

# **NONSMOOTH/NONCONVEX MECHANICS**

## **WITH APPLICATIONS IN ENGINEERING**

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*A VOLUME DEDICATED TO THE MEMORY  
OF PROFESSOR P. D. PANAGIOTOPoulos*

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PROCEEDINGS OF THE 2ND INTERNATIONAL CONFERENCE  
ON NONSMOOTH/NONCONVEX MECHANICS WITH APPLICATIONS IN ENGINEERING  
*IN MEMORIAM OF PROFESSOR P. D. PANAGIOTOPoulos*

PHASE KINETICS IN MODELLING SHAPE MEMORY ALLOYS

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1 SUMMARY

In this paper we propose a Ginzburg-Landau free energy model of multivariant phase transformation in shape memory alloy and its linkage with the atomistic reordering process which finally gives rise to self-accommodating microstructure. We analyze 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. Based on the variational formulation of the problem, we simulate phase transformations in a Ni-Al thin film. The results capture well a qualitative picture of the onset of microstructure formation.

2 INTRODUCTION

It is known that shape memory effects in alloys are due to the existence of large differences in the variants of the crystal lattice transformation strain tensors [1]. Hence, for practical engineering applications of shape memory effects, the understanding of the self-accommodation of the crystallographic variants in a particular geometry under thermomechanical constraints is of great importance. The related topics have been extensively discussed in the literature over the last three decades, including theoretical aspects (e.g., [2, 1, 3, 4, 5]), computational aspects (e.g., [6, 7, 8]), as well as experimental aspects (e.g., [9]).

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 or larger, it is natural to employ the variational methodology where one first defines an appropriate energy density and then thermodynamic conservation laws. To develop such a variational method, one requires to describe the non-equilibrium thermodynamics for a particular type of alloys involving entropy changes due to phase transformations. In contrast to the standard phenomenological description (e.g., [2]), where a large number of parameters have to be adjusted considering the dynamics of the phase evolution *a priori*, our thermodynamic approach in this based is based on the Ginzburg-Landau theory, which is microscopic in nature. In order to perform numerical simulations, we have developed a variational framework and a finite element code, where general thermo-mechanical loadings can be handled while studying the lattice-based kinetics of the microstructures. Here, the thermodynamic conservation laws couple the mechanical deformation, temperature and the order variables. The order variables describe the type of the phase (the parent austenite phase or a martensitic variant) at a material point. The outline of the paper is as follows. In Sec. 2 we highlight atomistic order variables and formulate the Ginzburg-Landau free

energy model. Thermodynamic conservation laws are discussed in Section 3 where we also discuss the variational framework and the finite element formulation of the problem. Numerical results for cubic to tetragonal phase transformations in Ni-Al thin films are presented in Section 4.

### 3 ATOMISTIC ORDER VARIABLES AND THE FREE ENERGY MODEL

Phase transformations in shape memory alloys are first order diffusion-less transformations where 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. We start our consideration from the molecular dynamic model [10] 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

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

where  $\mathbf{r}_i = \mathbf{h}\mathbf{s}_i$  denotes the position vector of the  $i$ th atom in the ensemble with  $\mathbf{s}$  as the atomic coordinate with respect to the lattice and the three components of the lattice vector in the columns of  $\mathbf{h}$ . 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

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

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

where  $\boldsymbol{\sigma}$  is the stress tensor,  $\theta$  is the temperature and  $\tau$  denotes time in the atomistic scale dynamics. Integrating Eq. (2a) over the characteristic time  $\tau_0$  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. The phase transition occurs within the time interval  $\tau_0$  and the atomic coordinate relative to the lattice changes from  $\mathbf{s}(0)$  to  $\mathbf{s}(b\tau_0)$ ,  $b > 1$ . Note that  $\mathbf{s}(0)$  can be expressed in terms of the lattice constants of the parent phase (austenite phase) and  $\mathbf{s}(b\tau_0)$  can be expressed in terms of the lattice constants of one of the transformed phase (martensite phase). An intermediate or diffused phase may exist which are unstable and may lead to defects and dislocations. We now consider a control volume  $\bar{V} = V^q$ ,  $q \leq 1$  and define the vector  $\boldsymbol{\eta}(t)$ ,  $t = b\tau$ ,  $b > 1$  of the order variables such that

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

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.

