Phase-field Approach to Studying Shape Memory Effects and Thermomechanical Properties of Low Dimensional Nanostructures

Melnik. R., Wang, L.X.

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Phase-field Approach to Studying Shape Memory Effects and Thermomechanical Properties of Low Dimensional Nanostructures

RODERICK MELNIK
Wilfrid Laurier University
M2NeT Laboratory, Department of Mathematics
75 University Ave W., Waterloo, ON N2L 3C5
CANADA
rmelnik@wlu.ca

LINXIANG WANG
Hangzhou Dianzi University
Faculty of Mechanical Engineering
Xiasha, Hangzhou, 310018
P.R. CHINA

Abstract: We focus on the development of mesoscopic models for the description of strongly nonlinear coupled thermomechanical effects, such as shape memory effects, in low dimensional nanostructures. The main model is a result of the phase-field approach which we extend to the present problems from our previous works on ferroelectrics. The resulting coupled system of partial differential equations is solved based on a combination of the Chebyshev collocation method and the extended proper orthogonal decomposition. The developed model and its numerical implementation allow us to study properties of nanostructures and we present macrostructure computations for nanowires and nanoplates.

Key–Words: Nanostructures, Shape Memory Effect, Nonlinear Thermomechanics, Mesoscopic Models, Size-dependent Effects, Dynamics, Phase Transformations, Galerkin projection, Coupled Problems.

1 Introduction

Low dimensional semiconductor nanostructures have many applications in nanotechnology, but they provide serious theoretical and computational challenges when it comes to the prediction of their properties [4]. This especially true when we need to account for finite size effects as it is the case, for example, for finite length nanowires [14]. Coupled effects in nanostructures are also their intrinsic feature that must be accounted for bette [12]. One such effect, namely piezoelectric, has been studied for a long time and is known to have importance consequences on bandstructure calculations of low dimensional nanostructures. More recently, the importance of thermal effects has been demostrated in the context of their coupling to electromechanical fields [15, 16]. While many such effects are linear, the importance of nonlinear effects have recently been also emphasized in [13]. It was shown that the applicability of linear models is limited for low dimensional nanostructures, in particular quantum dots, and both coupled and nonlinear effects need to be accounted for in the analysis of more realistic structures. In this contribution, we continue research along this direction and analyze the nonlinear coupling between mechanical and thermal fields in SMA-based nanowires. We use some generalizations of ideas originally developed for ferroelectric materials to arrive to a model based on a system of coupled partial differential equations [24, 25]. The resulting system can be solved efficiently by several different methodologies such as finite volume [20] or finite element methods [5]. In this paper, we apply the Chebyshev collocation method for the solution of the resulting problem, followed by the application of an extended proper orthogonal decomposition as was proposed in [18, 19].

To get started, we recall that it has been known for some time that in gold (Au) nanowires, the energy as a function of lattice spacing exhibits two distinct minima that correspond to fcc and bct phases. The fact that these nanowires exhibit shape memory effects has also been confirmed computationally with such methodologies as tight-binding and density functional theory. A similar situation holds for many other nanowires that show substantial potential for many applications in nano- and bio-nanotechnologies, including Cu, Ni, ZnO, FePd, Al, Ag, etc.

While many results up to date have been obtained for infinitely long nanowires (as well as for infinitely large nanoplates), including those obtained with ab initio calculations, the question has remained on whether phase transformations is a generic effect for the same material-type nanowires of finite length. Recently, there has been mounting evidence towards a positive answer to this question. However, comprehensive studies of finite nanowires and nanoplates are limited due to the fact that the methodologies applied for their studies are computationally expensive.

In this contribution, we present a relatively simple and computationally inexpensive model to study phase transformations in finite nanostructures with our major focus given here to finite nanowires and nanoplates. Based on our previous results, the models describing shape memory effects at the mesoscopic level for the case of square-to-rectangle transformations can be reduced to a two-dimensional case.

Before moving to the model construction, we shall note that martensitic transformations at the nanoscale have received substantial attention from experimentalists. A number of alloys that undergo these transformations have recently been studied in [17] where the results of transmission electron microscopy studies were reported.

