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# Nanostructures with Shape Memory Effect: Modelling Coupled Dynamics

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**Abstract** — In this contribution we apply a phase-field (PF) modeling approach for the analysis of properties of shape-memory alloy (SMA) nanostructures, focusing on their complex microstructures and thermo-mechanical behavior. We have developed a model that includes domain walls, treated as a diffuse interface, which leads to a fourth-order differential equation in a strain based order parameter PF model. Arising numerical challenges have been overcome based on the isogeometric analysis (IGA). Microstructure evolutions for different geometries of SMA nanostructures under temperature- induced phase transformations have been studied and some typical examples are presented here.

**Keywords** — *Ginzburg-Landau theory; isogeometric analysis; phase- field models; nonlinear thermo-elasticity; low dimensional nanostructures; coupling*

## I. INTRODUCTION

There has been an increasing interest in using SMA nanotubes and other low dimensional nanostructures for nano-electromechanical (NEMS) and micro-electromechanical systems (MEMS), various engineering systems and devices, as well as for biomedical applications [1, 2]. These applications involve designing different geometries and using domain patterns for controlling distortions. In its turn, this motivates the need for a better of understanding of domain patterns and their thermo-mechanical properties in realistic and complex geometries for application development.

Among modeling approaches that have been used to study SMA dynamics [3, 4], we would like to especially emphasize the phase-field (PF) approach. Indeed, PF-based models have been used to study the phase transformations in SMA meso- and nano- structures [5, 6]. Broadly speaking, the PF models for SMAs can be divided into two groups. One is based on the kinetic model by using independent order parameter(s) (OPs). The second group combines the strain-based OP PF models. The implementation of models from the first group typically leads to models based on second-order differential equation(s) for microstructure evolution, while the implementation of models from the second group requires dealing with fourth-order differential equations in space. Due to strong (hysteretic-type) nonlinearities and coupling with structural and/or thermal physics, this leads to several computational challenges in both of these cases. The fourth order equations, in

particular, introduce a number of especially severe numerical challenges such as restrictions on the time-step (for discretization) and stencil (or grid) size [7].

Most of the above studies were carried out using traditional numerical methods, such as spectral collocation or the finite difference method. These methods typically lack geometrical flexibility, and most of the simulations based on these methods were performed on a cubic domain with periodic boundary conditions. However, other geometries become increasingly important in applications of SMAs, and there is a need for more flexible methods which can allow to model complex bigger domains with different boundary conditions. Another difficulty we face when designing computational methods for strain-based OP PF theories is to find an efficient discretization procedure for fourth-order spatial differential operators. Due to its geometrical flexibility and the possibility of generating globally smooth basis functions, we propose isogeometric analysis (IGA) as an efficient numerical method to solve the fourth-order PF model on various geometries.

IGA is a new computational method originally developed to avoid mesh generation bottle-necks during engineering analysis. It uses non-uniform rational B-splines (NURBS), a back-bone of CAD and animation technology, as basis functions. The use of rich basis functions provides the IGA with a unique capability to model geometry exactly, in many instances, while field variables can be approximated with enhanced accuracy. The IGA provides unique attributes of higher-order accuracy and robustness with the C 1- or higher-order continuity necessary for solving higher-order differential equations. The IGA has been successfully used to solve models based on the PF theories and higher-order differential equations (see [8, 9, 10] and references therein).

In this contribution we apply the IGA to study SMA nanostructures. Our PF model has been developed on the basis of the Ginzburg-Landau theory and consists of coupled equations of nonlinear thermoelasticity. The governing laws are introduced in the IGA framework using the variational formulation.

## II. MATHEMATICAL MODEL

All our results here are exemplified on the cubic-to-tetragonal phase transformations that occur in SMA alloys like

NiAl, FePd, InTl, etc. The cubic austenite phase is converted into tetragonal martensitic variants upon mechanical or thermal loadings (see Fig. 1).

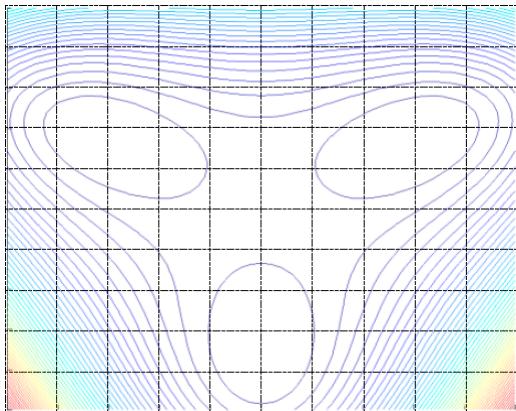


Fig. 1. Typical minima of the free energy function that corresponds to cubic-to-tetragonal phase transformation.

