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ISOGEOMETRIC ANALYSIS IMPLEMENTATION OF THE PHASE-FIELD MODEL FOR 3D CUBIC-TO-TETRAGONAL TRANSFORMATIONS IN SHAPE MEMORY ALLOYS

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Key words: Shape memory alloys, Thermo-mechanical modeling, Isogeometric analysis, Phase-field model, Microstructure evolution.

Summary. In this contribution, we present the isogeometic analysis implementation of a 3D shape memory alloy (SMA) model based on the phase-field theory. The 3D phase-field model is developed for the cubic-to-tetragonal transformations using the Ginzburg-Landau framework. The developed model has a bi-directional coupling via strain, strain rate, and temperature, which is usually neglected in the models for SMAs in the literature. In addition to thermo-mechanical coupling, the model is characterized by inherent nonlinearity and higher (fourth) order differential terms. The isogeometric analysis, a finite element methodology based on the non-uniform rational B-spline (NURBS) basis functions, offers several advantages in solving complex problems with higher order differential terms. Here we report new results on microstructure evolution for the 3D cubic-to-tetragonal transformations in SMAs. In particular, based on the isogeometric analysis implementation, we present the results on numerical simulations of a SMA domain subjected to externally applied body loads.

1. INTRODUCTION

The atomic rearrangements in shape memory alloys cause solid-to-solid phase transformations and impact interesting properties of shape recovery upon thermal and/or mechanical loadings. As the phase transformations occur fast (at the speed of sound) in the SMA materials, it is difficult to observe them experimentally. The mathematical models have been developed to describe phase transformations to gain insights into dynamics and thermo-mechanical behavior of SMAs.

In this contribution, we use the phase-field (PF) theory to study the martensitic phase transformations in SMAs. The PF theory has been widely used to derive mathematical models in order to describe complex microstructures, stress and temperature induced phase transformations of materials. The resulting mathematical models are usually formulated in the variational settings. We are particularly interested here in the cubic-to-tetragonal phase transformations of FePd alloy due to its thermal, mechanical, and magnetic coupling and biocompatibile properties [1, 2]. Several PF approaches have been developed to understand the dynamic properties of SMAs (see, e.g., the review paper [3]). Here, we use the PF theory developed on strain based order parameters (OPs). Most of the models developed on this theory have used various isothermal assumptions [4, 5, 6], despite the fact that SMAs exhibit temperature dependent thermo-mechanical behavior. In the meantime, recently developed fully coupled 2D and 3D thermo-mechanical models based on the PF theory and the Ginzburg-Landau free energy for SMAs are now available [7, 8, 9].

The SMA phase transformations lead to development of interfaces between two phases, either between the austenite-martensite or martensite variants. The variations between different phases in a domain can be modeled by a sharp or diffuse interface models, of which diffuse interfaces tend to be quite popular [10]. In the PF model, using a strain based OP, this can be mathematically achieved by introducing a smooth continuously varying (diffused) interface via higher (fourth) order differential terms. Traditionally, the fourth-order partial differential terms have been treated numerically by using finite-difference, finite-volume, or spectral methods [5, 11]. We have developed a new numerical formulation based on the finite element method, called isogeometric analysis (IGA), using non-uniform rational B-spline (NURBS) basis functions. IGA can numerically solve the fourth order differential equations directly, with C^1 continuous elements as compared to the traditional approach of splitting the fourth-order terms into two second-order terms. Apart from this, IGA also offers advantages in exact geometric representations, higher-order continuity, accuracy and robustness [12]. In [7], we presented the first results of microstructure evolution for the 3D cubic-to-tetragonal phase transformations in SMAs using the IGA. In this paper, we study the microstructure evolution of a SMA domain subjected to externally applied body loads.

In the following sections, we describe the mathematical model and its numerical implementation based on the IGA. We present the description of martensitic PTs in SMAs subjected to externally applied body loads followed by the conclusions.