2 Mathematical Model

To account for the first order phase transformations in ferroelastic materials such as shape memory alloys, time-dependent models of coupled dynamic thermoelasticity must account for a nonconvex highly nonlinear character of the associated free energy function. We start with the following 1D mathematical model [10, 7]:

$$\begin{aligned}
&\rho\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(k_1\left(\theta-\theta_1\right)\frac{\partial u}{\partial x} - k_2(\frac{\partial u}{\partial x})^3 + \right.\\
&\left. k_3(\frac{\partial u}{\partial x})^5\right) + \nu\frac{\partial}{\partial t}\frac{\partial^2 u}{\partial x^2} - \delta\frac{\partial^4 u}{\partial x^4} + F, \qquad (1)\\
&c_v\frac{\partial\theta}{\partial t} = k\frac{\partial^2\theta}{\partial x^2} + k_1\theta\frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + G,
\end{aligned}$$

where u is displacement, θ temperature, ρ density, k_1, k_2, k_3, c_v, ν, δ and k are normalized material-specific constants, θ_1 is the reference temperature for 1D martensitic transformations, and F and G are distributed mechanical and thermal loadings. The interested reader can find efficient numerical procedures for reducing systematically the general 3D model to models such as (1) in [10].

Although this is only a 1D model for the nonlinear dynamics of ferroelastic materials, it presents a number of challenges in its analysis and numerical implementation due to the coupling between thermal and elastic fields and strong nonlinearities. Furthermore, the inclusion of thermal and mechanical hystereses and the first order martensitic transformations into the model gives additional difficulties. First, we re-write the above system for numerical convenience as follows [7]:

$$\begin{aligned}
&c_v\frac{\partial\theta}{\partial t} = k\frac{\partial^2\theta}{\partial x^2} + k_1\theta\epsilon\frac{\partial v}{\partial x} + G, \quad \frac{\partial\epsilon}{\partial t} = \frac{\partial v}{\partial x}\\
&\rho\frac{\partial v}{\partial t} = \frac{\partial}{\partial x}\left(k_1\left(\theta-\theta_1\right)\epsilon - k_2\epsilon^3 + k_3\epsilon^5\right) + \qquad (2)\\
&\nu\frac{\partial}{\partial t}\frac{\partial^2 u}{\partial x^2} - \delta\frac{\partial^3\epsilon}{\partial x^3} + F,
\end{aligned}$$

where $\epsilon = \partial u/\partial x$ is the strain, and $v = \partial u/\partial t$ is the velocity. Note that this representation is convenient for a reduction of the original PDE-based model to a system of differential-algebraic equations the approach that was initiated in [8].

More generally, our consideration in this paper is based on the nonlocal model developed in [10] based on the equation of motion

$$\rho\frac{\partial^2\mathbf{u}}{\partial t^2} = \nabla_{\mathbf{x}}\cdot\mathbf{s} + \mathbf{F} \quad \text{with} \quad \mathbf{F} = \rho(\mathbf{f}+\hat{\mathbf{f}}) - \hat{\rho}\mathbf{v}\,, \quad (3)$$

and the energy balance equation

$$\rho\frac{\partial e}{\partial t} - \mathbf{s}^T : (\nabla\mathbf{v}) + \nabla\cdot\mathbf{q} = g\,, \qquad (4)$$

where $\mathbf{u}$ is the displacement vector, ρ is the density of the material, e is the internal energy (per unit mass), $\mathbf{q}$ is the heat flux, $\mathbf{f}$ is a given body force per unit mass, $\hat{\rho}$ and $\hat{\mathbf{f}}$ are nonlocal mass and force residuals respectively (similarly, g accounts for both local and non-local contributions), $\mathbf{v} = \partial\mathbf{u}/\partial t$ is the velocity vector, $\mathbf{s}$ is the stress tensor, $\mathbf{a}^T : \mathbf{b} = \sum_{i,j=1}^{3} a_{ij}b_{ij}$ is the standard notation for the rank 2 tensors $\mathbf{a}$ and $\mathbf{b}$ (further details can be found in [10]). The constitutive relationships that couple stresses, deformation gradients, temperature and heat fluxes have the following general form:

$$\Phi_1(\mathbf{s},\boldsymbol{\epsilon}) = 0\,, \quad \Phi_2(\mathbf{q},\theta) = 0\,, \qquad (5)$$

where it is implicitly assumed that these relations may involve spatial and temporal derivatives of the functions. Particular forms for Φ_1 and Φ_2 are problem specific. In dealing with phase transformations, the approach adopted in this paper is based on the Landau criterion stating that any isothermal equilibrium configuration of the lattice corresponds to a minimum (global or local) of the free energy function.