Next, we denote the order variables  $\eta_k \in [0, 1]$ , where  $k = 1, \dots, N$  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  $k$ th 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  $\boldsymbol{\eta} = \{\eta_1, \dots, \eta_N\}^T$ , the Gibbs free energy density is defined as  $G(\boldsymbol{\sigma}, \theta, \boldsymbol{\eta})$ . Here  $\boldsymbol{\sigma}$  is the stress tensor,  $\theta$  is the temperature. The finite strain tensor  $\boldsymbol{\varepsilon}$  is decomposed into the elastic part and the transformation-induced part as

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

where  $\varphi(\eta_k)$  is a polynomial in  $\eta_k$  and  $\boldsymbol{\varepsilon}_k^t, k = 1, \dots, N$  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.

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

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

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

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.

$$\begin{aligned} G(\boldsymbol{\sigma}, \theta, \boldsymbol{\eta}) = & -\frac{1}{2} \boldsymbol{\sigma} : \left[ \boldsymbol{\lambda}_0 + \sum_{k=1}^N (\boldsymbol{\lambda}_k - \boldsymbol{\lambda}_0) \varphi(\eta_k) \right] : \boldsymbol{\sigma} - \boldsymbol{\sigma} : \sum_{k=1}^N \boldsymbol{\varepsilon}_k^t \varphi(\eta_k) \\ & - \boldsymbol{\sigma} : \left[ \boldsymbol{\varepsilon}_{\theta 0} + \sum_{k=1}^N (\boldsymbol{\varepsilon}_k^\theta - \boldsymbol{\varepsilon}_0^\theta) \varphi(\eta_k) \right] + \sum_{k=1}^N f(\theta, \eta_k) + \sum_{i=1}^{N-1} \sum_{j=i+1}^N F_{ij}(\eta_i, \eta_j), \end{aligned} \quad (7)$$

where  $\boldsymbol{\lambda}_k$  is the second-order forth-rank compliance tensor for the  $k$ th martensitic variant ( $M_k$  phase),  $\boldsymbol{\lambda}_0$  is for austenite phase ( $A$  phase),  $\boldsymbol{\varepsilon}_0^\theta = \boldsymbol{\alpha}_0(\theta - \theta_e)$ ,  $\boldsymbol{\varepsilon}_k^\theta = \boldsymbol{\alpha}_k(\theta - \theta_e)$ .  $\theta_e$  is the temperature at which the stress-free martensite loses 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.,

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

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

$$\frac{\partial^2 G}{\partial \eta_k^2} \leq 0, \quad \boldsymbol{\eta} = \bar{1} \quad (M_k \rightarrow A). \quad (10)$$

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

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

where  $\Delta G^\theta$  is the jump in the free energy due to phase transformation. With the help of Eqs. (5)-(11), we determine  $\varphi(\eta_k)$  and  $f(\theta, \eta_k)$  (see [11] 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 [12] for the details)

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

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  $f(\theta, \eta_k)$ .

#### 4 THERMODYNAMIC CONSERVATION LAWS, VARIATIONAL FRAMEWORK AND FINITE ELEMENT DISCRETIZATION

We note that a jump in the free energy  $\Delta G^\theta$  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 non-negativity 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

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

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

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

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

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

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

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

and the momentum balance equation

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

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

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

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

We relate the elastic part of displacements to the elastic strain  $\boldsymbol{\epsilon}_{el}$  via the linear strain-displacement relation, i.e.  $\boldsymbol{\epsilon}_{el} = ((\nabla \boldsymbol{u}) + (\nabla \boldsymbol{u})^T)/2$ . It is now obvious that the order variables  $\eta_k, k = 1, \dots, N$  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  $\text{diam}(\Omega)^3 = \bar{V}$ . We are interested in fixed-order finite elements with  $h$ -refinement. We consider the Lagrangian isoparametric interpolation function  $\mathbf{N}$ ,

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

$$\boldsymbol{v} = \{u_1 \ u_2 \ u_3 \ \theta \ \eta_1 \ \dots \ \eta_n\}^T . \quad (20)$$

