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3D coupled thermo-mechanical phase-field modeling of shape memory alloy dynamics via isogeometric analysis

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ABSTRACT

The paper focuses on numerical simulation of the 3D phase-field (PF) equations for modeling cubic-to-tetragonal martensitic transformations in shape memory alloys (SMAs), their complex microstructures and thermo-mechanical behavior. The straightforward solution to the fourth-order diffuse interface 3D PF equations, based on the Landau–Ginzburg potential, is numerically solved using an isogeometric analysis. We present microstructure evolution in different geometries of SMA nanostructures under temperature-induced phase transformations to illustrate the geometrical flexibility, accuracy and robustness of our approach. The simulations successfully capture the dynamic thermo-mechanical behavior of SMAs observed experimentally.

1. Introduction

As a result of their interesting solid-to-solid phase transformations and coupled-physics (thermo-mechanical, magnetostrictive) properties, shape memory alloys (SMAs) have been used as micro- and nano-actuators and sensors for a broad spectrum of applications. Recently, there has been a major research focus on using SMA nanostructures [1–7] for nanoelectromechanical (NEMS) and microelectromechanical systems (MEMS) and biomedical applications. These applications involve designing different geometries and using domain patterns for controlling distortions [2]. All of these motivate the need for understanding domain patterns and their thermo-mechanical properties in realistic and complex geometries for better application development.

Several modeling approaches have been used to study the SMA behaviors [8–13]. In particular, phase-field (PF) models have been widely used to study the phase transformations in SMA meso- and nano-structures [14–17]. Broadly, PF models for SMAs can be divided into two approaches: the kinetic model using independent order parameter(s) (OPs) (see, for example, [18,19]) and the strain-based OP PF models (e.g., [14,20]). The first approach often leads to a second-order differential equation for microstructure evolution, while the second approach typically leads to a fourth-order differential equation in space.

Here, we focus on the second approach and use the PF methodology. Several 3D PF models for SMAs have been proposed in the literature. The majority of these models do not account for the dynamics of SMAs, but only relax the quasi-static microstructures using a dissipation potential or directly assume a quasi-static response. Moreover, most models assume isothermal conditions, which neglects the thermo-mechanical coupling of SMAs, a significant modeling limitation. The nucleation and growth of martensitic transformations have been widely studied by using the kinetic time-dependent Ginzburg–Landau models [18,19,21–24,16,25,26]. Using the strain-based OP PF models, the temperature- and stress-induced phase transformations have been studied for SMAs [27,14]. The full 3D dynamic model in its generality was first formulated by Melnik et al. [28] and the first model-based explanation of thermally-induced hysteresis was discussed in [29,30]. From a computational perspective, most of the above studies used traditional numerical methods, such as spectral collocation or the finite difference method. These algorithms typically lack geometrical flexibility, as the majority of the above studies were performed on a cubic domain with periodic boundary conditions. However, complex geometries exist in real life, and there is a need for more flexible methods which can allow to model geometrically complex and large domains with different boundary conditions. When geometrical flexibility is needed, the finite element method is the natural choice. However, if we do not want to include additional

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variables, solving fourth-order equations with the finite element method requires globally smooth basis functions, and this has proved very difficult to achieve with traditional finite elements. Due to its geometrical flexibility and the possibility of generating globally smooth basis functions, we propose isogeometric analysis (IGA) as an effective numerical method to solve the fourth-order PF model on non-trivial geometries.

IGA is a new computational method originally developed to avoid mesh generation bottlenecks during engineering analysis [31,32]. It was originally developed using non-uniform rational B-splines (NURBS), a backbone of CAD and animation technology, as basis functions, but it was later extended to accommodate other widely-used functions in the CAD community, such as, for example, T-Splines [33–36]. IGA has been successfully applied to problems of fluid mechanics [37–40], solid mechanics [41–46], fluid–structure interaction [47,48], and condensed-matter physics [49–52]. The use of rich basis functions provides IGA with a unique capability to model geometry exactly, in many instances, while field variables can be approximated with enhanced accuracy [53,54]. IGA provides unique attributes of higher-order accuracy and robustness with the $\mathcal{C}^1$- or higher-order continuity necessary for solving higher-order differential equations in a variational formulation. IGA has been successfully used to solve the PF theories and higher-order differential equations using Galerkin variational formulations [55–59,44,60–62]. Additionally, it has been recently shown by Gomez et al. [63] that the possibility of generating highly-smooth basis functions also permits deriving collocation methods that approximate directly the strong form of the equations, an approach that is not pursued in this work.

We recently illustrated the flexibility of the IGA approach by applying it to a 2D PF model for SMAs [64]. Here, we solve a 3D theory for cubic-to-tetragonal phase transformations in nanostructured SMAs using IGA. As the 2D model [64] and 3D models have distinct requirement related to the symmetry of martensitic variants, their free energy functional have distinct expressions. As a consequence, the expressions for constitutive relationships and the thermo-mechanical coupling term are distinct. The 3D constitutive relationships and the thermo-mechanical coupling term do not reduce to the 2D constitutive relationships and the thermo-mechanical coupling term. As a result, the models and numerical implementations of the 2D and 3D models are distinct.