In order to characterize both, austenite at high temperature and martensite at low temperature, having in mind the analysis of finite length nanowires and other low dimensional nanostructures, by using a generic expression, the potential energy is constructed

on the basis of the modified Ginzburg-Landau free energy function. We follow [23] to get the evolution equations for our case as follows:

$$\frac{\partial^2 u_1}{\partial t^2} = \frac{\partial \sigma_{11}}{\partial x} + \frac{\sigma_{12}}{\partial y} + f_1, \tag{6}$$

$$\frac{\partial^2 u_2}{\partial t^2} = \frac{\partial \sigma_{12}}{\partial x} + \frac{\sigma_{22}}{\partial y} + f_2, \tag{7}$$

$$c_v \frac{\partial T}{\partial t} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + \tag{8}$$

$$a_2 T e_2 \frac{\partial e_2}{\partial t} + g \tag{9}$$

with

$$\sigma_{11} = \frac{\sqrt{2}}{2}\rho\left(a_1 e_1 + a_2(T - T_0)e_2 - a_4 e_2^3 + \right. \tag{10}$$

$$\left. a_6 e_2^5\right) + \frac{d_2}{2}\nabla_x^2 e_2,\ \sigma_{12} = \frac{1}{2}\rho a_3 e_3 = \sigma_{21}, \tag{11}$$

$$\sigma_{22} = \frac{\sqrt{2}}{2}\rho\left(a_1 e_1 - a_2(T - T_0)e_2 + a_4 e_2^3 + \right. \tag{12}$$

$$\left. a_6 e_2^5\right) + \frac{d_2}{2}\nabla_y^2 e_2, \tag{13}$$

where all the notation here are identical to those of [23].

3 Numerical approximations

A similar model has been recently applied in [1]. As we have already mentioned, under appropriate boundary and initial conditions, the models like this can be efficiently solved with several recently developed numerical methodologies, including the Chebyshev collocation procedure [21], the proper orthogonal decomposition [19], the genetic algorithm based optimization procedure [22], and the finite volume methodology [20], as well as finite element techniques [6].

For the sake of convenience, the governing equations are re-written in the form of evolution operator equation:

$$\frac{d\mathcal{U}}{dt} = \mathcal{M}(\mathcal{U}), \tag{14}$$

where $\mathcal{U}$ is the solution and $\mathcal{M}(\mathcal{U})$ is an operator which contains all the spatial derivatives of $\mathcal{U}$. In general, the approximation given by our model will not satisfy Eq.(14), i.e., the residual

$$\mathcal{R} = \frac{d\mathcal{U}^N}{dt} - \mathcal{M}(\mathcal{U}^N) \tag{15}$$

will not vanish everywhere. To determine all the expansion coefficients, the Galerkin method requires the following condition to be satisfied:

$$\int_0^L \left(\frac{d\mathcal{U}^N}{dt} - \mathcal{M}(\mathcal{U}^N)\right)\psi_i(x)dx = 0, \tag{16}$$

where $\psi_i(x)$ are the test functions.

In the Chebyshev collocation methods the trial functions are chosen to satisfy the following conditions:

$$\phi_i(x_j) = \begin{cases} 1, & \text{i = j,} \\ 0, & \text{i} \neq \text{j}\,. \end{cases} \tag{17}$$

and the test functions are chosen as:

$$\psi_i(x) = \delta(x_i) = \begin{cases} 1, & \text{x=}x_i, \\ 0, & x \neq x_i, \end{cases} \tag{18}$$

where $\{x_i\}$ is a set of chosen discretization points in the computational domain. For the Chebyshev approximation, it is chosen as follows:

$$x_i = L\left(1 - \cos(\frac{\pi i}{N})\right)/2, \quad i = 0, 1, \ldots, N, \tag{19}$$

where L is the length of the considered ferroelastic rod.