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

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

where

$$\begin{aligned} \delta\Pi_{PT} &= \int_{\Omega} \sum_{k=1}^N \delta\bar{\eta}_k \left[ \frac{\partial \eta_k}{\partial t} - \theta_k \right] d\mathbf{x} + \int_{\Omega} \sum_{k=1}^N \sum_{p=1}^N \delta\bar{\eta}_k \left[ L_{kp} \left( \frac{\partial G}{\partial \eta_p} + \beta_p : \nabla \nabla \eta_p \right) \right] d\mathbf{x} \\ &\quad - \int_{\partial\Omega} \sum_{k=1}^N \sum_{p=1}^N \delta\bar{\eta}_k L_{kp} \frac{\partial G}{\partial \eta_p} ds(\mathbf{x}) , \end{aligned} \quad (22)$$

$$\begin{aligned} \delta\Pi_\theta &= \int_{\Omega} \delta\bar{\theta} \left[ \frac{\partial}{\partial t} \left( \mathcal{W} - \theta \frac{\partial \mathcal{W}}{\partial \theta} \right) - \nabla \cdot (\boldsymbol{\sigma} \cdot \frac{\partial \boldsymbol{u}}{\partial t}) \right] d\mathbf{x} \\ &\quad + \int_{\Omega} \delta\bar{\theta} \left[ \nabla \cdot \left( -\kappa \nabla \theta - \alpha' \kappa \nabla \frac{\partial \theta}{\partial t} \right) \right] d\mathbf{x} - \int_{\partial\Omega} \delta\bar{\theta} \boldsymbol{q}_\perp ds(\mathbf{x}) , \end{aligned} \quad (23)$$

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

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

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

with initial state and microstructure

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

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 NUMERICAL SIMULATIONS

We are interested in cubic to tetragonal transformations of a Ni-Al thin film, considered in a two-dimensional domain of rectangular shape. There are three tetragonal martensitic variants in this case and  $N = 3$ . The transformation strain tensors for these three variants are, respectively,

$$\boldsymbol{\varepsilon}_1^t = \begin{pmatrix} \gamma & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}, \quad \boldsymbol{\varepsilon}_2^t = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \gamma & 0 \\ 0 & 0 & \alpha \end{pmatrix}, \quad \boldsymbol{\varepsilon}_3^t = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \gamma \end{pmatrix}, \quad (27)$$

where the transformation stretches are given by

$$\alpha = \frac{a}{a_0}, \quad \gamma = \frac{c}{a_0}, \quad (28)$$

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  $\eta_k$ .

$$\phi(\eta_k) = 3\eta_k^2 - 2\eta_k^3. \quad (29)$$

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

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

where

$$\Delta G^\theta \approx (-\Delta s^e + \Delta c)(\theta - \theta_e), \quad (31)$$

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

where  $\Delta G^\theta(\theta_e) = 0$ ,  $\theta_e$  is the equilibrium temperature,  $\theta_c > \theta_e$  is the critical temperature for transformation under the applied thermo-mechanical loading,  $\Delta c$  is jump in the specific heat capacity during transformation,  $-\Delta s^e > 0$  is the jump in the specific entropy at

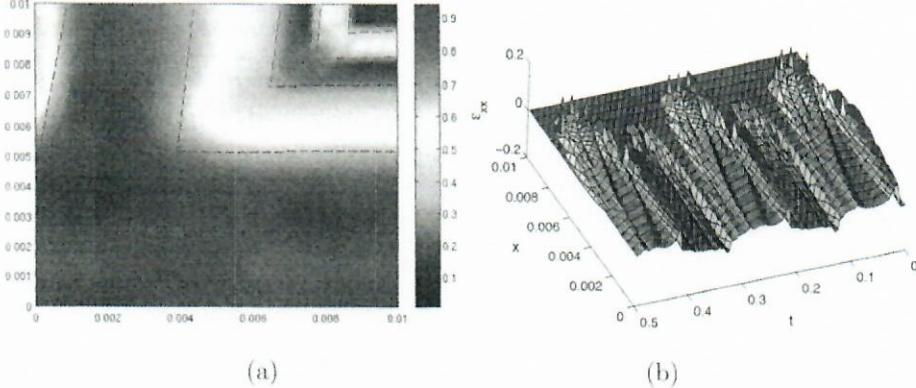


Figure 1: (a) Evolved microstructure with martensitic variant  $\eta_1 \rightarrow 1$  and (b) time history of  $\varepsilon_{xx}$  along the  $y = 0$  line.

