. (14) and (16) with similar steps described in Sec. 2, we get

$$\eta_{bk} = -6\boldsymbol{\sigma} : \boldsymbol{\varepsilon}_{tk} + 6\Delta G^{\theta} + 1/2 \tag{17}$$

Following the steps given in [11], we arrive at the symmetry preserving polynomial structure of the interaction potential

$$F_{ij} = \eta_i\eta_j(1-\eta_i-\eta_j)\left[B\left\{(\eta_i-\eta_j)^2-\eta_i-\eta_j\right\}+D\eta_i\eta_j\right]+\eta_i^2\eta_j^2(\eta_i Z_{ij}+\eta_j Z_{ji}) \tag{18}$$

such that

$$G = \sum_{k=1}^{3}\left[\frac{1}{2}\eta_{bk}\eta_k^2 - \frac{1}{3}(\eta_{bk}+1)\eta_k^3 + \frac{1}{4}\eta_{bk}^4\right] + \sum_{i=1}^{2}\sum_{j=i+1}^{3} F_{ij}(\eta_i,\eta_j) \tag{19}$$

leads to a 2-3-4-5 polynomial structure, where B, D are constants estimated from experiments. The transformation energy associated with $M_i \rightarrow M_j$ requires

$$G(\boldsymbol{\sigma},\theta,\bar{\eta}_i) - G(\boldsymbol{\sigma},\theta,\bar{\eta}_j) = \boldsymbol{\sigma} : (\boldsymbol{\varepsilon}_{tj} - \boldsymbol{\varepsilon}_{ti}) \tag{20}$$

which is already satisfied through Eq. (17). The uniqueness of PT at a material point is now imposed through similar steps described in context of Eq. (6).

4 Strongly Coupled Dynamics of the Phase Transformation and Coupled Thermoelasticity in a Rectangular NiAl Bar

The link between microstructure of SMA and its macroscopic behaviour is realized via the coupled field model in which the phase kinetics is governed by the Ginzburg-Landau equation

$$\frac{\eta_k}{\partial t} = -\sum_{p=1}^{3} L_{kp}\left[\frac{\partial G}{\partial \eta_p} - \boldsymbol{\beta}_p : \boldsymbol{\nabla}\boldsymbol{\nabla}\eta_p\right] + \theta \ , \tag{21}$$

where L_{kp} are positive definite kinetic coefficients, $\boldsymbol{\beta}_k$ are positive definite second rank tensor, and the macroscopic energy conservation law is governed by the heat transfer equation

$$\rho\frac{\partial \bar{G}}{\partial t} - \boldsymbol{\sigma} : \boldsymbol{\nabla}\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{q} = h_\theta \ , \tag{22}$$

and the momentum balance equation

$$\rho\frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} + \boldsymbol{f} \ , \tag{23}$$

where $\bar{G} = G - \theta\partial G/\partial\theta$ is the internal energy, ρ is the mass density, $\boldsymbol{u}$ is the displacement vector, $\boldsymbol{q}$ is the heat flux, h_θ and $\boldsymbol{f}$ are the thermal and mechanical loading, respectively. The displacement is related to the Green strain tensor

as $\boldsymbol{\varepsilon} = (1/2)[\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}]$ where $\boldsymbol{F}$ is the deformation gradient. For the purpose of numerical simulation we consider a rectangular NiAl bar with macroscopic domain $([0, L], [y^-, y^+], [z^-, z^+])$ undergoing single variant cubic to tetragonal transformation under uniaxial stress (σ_{11}) due to boundary conditions $f_1(0,t) = (y^+ - y^-)(z^+ - z^-)\sigma_0(t)$, $u_1(0, y, z, t) = 0$, traction-free surfaces, thermal boundary conditions at the ends $\partial\theta(x = 0, t)/\partial x = \bar{\theta}(t)_0$, $\partial\theta(x = L, t)/\partial x = \bar{\theta}(t)_L$, on the surface $(y = y^+, y^-)$, $\partial\theta/\partial y = \bar{\theta}_S$ and on the surface $(z = z^+, z^-)$, $\partial\theta/\partial z = \bar{\theta}_S$. The initial conditions are $\theta(x, 0) = \eta_0(x)$, $\theta(x, y, z, 0) = \theta_0(x)$, $u(x, y, z, 0) = u_0(x)$ and $\partial u(x, y, z, 0)/\partial t = 0$. A consistent form of the temperature field is obtained as

$$\theta(x, y, z, t) = \theta_1(x, t) + (y + z)\bar{\theta}_s \ . \tag{24}$$

The longitudinal displacement and strain fields are approximated as

$$u_1 = u(x, t) \ , \quad \varepsilon_{11} = \frac{\partial u}{\partial x} + \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2 \ , \quad \varepsilon_{22} = \frac{\partial u_2}{\partial y} \ , \quad \varepsilon_{33} = \frac{\partial u_3}{\partial z} \ . \tag{25}$$

In the present example we assume that the habit planes are normal to e_1, such that $\eta = \eta(x, t)$. For microscopic deformation, the fine graining of strain requires the property of cubic to tetragonal transformation. For this model, we obtain the consistent form of the unknown fields $u_2(x, y, z, t)$ and $u_3(x, y, z, t)$ by imposing the geometric constraints for effectively one-dimensional dynamics, which leads to

$$u_2 = \frac{\mu}{2}y + \frac{\lambda_{21}}{\lambda_{11}}y\varepsilon_{11} - \left(\frac{1}{2} + \frac{\lambda_{21}}{\lambda_{11}}\right)\varepsilon_t\varphi(\eta)y + \alpha\left(1 - \frac{\lambda_{21}}{\lambda_{11}}\right)\int(\theta - \theta_0)dy \ , \tag{26}$$

$$u_3 = \frac{\mu}{2}z + \frac{\lambda_{31}}{\lambda_{31}}y\varepsilon_{11} - \left(\frac{1}{2} + \frac{\lambda_{31}}{\lambda_{11}}\right)\varepsilon_t\varphi(\eta)y + \alpha\left(1 - \frac{\lambda_{31}}{\lambda_{11}}\right)\int(\theta - \theta_0)dz \ , \tag{27}$$

where μ is the prescribed error in the volumetric strain. This quasi-continuum model with discontinuous distribution of $\eta(x, t)$, and continuous fields $u_1(x, t)$, $\theta_1(x, t)$ is then solved by variational minimization of Eqs. (21)-(23).

5 Concluding Remarks

In this paper, a new dynamic multiscale model for simulation of 3D SMA samples has been developed by linking an improved version of the microscopic Landau theory and macroscopic conservation laws. Essential properties of the $A \leftrightarrow M_j$ as well as $M_j \leftrightarrow M_i$ PTs are recovered using consistent steps, which eliminates the problem of non-uniqueness of energy partitioning during PTs and relaxes the over-sensitivity of the free energy due to many unknown material constants in previously reported models. It has been shown how the new 3D model can be reduced to a low dimensional model for simulating the strongly coupled phase kinetics and thermoelasticity in a rectangular bar undergoing cubic to tetragonal phase transformations.

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