2. MATHEMATICAL MODEL

The temperature dependent properties of SMAs can be modeled by describing the free energy as a function of temperature and order parameter (OP). The mathematical model of SMA dynamics can be described by conservation equations of mass, linear momentum, and energy balance [13]. The thermo-mechanical coupled SMA model is given as follows

$$\dot{\mathbf{u}} = \mathbf{v}, \tag{1}$$

$$\rho\dot{\mathbf{v}} = \nabla\cdot\boldsymbol{\sigma} + \nabla\cdot\boldsymbol{\sigma}' + \mathbf{f}, \tag{2}$$

$$\rho\dot{e} - \boldsymbol{\sigma}^T : (\nabla\mathbf{v}) + \nabla\cdot\mathbf{q} = g, \tag{3}$$

where ρ is the mass density, $\mathbf{q}$ is the Fourier heat flux vector, $\boldsymbol{f}$, and g are external mechanical (body) and thermal loadings. The stress tensors $\boldsymbol{\sigma}$ and dissipation stress tensors $\boldsymbol{\sigma}'$ are defined as

$$\boldsymbol{\sigma} = \frac{\partial\mathscr{F}}{\partial e_{ij}}, \qquad \boldsymbol{\sigma}' = \frac{\partial\mathscr{R}}{\partial\dot{e}_{ij}}. \tag{4}$$

The appropriate free energy potential well is chosen to represent the 3D cubic-to-tetragonal phase transformations in SMAs. The potential well $\mathscr{F}$ with one minima above the threshold temperature, three minima below the threshold temperature, and the degenerate state existing near the critical temperature can be described as

$$\begin{aligned}\mathscr{F} = \quad & \frac{a_{31}}{2}\left[e_1 - E_0(e_2^2+e_3^2)\right]^2 + \frac{a_{36}}{2}\left[e_4^2+e_5^2+e_6^2\right] + \frac{a_{32}}{2}\tau(e_2^2+e_3^2) + \frac{a_{33}}{2}e_3(e_3^2-3e_2^2) \\ & + \frac{a_{34}}{2}(e_2^2+e_3^2)^2 + \frac{k_g}{2}\left[(\nabla e_2)^2 + (\nabla e_3)^2\right],\end{aligned} \tag{5}$$

where a_{ij}, E_0, k_g are the material parameters and τ is the rescaled temperature coefficient [4]. The e_i are the strain components following the Voigt's notation defined by using the Cauchy-Lagrange strain tensor $e_{ij} = \left[(\partial u_i/\partial x_j) + (\partial u_j/\partial x_i)\right]/2$ (using the repeated index convention) and $\mathbf{u} = \{u_i\}|_{i=1,2,3}$ are the displacements along *x*, *y*, and *z* directions, respectively. We use the Rayleigh dissipation function $\mathscr{R}$ defined as

$$\mathscr{R} = \frac{\eta}{2}\sum_{i=1}^{n}\dot{e}_i^2, \tag{6}$$

where η is the dissipation coefficient [4].

The bi-directional thermo-mechanical coupling is established between equations (1)-(3) via temperature θ, strain, and strain rate. The weak form of the governing equations is numerically implemented in the isogeometric analysis framework (refer to [7] for more details). The domain is discretized by using a Galerkin finite element scheme with C^1-continuous NURBS basis functions, necessary in this case for solving the fourth-order PDEs [12, 14].

3. NUMERICAL SIMULATIONS

The numerical simulations have been conducted on the SMA nano-cube domain of side 80 nm, a sufficient domain size to study the phase evolution phenomena [7]. The material parameters of FePd can be found in [4]. These materials are used in nano- and bio-nanotechnology, including the development of nanotubes for drug delivery [2] and other applications [1]. The domain consists of 80 univariate second-order NURBS basis functions in each direction. The computations have been carried out on the 64 processors (4 processors in each direction) at the high-performance clusters of the Sharcnet computational facilities in Canada. The total number of elements, global, and local basis in a typical run are 512k, 681k, and 27, respectively. Here we provide results of one of the considered examples. The external body load $\boldsymbol{f} = \{10^{-4}, 0, 0\}$ is applied in the domain in the dimensionless units and the system is allowed to evolve. The microstructure at the 700'th time step is shown in Figure 1. The fully coupled 3D thermo-mechanical equations have been solved under the fully periodic boundary conditions, starting from the initial random condition corresponding to the austenite phase at temperature 295 K as shown in Figure 1(a). The three tetragonal martensitic variants (strains) are self-accommodated in the x, y, and z directions in favor to the applied body loading as shown in Figures 1(b)–1(d).