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 [12]. The film is subjected to 5Hz sinusoidal stress applied in longitudinal direction throughout the left and the right edges. The other two parallel edges are left free. The stress distribution over the edge has triangular shape. Constant temperature of 300K with cubic phase (austenite) is assumed to be the initial state. Fig. 1(a) shows the nucleated tetragonal phases  $\eta_1 \rightarrow 1$  when the peak tensile stress is attained during the first half cycle. The corresponding time history of the longitudinal strain distribution along the  $y = 0$  line is shown in Fig. 1(b). In this figure, the jumps in the strain due to phase transformation is captured. The results shown here provides a qualitative picture of the phase transformation and the onset of microstructure formation. It is known that due to the non-convex nature of the problem, there are multiple energy wells and a continuum solution based on proper rotation of the lattice vectors alone do not produce a unique transformation path. However, with the introduction of the atomic reordering process through the kinetics, we have arrived at a dynamic model, by which it becomes possible to simulate the microstructures which are computationally reproducible. The accuracy of the solution is dominated by the accuracy of interpolation of the order parameters.

## 6 CONCLUSIONS

We proposed an approach to couple the atomistic scale dynamics with the microscopic kinetics based model of phase transformation in shape memory alloys. A Ginzburg-Landau free energy description has been employed in a variational framework to simulate cubic to tetragonal phase transformation in thin films under mechanical loadings. The computational model reported here is one step forward in attempts to combine numerical simulations with experiments to characterize various properties of multivariant phase transformations. While the results presented here provide a qualitatively correct picture of the phase transformation and the onset of microstructure formation, further studies

with refined finite element meshes are required to capture smaller-scale features in the dynamics.

## References

- [1] Bhattacharya K., Microstructure of Martensite, Oxford University Press, NY (2003).
- [2] Boyd J.G. and Lagoudas D.C., A thermodynamical constitutive model for shape memory materials. Part I. the monolithic shape memory alloy, *Int. J. Plasticity*, 12(6), (1996), 805-842.
- [3] Brocca M., Brinson L.C. and Bazant Z.P., Three-dimensional constitutive shape memory alloys based on microplane model, *J. Mech. Phys. Solids*, 50, (2002), 1051-1077.
- [4] Artemev A., Wang Y., Khachaturyan A.G., Three-dimensional phase field model and simulation of martensitic transformation in multilayer systems under applied stresses, *Acta Mater.*, 48, (2000), 2503-2518.
- [5] Levitas V.I. and Preston D.L., Three-dimensional Landau theory for multivariant stress-induced martensitic phase transformations. I. Austenite  $\leftrightarrow$  martensite. *Phys. Rev. B*, 66, (2002), 134206.
- [6] Belik P. and Luskin M., Computational modeling of softening in a structural phase transformation, *Multiscale Model. Simul.*, 3(4), (2005), 764-781.
- [7] Auricchio F. and Petrini L., A three-dimensional model describing stress-temperature induced solid phase transformations: solution algorithm and boundary value problems, *Int. J. Numer. Meth. Engng.*, 61, (2004), 807-836.
- [8] Melnik R.V.N., Roberts A.J., Thomas K., Computing dynamics of copper-based shape memory alloys via center manifold reduction of 3D models, *Computational Materials Science*, 18, (2000), 255-268.
- [9] Boullay P., Schryvers D., and Ball J.M., Nano-structures at martensite macrotwin interfaces in Ni<sub>6</sub>Al<sub>3</sub>5, *Acta Mater.*, 51, (2003), 1421-1436.
- [10] Entel P., Meyer R. and Kadau K., Molecular dynamic simulations of martensitic transitions, *Phil. Mag. B*, 80(2), (2000), 183-194.
- [11] Mahapatra D.R. and Melnik R.V.N., A dynamic model for phase transformations in 3D samples of shape memory alloys, Lecture Notes in Computer Science, Springer-Verlag, 3516, 25-32, (2005).
- [12] Levitas V.I., Preston D.L., and Lee D.W., Three-dimensional Landau theory for multivariant stress-induced martensitic phase transformations. III. Alternative potentials, critical nuclei, kink solutions, and dislocation theory, *Phys. Rev. B*, 68, (2003), 134201.