We have recently developed a mathematical model for the three-dimensional coupled thermo-mechanical analysis of SMAs [9, 10]. Our model has been derived from a free-energy functional using the Hamiltonian principle. Components of this functional in the 3D case are:

$$\begin{aligned}\mathcal{F}_{nop_{3D}} &= \frac{a_{31}}{2} [e_1 - E_0(e_2^2 + e_3^2)]^2 + \frac{a_{36}}{2} [e_4^2 + e_5^2 + e_6^2], \\ \mathcal{F}_{op_{3D}} &= \frac{a_{32}}{2} \tau(e_2^2 + e_3^2) + \frac{a_{33}}{2} e_3(e_3^2 - 3e_2^2) + \frac{a_{34}}{2} (e_2^2 + e_3^2)^2, \\ \mathcal{F}_{gradient_{3D}} &= \frac{k_g}{2} [(\nabla e_2)^2 + (\nabla e_3)^2],\end{aligned}$$

where  $e_j$  are components of strain tensor and  $a_{ij}$  are material-specific coefficients.

The unknowns are the displacement field  $\mathbf{u} = \{u_1, u_2, u_3\}^T$  and the temperature  $\theta$ . The problem is analyzed in the physical domain  $\Omega \subset R^3$ , which is an open set parameterized by Cartesian coordinates  $\mathbf{x} = \{x_1, x_2, x_3\}^T$ . We use of the Cauchy-Lagrange infinitesimal strain tensor. The governing equations can be written as follows (see [9,10] for details):

$$\begin{aligned}\dot{\mathbf{u}} &= \mathbf{v}, \\ \rho \dot{\mathbf{v}} &= \nabla \cdot \boldsymbol{\sigma} + \nabla \cdot \boldsymbol{\sigma}' + \boldsymbol{\sigma}_g + \mathbf{f}, \\ \rho \dot{\mathbf{e}} - \boldsymbol{\sigma}^T : (\nabla \mathbf{v}) + \nabla \cdot \mathbf{q} &= g,\end{aligned}$$

where the constitutive equations take the form:

$$\begin{aligned}\boldsymbol{\sigma} &= \frac{\partial}{\partial e_{ij}} (\mathcal{F}_{nop} + \mathcal{F}_{op}), \quad \boldsymbol{\sigma}' = \frac{\partial \mathcal{R}}{\partial \dot{e}_{ij}}, \quad \boldsymbol{\sigma}_g = \frac{\partial}{\partial e_{ij}} (\mathcal{F}_{gradient}) \\ \mathcal{R} &= \frac{\eta}{2} \sum_{i=1}^n \dot{e}_i^2,\end{aligned}$$

with the dissipation

where  $\mathbf{v}$  is the velocity and other notions are standard (see, e.g., [9, 10] and references therein).

### III. NUMERICAL FORMULATION

For its numerical implementation, the problem is reformulated in a weak form. We seek  $S = \{\mathbf{u}, \theta\} \in X$  such that  $B(W, S) = 0$  for all  $W \in X$ , with

$$\begin{aligned}B(W, S) = & \left( \mathbf{U}, \frac{\partial \mathbf{u}}{\partial t} \right)_\Omega + \left( \mathbf{V}, \rho \frac{\partial \mathbf{v}}{\partial t} \right)_\Omega + \left( \Theta, c_v \frac{\partial \theta}{\partial t} \right)_\Omega - (\mathbf{U}, \mathbf{v})_\Omega \\ & + (\nabla \mathbf{V}, \boldsymbol{\sigma})_\Omega + (\nabla \mathbf{V}, \eta \mathbf{v})_\Omega - (\mathbf{V}, \mathbf{f})_\Omega + (\mathbf{V}, \boldsymbol{\sigma}_g)_\Omega \\ & + (\nabla \Theta, \kappa \nabla \theta)_\Omega - (\Theta, g)_\Omega - (\chi_d)_\Omega,\end{aligned}$$

where the interested reader can consult [9, 10] for additional details.

For the space discretization of the model we have used the Galerkin with the NURBS basis functions. We have also used the generalized- $\alpha$  method for time integration. This method has already found a wide range of applications in the computations where control over high frequency dissipation is useful, such as, for example, nonlinear structural dynamics and turbulence (e.g., [8] and references therein). We also note that it has been applied (in the IGA framework) for the computations of other nonlinear models such as the Cahn-Hilliard equation and the isothermal Navier-Stokes-Korteweg equation. Here, we also take advantage of the fact that generalized- $\alpha$  method permits a straightforward one-step discretization of a coupled system of first- and second-order ordinary differential equations, which is precisely the structure of our semi-discrete form.

### IV. RESULTS AND DISCUSSION

In this section, we present numerical studies on nanostructured SMAs subjected to temperature induced loadings. The microstructure evolution and its effect on thermo-mechanical properties in SMA specimens have been analyzed. The developed thermo-mechanical model described has been rescaled in the spatio-temporal domains for numerical convenience, and the rescaled equations have then been converted into the rescaled weak formulation, as described in the previous section. The scaling constants for the spatial and temporal domains are 1.2645 nm, and 0.901 ps, respectively. All calculations presented here have been carried out for  $Fe_{70}Pd_{30}$ .