4. CONCLUSIONS

The fully coupled thermo-mechanical 3D model has been developed for the cubic-to-tetragonal phase transformations in SMAs. The model is numerically implemented based on the isogeometric analysis. The numerical simulation results, using external body loads, indicate the accommodation of three tetragonal variants in favor of the mechanical loading. The 3D simulations with complex loading on SMA domains are being investigated.

Acknowledgments

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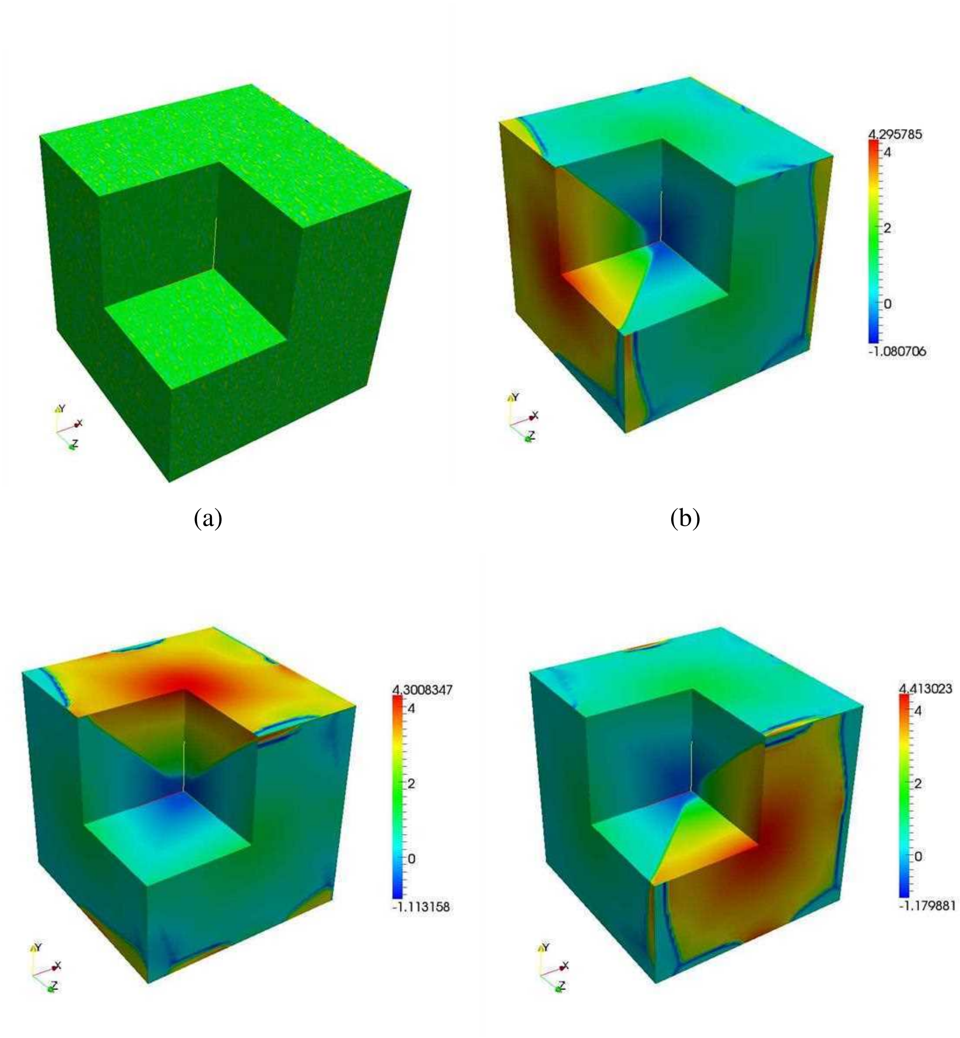

(a) (b)

(c) (d)

Figure 1. (Color online) Microstructure evolution in a cube domain: (a) starting with random initial condition, and evolved martensitic variants (strains) in the (b) x, (c) y, and (d) z direction on application of external body load (a portion of cube is not shown for better clarity).