The 3D coupled equations of nonlinear thermoelasticity are developed using the PF model and the Ginzburg–Landau theory. The governing laws are introduced in the IGA framework using a variational formulation. Several numerical studies have been performed to illustrate the flexibility, accuracy and stability of the approach. Based on the above tasks, the paper is organized as follows. In Section 2, the governing coupled equations of nonlinear thermoelasticity and solid–solid phase transformations are presented. The details of the numerical implementation of the SMA governing equations in the IGA framework are given in Section 3. The developed methodology is exemplified with 3D numerical simulations on nanostructured SMA domains subjected to thermally-induced phase transformations in Section 4. Finally, the conclusions are given in Section 5.

2. Mathematical model of SMA dynamics

The cubic-to-tetragonal phase transformations occur in SMA alloys like NiAl, FePd or InTl. The cubic austenite phase is converted into tetragonal martensitic variants upon mechanical or thermal loadings as schematically shown in Fig. 1(a).

We have recently put forward a mathematical model for the 3D coupled thermo-mechanics of SMAs [65]. Our model can be derived from a free-energy functional using Hamiltonian mechanics. The unknowns are the displacement field $\boldsymbol{u} = \{u_1, u_2, u_3\}^T$ and the temperature θ. We assume that the problem takes place on the physical domain $\Omega \subset \mathbb{R}^3$, which is an open set parameterized by Cartesian coordinates $\boldsymbol{x} = \{x_1, x_2, x_3\}^T$. We will make use of the Cauchy–Lagrange infinitesimal strain tensor $\boldsymbol{\epsilon} = \{\epsilon_{ij}\}$, whose components are defined as $\epsilon_{ij} = (u_{i,j} + u_{j,i})/2$, $i,j \in \{1,2,3\}$, where an inferior comma denotes partial differentiation (e.g., $u_{i,j} = \partial u_i / \partial x_j$). Using the strain tensor, we define the strain measures e_i, for $i = 1, \ldots, 6$ as follows:

$$\begin{Bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \\ e_6 \end{Bmatrix} = \left[\begin{array}{c|c} \mathbb{D}_3 & \mathbb{O}_3 \\ \hline \mathbb{O}_3 & \mathbb{I}_3 \end{array}\right] \begin{Bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \epsilon_{23} \\ \epsilon_{13} \\ \epsilon_{12} \end{Bmatrix}, \tag{1}$$

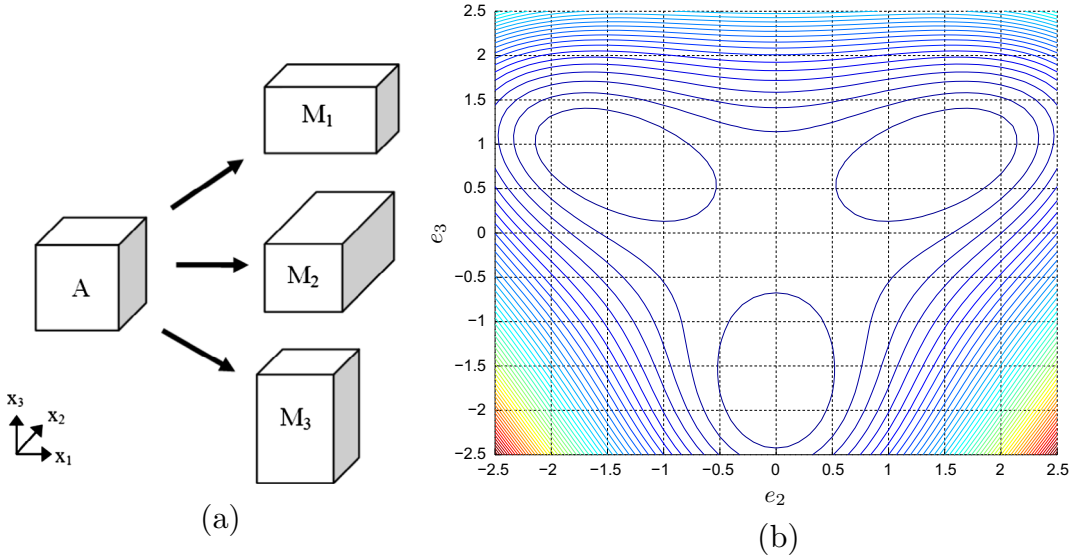

Fig. 1. Cubic-to-tetragonal phase transformations (a) schematic of microstructures: austenite (A), and martensite variants (M_1, M_2, M_3) (b) free energy function plot at $\tau = -1.2$ (see Eq. (4)).