As mentioned earlier, applications exist where different geometries are required, often beyond cubic domains. While we carried out a series of numerical experiments for different nanostructured SMA geometries, we provide here typical examples for slab geometries. For the thermal physics, insulated boundary conditions have been used for all the simulations. We discretized the domains using B-spline or NURBS basis functions with  $C^k$  global continuity for  $k \geq 1$ .

Firstly, we performed a refinement study of the spatial mesh, holding the time step fixed at a sufficiently small value. The spatial mesh has been refined using the classical h-refinement and the new paradigm for mesh refinement introduced by IGA, k-refinement, in which the order of the basis functions is elevated, but their global continuity is likewise increased. The mesh convergence studies have been carried out on a cube with its side equal to 32nm, periodic boundary conditions and starting with initial random conditions. The cube was discretized using three meshes: two meshes with uniform

$C^1$ -continuous quadratic B-spline with 34 and 50 basis functions in each direction and third mesh with uniform cubic  $C^2$ -continuous B-splines with 69 basis functions in each direction. Then, the cube was quenched to (non-dimensional) temperature corresponding to  $\tau = -1.2$  and allowed to evolve for a sufficiently long time till it was stabilized. We analyzed the cut lines of OP deviatoric strains  $e_2$  and  $e_3$  along the normalized distance  $\hat{x}$  between two points (0,15,15) nm and (32,15,15) nm on the opposite surfaces of the cube, for all three meshes. The maximum error of the coarsest mesh is 2 % with respect to the fine mesh, thus indicating that good results can be obtained by using the IGA even with the coarsest mesh.

Secondly, we analyzed the impact of the time step size on the solution holding the spatial discretization fixed. The simulations have been performed on a cube with its sides equal to 50 nm by using periodic boundary conditions and starting with an initial random condition. We have used three different fixed time steps 0.225 ps, 0.4505 ps, and 0.901 ps. Cut lines of the OPs  $e_2$  and  $e_3$  have been analyzed along the diagonal (0,0,0) – (50,50,50) nm, at time 0.427 ns, and the time evolution of the average temperature coefficient  $\tau$  was studied. The maximum error in the OPs of the largest time step (0.901 ps) with respect to the smallest one (0.225 ps) is just 0.02 %. Hence, the largest time step can be safely used.

Finally, we generated a thermally induced microstructure in SMA specimens of different geometries, by quenching them to the temperature corresponding to  $\tau = -1.2$  and allowing the system to evolve. All the simulations have been started with a small amplitude random initial condition, corresponding to the austenite phase, for the displacement vector  $u$ . Periodic, constrained or stress-free boundary conditions have been used on different surfaces for the structural physics. Our example is for a slab geometry which was discretized using uniform  $C^1$ -quadratic B-spline basis functions (while for other geometries, e.g. the cylindrical tube and tubular torus, we used the NURBS basis functions).

Now, if the domain size is reduced to half in one of the directions ( $L_{x1} = L_{x3} = 60$  nm and  $L_{x2} = 30$  nm) and microstructures are allowed to evolve in the slab domain, we obtain morphology evolution as shown in Fig. 2. The three variants exist in approximately equal proportions forming chevron patterns as shown in the last sub-plot of Fig. 2. The microstructure in slab domain (the last sub-plot) is morphologically different than the cube domain. The primary bands of  $M_1$  and  $M_3$  variants are prominent and intersected by a thin secondary band of the  $M_2$  variant at  $90^\circ$ . The width ratios of primary and secondary bands are in agreement with the cube specimen. These results clearly demonstrate the influence of geometry on microstructure evolution and morphology in SMA nanostructures.

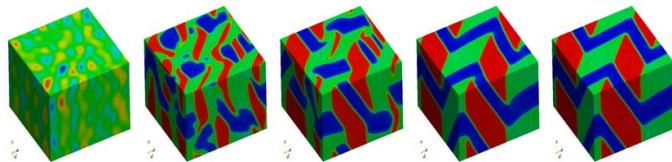


Fig. 2. (Color online) Microstructure morphology evolution in a slab specimen with  $L_{x1} = L_{x3} = 60$  nm and  $L_{x2} = 30$  nm at time  $t$  (red, blue, and green colors represent  $M_1$ ,  $M_2$ , and  $M_3$  variants, respectively). (a)  $t = 0.036$  ns, (b)  $t = 0.09$  ns, (c)  $t = 0.18$  ns, (d)  $t = 0.27$  ns, (e)  $t = 1$  ns

## V. CONCLUSIONS

We have applied a newly developed phase-field model in the analysis of properties of shape memory alloy nanostructures, paying a special attention to complex microstructure evolution and coupled thermo-mechanical behavior. Since the model includes domain walls, treated as a diffuse interface, we had to deal with high order derivatives in our strain-based order parameter phase-field model. This led to a range of computational difficulties which were overcome by using the isogeometric analysis. Shape memory alloy nanostructures of different geometries were studied with the major focus given to microstructure evolution, and some typical examples of these studies were presented. These results can be used in coupling thermo-mechanical properties with band structure studies of shape memory alloy nanostructures, leading to more precise prediction of optoelectronic properties of these structures for application development.

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