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1035 Abstract 198	1100 Abstract 11	1125 Abstract 13	1150 Abstract 19	1215 Abstract 37	1240 Abstract 51
Mechanical and functional response of NiTi based Belleville washers	Use of shape memory alloys for structural fire protection - experimental and parametric study	Effect of heating speed and degree of transformation on the functional fatigue of Ni-Ti shape memory wires	Effect of pressure on magnetorheological fluids in shear and flow mode	Isogeometric analysis implementation of the phase-field model for 3d cubic-to-tetragonal transformations in shape memory alloys	Design and manufacturing of a morphing flap for wind turbine blades
F. Furgiuele, C. Maletta, E. Sgambitterra	M.B. Wong, H. Sadiq, J. Liu	G. Scirè Mammano, E. Dragoni	A. Spaggiari, E. Dragoni	R. Dhote, H. Gomez, R. Melnik, J. Zu	P. B. Andersen, H.A. Madsen

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Key words: Shape memory alloys, Thermo-mechanical modeling, Isogeometric analysis, Phase-field model, Microstructure evolution.

Summary. *Shape memory alloys (SMAs) are a prime example of materials exhibiting multi-scale and multiphysics behaviors and complex microstructures. This contribution focuses on the multiphysics (thermo-mechanical) behavior of SMAs and has the dual objectives of model development and its numerical implementation. The phase-field model can describe the complex microstructure, stress and temperature induced phase transformations in the variational framework. The strain based order parameter 3D phase-field model is developed for the cubic-to-tetragonal transformations using the Ginzburg-Landau theory [1]. The developed model has a bi-directional coupling via strain, strain rate, and temperature. In addition to thermo-mechanical coupling it is characterized by inherent nonlinearity and higher (fourth) order differential terms. The bi-directional coupling has been usually neglected in a studies of SMA properties in the literature, and most of the model developments have been carried out under*

the assumption of isothermal phase transformations (e.g. [2]). The isogeometric analysis, a finite element methodology based on the non-uniform rational B-spline (NURBS) basis functions, offers several advantages in solving complex problems with higher order differential terms [3]. Here we report new results on microstructure evolution for the cubic-to-tetragonal transformations in SMAs. The tensile test on the 3D specimens has shown a significant impact of thermo-mechanical coupling on the mechanical properties.

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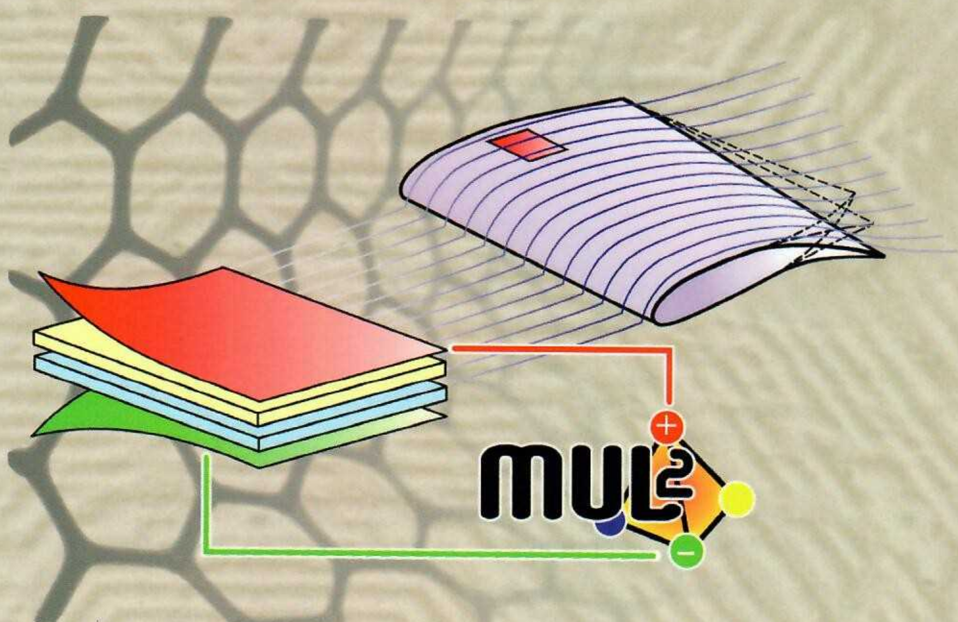

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