Following the standard procedure, our equation can be written in a matrix form as:

$$\mathrm{U}_x = \mathrm{DU}. \tag{20}$$

By substituting corresponding approximations of the spatial derivatives, the PDE-based model is converted into a set of Differential-Algebraic Equations (DAEs). The idea of a reduction of the original PDE model to a system of DAEs was first proposed in [8], followed by a subsequent development of low dimensional models based on the center manifold technique [10]. The application of an efficient time integrator can finally solve the problem in a way similar discussed earlier [7, 19]. The described methodology allows us to determine the temperature, stress, strain and displacement of the material at any point of the computational domain at any time. Then, the resultant data can be used for the POD analysis. It is carried out in a way similar to that described in [18, 19].

Having obtained optimal basis functions for the dynamical system, its lower dimensional approximation can be obtained by projecting the full system orthogonally onto the subspace spanned by the chosen basis functions (by the Galerkin projection). The model reduction can be achieved due to the fact that much smaller number of basis functions is needed for the approximation of the full system provided the chosen basis functions are optimal in a sense specified above.

3.1 Extended POD with Galerkin Projection

From the above described procedure, we obtain a collection of system states, so that the eigenmode series for the approximation to the system dynamics can be constructed using the extended POD method. First we obtain optimal basis functions for our dynamical system, and then its lower dimensional approximation can be obtained by projecting the full system orthogonally onto the subspace spanned by the chosen basis functions. For the current problem, the phase transformation can take place at different temperatures, by either mechanical or thermal stimulations. There may be no phase transformation if the temperature is sufficiently high. In order to model the dynamics of the ferroelastic material correctly, the empirical eigenfunctions have to take into account the temperature influence. Following [26], we choose a few (three) representative temperature values to demonstrate the analysis, in particular those for which the system has only martensite phase (low temperature θ_1), metastable austenite and martensite phases (medium temperature θ_2), or only austenite phase (high temperature θ_3), respectively. We denote the collection of snapshots with initial temperatures θ_i as $\boldsymbol{U}_i$, $i = 1, 2, 3$. If one employs the POD method directly to all the overall snapshots $\boldsymbol{U} = [\boldsymbol{U}_1, \boldsymbol{U}_2, \boldsymbol{U}_3]$ by putting all snapshots together, the characteristics of different blocks will be mixed and dispersed with each other, and that is why we are using the extended POD method to construct the eigenmodes using the snapshots collected in all the blocks. Taking all the blocks of snapshots simultaneously into account, the extended POD analysis can be formally represented in the following matrix form:

$$\boldsymbol{U} = \boldsymbol{\phi}\boldsymbol{C}, \tag{21}$$

where

$$\boldsymbol{U} = [\boldsymbol{U}_1\, \boldsymbol{U}_2\, \boldsymbol{U}_3], \qquad \boldsymbol{\phi} = [\boldsymbol{\phi}_1\, \boldsymbol{\phi}_2\, \boldsymbol{\phi}_3] \tag{22}$$

is a collection of snapshots and eigenmodes from each block, while the coefficient matrix is given as follows [3]:

$$\boldsymbol{C} = \begin{bmatrix} \boldsymbol{C}_1 & \boldsymbol{\phi}_1^T\boldsymbol{U}_2 & \boldsymbol{\phi}_1^T\boldsymbol{U}_3 \\ 0 & \boldsymbol{C}_2 & \boldsymbol{\phi}_2^T\boldsymbol{U}_3 \\ 0 & 0 & \boldsymbol{C}_3 \end{bmatrix}, \tag{23}$$

where all the entries in the matrix can be obtained once the blocks of snapshots are provided. For those situations where more snapshot blocks are available, the extended POD can be carried out in a similar manner.

4 RESULTS

A number of examples for nanostructures of different geometry and materials have been analyzed with the above model, and in what follows we present only a few representative calculations carried out for iron-based (FePd) nanostructures. Values of parameters for FePd can be found in [1]. In Fig. 1 we observe the formation of microstructures in two nanowires with increasing diameter-to-length ratio (same length, increasing diameter). With decreasing length of the nanowire, the microstructure acquires a more regular pattern as seen in Fig. 2 (left). In all these three cases $K_g = 1 \times 10^{-4}$. The analysis of the evolution of the microstructure for a square nanoplate is given in Fig. 2 (right) and Fig. 3. In this case, $K_g = 5 \times 10^{-5}$. All the results here have been obtained for $\theta_0 = 265K$ and presented for $\theta = 250K$. A typical number of degree of freedom in these finite element calculations is on the order of 100,000. Results on critical diameters of finite length nanowires will be presented elsewhere. Finally, we note that some initial three-dimensional modelling results with mesoscopic models were presented in [5].