## CONTENTS

Preface .....	vii
Introduction .....	xv
<b>C. C. Baniotopoulos:</b> The impact of Nonsmooth/Nonconvex Mechanics and the work of Panagiotopoulos .....	xvii

### MATHEMATICAL MODELLING AND MECHANICS

<b>J. J. Moreau:</b> Facing the plurality of solutions in Nonsmooth Mechanics .....	3
<b>D. Gao:</b> Multi-scale modeling and duality theory in phase transitions of solids .....	13
<b>M. Sofonea:</b> A quasistatic contact problem for electro-elastic materials .....	21
<b>D. Sfyris, N. Charalambakis and V. K. Kalpakides:</b> On the force acting on dislocations within nonlinear elastostatics .....	29
<b>L. Gasiński:</b> Semilinear hemivariational inequalities with hysteresis .....	37
<b>M. Ait Mansour:</b> On the Panagiotopoulos inequality and nonmonotone network flow problems .....	45
<b>K. Hackl and U. Hoppe:</b> Relaxed potentials and evolution equations for inelastic microstructures .....	53
<b>N. Charalambakis and F. Murat:</b> Existence, uniqueness and homogeni- zation for a class of stratified thermoviscoplastic materials .....	61
<b>W. R. Bielski, B. Gabin and E. Kruglenko:</b> Selected problems of rigid and deformable micromagnetics .....	69
<b>G. Chatzigeorgiou, V. Kalpalides and N. Charalambakis:</b> Biaxial loading of continuously graded thermoviscoplastic materials .....	77

<b>J. M. Viaño, C. Ribeiro and J. Figueiredo:</b> Limit of the Kirchhoff-Love model for plates: The Bernoulli-Navier model for beams .....	85
<b>S. Migórski and A. Ochal:</b> Evolution hemivariational inequalities for Navier-Stokes type operators .....	93
<b>M. Wilko, L. Jankowski and J. Holnicki:</b> Impact load identification – Forensic engineering .....	99
<b>P. Nazarko and L. Ziemianski:</b> Damage identification in rods using neural networks .....	107
<b>Ch. Efstathiades, C. C. Baniotopoulos, P. Nazarko, L. Ziemianski and G. E. Stavroulakis:</b> Structural health monitoring in aluminium curtain-walls by applying neural networks techniques .....	115
<b>Y. Abdel-Jawad, M. Daoud and Y. Hunaiti:</b> Optimization of prestressed concrete simply supported beams using genetic algorithms .....	123
<b>D. Roy Mahapatra and R. V. N. Melnik:</b> Phase kinetics in modeling shape memory alloys .....	131
<b>L. G. Machado and D. C. Lagoudas:</b> Nonlinear dynamic response of a shape memory alloy oscillator .....	139
<b>M. E. Filippakis and N. S. Papageorgiou:</b> Degree theoretic methods in nonlinear elliptic equations .....	147

## COMPUTATIONAL MECHANICS

<b>J. Haslinger, Z. Morávková and C. C. Baniotopoulos:</b> Contact problems with nonmonotone friction and a solution dependent coefficient of friction .....	157
<b>M. Raous, M. Schryve and M. Cocou:</b> Recoverable adhesion and friction .....	165
<b>Ch. Glocker:</b> Reduction techniques for distributed set-valued force laws .....	173
<b>C. D. Bisbos:</b> Semidefinite programming in the Limit and Shakedown Analysis of structures .....	181
<b>T. Geier, M. Foerg, R. Zander, H. Ulbrich, F. Pfeiffer, A. Brandsma and A. Van der Velde:</b> Modeling of contacts in a push belt CVT .....	189
<b>C. D. Bisbos and G. Papaioannou:</b> Shakedown Analysis of FEM-discretized steel shell structures under the Ilyushin yield criterion .....	197

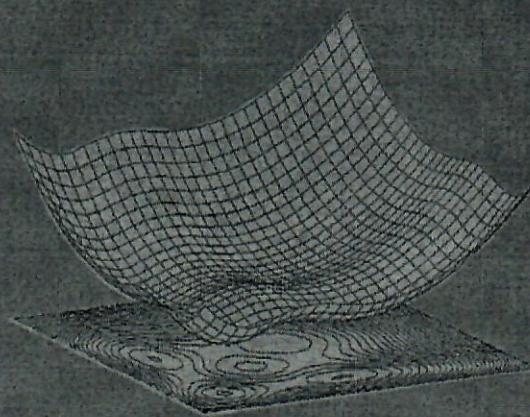
DEPARTMENT OF CIVIL ENGINEERING  
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*IN MEMORIAM OF*  
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