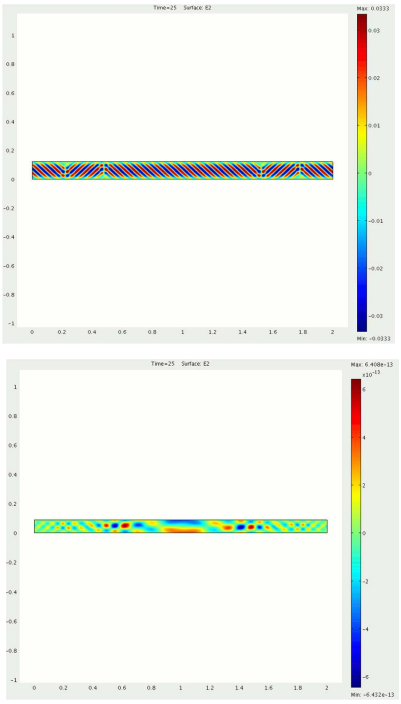

Figure 1: Size dependency of nanowires with increasing diameter-length ratio.

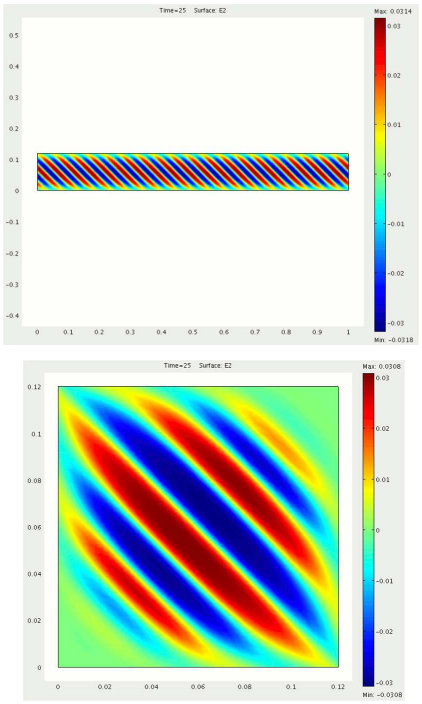

Figure 2: Microstructures in the nanowire of smaller length (left) and in the square nanoplate.

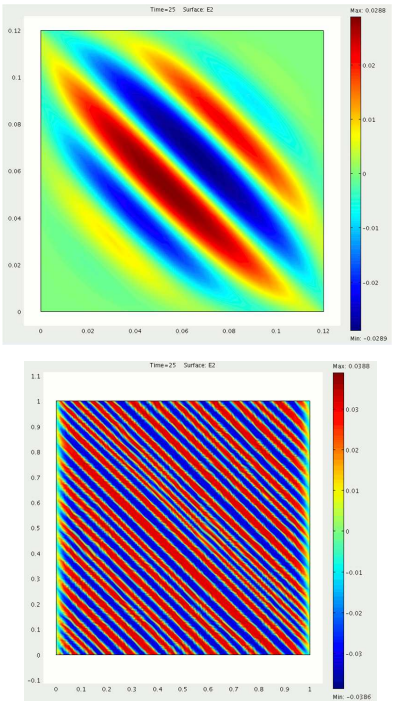

Figure 3: Evolution of microstructure in the square nanoplate.

5 Conclusions

In this contribution, we focused on the development of mesoscopic phase-field-type models for the description of strongly nonlinear coupled thermomechanical effects. Our main attention was on shape memory effects and phase transformations in low dimensional nanostructures. The resulting model was successfully implemented and solved based on a combination of the Chebyshev collocation method and the extended proper orthogonal decomposition. We reported several representative examples presenting results on the analysis of microstructure evolution in finite nanostructures with the developed models for finite nanowires and nanoplates.

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