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Modeling of coupled phase transformation and reorientation in shape memory alloys under non-proportional thermomechanical loading

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ABSTRACT

In the present study, a new 3D thermodynamic coupled model is proposed for SMAs. The behavior of SMA structures is described through several strain mechanisms, each associated with its proper internal variables. This model is built to capture the particular behavior of SMAs when subjected to complex loading, namely non-proportional thermomechanical loading. To achieve this task, a new approach to describe the martensitic reorientation mechanism has been introduced in conjuction with a new method to account for forward and reverse transformation. Thermomechanical coupling, related to dissipation and latent heat is fully implemented. The validity of the model is demonstrated by comparing experimental results of complex thermomechanical loading paths of SMA structures with numerical simulations.

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1. Introduction

Shape memory alloys (SMAs) are metallic materials named after the discovery of their unique capability to retrieve their original shape when their temperature is increased after a mechanical loading. It is the result of the transformation at the crystallic level between the two key solid phases that the material can adopt, austenite and martensite. The difference between these two phases lies on the architecture of the crystalline structure, which varies between a cubic-like configuration in austenite and a less symmetric configuration in martensite (Patoor et al., 2006; Otsuka and Wayman, 1999). Several different effects have been investigated, for instance superelasticity and actuation, depending on the thermomechanical conditions imposed. Such capabilities rank those materials in the wider class of smart materials, according to their multiphysics (mechanical-thermal) coupling.

All those effects are based on the fact that such martensitic transformation can take place in both ways, and that the martensitic phase can be reoriented under the action of mechanical forces. The direction from austenite to martensite is systematically defined as forward transformation, whereas the inverse procedure is called reverse transformation. This phase transformation can be the result of a change in temperature between critical values, and/or a change in the mechanical state. In the absence of applied stress, forward transformation occurs between martensite start (M_s) and finish (M_f) temperatures and reverse transformation between austenite start (A_s) and finish (A_f) temperatures. The development of appropriate stress

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levels can also lead to phase transformation. In particular, applying a mechanical loading/unloading cycle above A_f demonstrates the effect of superelasticity in SMAs. During forward transformation, the transformation starts at a critical, temperature-dependent stress. A stress plateau is observed in the uniaxial stress-strain diagram, before the start of the elastic section of martensite. In the case of mechanical loading at temperatures above A_f, the strain that appears between the two elastic sections on the stress-strain diagram corresponds to a transformation strain. This strain is fully recovered after reverse transformation has finished during unloading.

Martensite is the phase that appears at low temperatures/high stress state and consists of zones with different orientation directions found in a single crystal, called variants. Two main forms, distinguished on the basis of the configuration of variants, are observed: twinned martensite, for which the variants appear in multiple directions and form a self-accommodated assembly; and detwinned or oriented martensite, for which a principal direction of variants dominates the martensitic composition (Merzouki et al., 2010). Contrary to the two-way direction of phase transformation, the transition between these two crystallic configurations occurs in one direction, resulting to detwinned martensite only and is called orientation or detwinning. This occurs with the help of mechanical working, when stress is increased between critical levels. Such oriented martensite can still be reoriented if the direction of mechanical forces change. Appropriate combination of orientation and phase transformation processes result in the characteristic shape memory effect (Lagoudas, 2008).

The properties of shape memory and superelasticity render SMAs an interesting material sought to be utilized in practical applications in the last twenty years (Lecce and Concilio, 2014; Barbarino et al., 2014). A significant increase in the interest given to SMAs in publications and patents has recently been observed (Mohd Jani et al., 2014). Specifically, innovative systems were introduced in automotive and aerospace industries (Hartl and Lagoudas, 2007; Van Humbeeck, 1999). SMAs have also found particularly extended use in biomedical applications (Auricchio et al., 2015; Morgan, 2004). This wide array of applications motivates research to develop mathematical models able to capture their particular thermomechanical behavior (Khandelwal and Buravalla, 2009). These models aim at being utilized in robust computational tools, mostly Finite Element Analysis (FEA) methods. Their contribution is associated with the assistance provided to engineers to design SMA actuators and conceive innovative products.

In recent years, various phenomenological models have been proposed to explain the physics behind SMA behavior (Cisse et al., 2015). They focus on the macroscopic variables, allowing for relatively simple numerical implementation with respect to micromechanical approaches based on the physics of the crystalline structure (Patoor and Berveiller, 1997; Lagoudas et al., 2006). The primary macroscopic variable taken in mind in such models is the martensitic volume fraction (MVF). The actual representation of phase transformation in the macroscopic level is the change of the concentration of martensite in the material, thus justifying this consideration (Hartl et al., 2010; Chemisky et al., 2011; Lexcellent et al., 2006). The direction of strain appearing during transformation is taken in mind using necessarily a tensorial variable that depends on the loading conditions (Luig and Bruhns, 2008). Generally, these models have proven sufficiently accurate in capturing the material behavior under unidirectional loading (Peultier et al., 2008).

The effect of orientation has also been investigated in recent works (Ameduri et al., 2015; Sedlák et al., 2012; Saleeb et al., 2011; Saint-Sulpice et al., 2009). These models add the feature of simulating three-dimensional loading paths to previous simpler models (Boyd and Lagoudas, 1994; Brinson, 1993; Saleeb et al., 2001). Interesting experimental work has been carried out with respect to such loading (Bouvet et al., 2004; Grabe and Bruhns, 2009; Sittner et al., 1995). Reorientation consists in the change of the orientation of the martensite variants in existing martensite volume, without inducing further transformation. The procedure of reorientation has a visible effect on the preferred direction of inelastic strains, whereas detwinning mostly concerns their magnitude (Liu and Favier, 2000; Popov and Lagoudas, 2007). In certain models (Panico and Brinson, 2007; Helm and Haupt, 2003; Arghavani et al., 2010) and subsequent works, two different volume fractions for martensite are considered as driving material properties, one for twinned and one for the detwinned part. This proves a useful consideration, since the evolution of the martensitic strain can be associated to thermally induced and stress induced forward transformation. However, most of these models operate under the assumption that there is a direct relation between the stress induced martensitic fraction and an equivalent transformation strain magnitude, as investigated in Souza et al. (1998); Juhász et al. (2001); Taillard et al. (2008).

In this paper, a phenomenological model based on the physical interpretation of the processes that occur inside a SMA polycrystal is developed. The notion of mean transformation strain inside the martensitic volume discussed in the articles of Peultier et al. (2008); Chemisky et al. (2011) is examined from a macroscopic point of view to redefine the principles of reorientation, forward and reverse transformation. This leads to the introduction of independent scalar rate variables which drive each of the three strain mechanisms. Accordingly, a robust formalism is presented in terms of thermodynamics which is based on a Gibbs free energy potential.

Moreover, the scope of this work extends to providing a general framework for addressing the numerical resolution of multiple strain mechanisms simultaneously activated, allowing for adding even more inelastic strain mechanisms. Motivated by the work of Auricchio et al. (2014), each mechanism is thought to have its proper activation criterion. These criteria take the form of yield functions, depending on internal variables. Based on simple observations, the methodology for carrying out the numerical algorithm is presented and the mechanical and thermal tangent moduli are calculated. Furthermore, recognizing the strong coupling of thermomechanical effects on SMA behavior (Peyroux et al., 1998; Morin et al., 2011), the heat caused by mechanical working is calculated under the scope of multiple mechanisms in play. This investigation is able to cover the issue of latent heat which affects mechanical tests in superelasticity (Brinson et al., 2004; Hartl and Lagoudas, 2008).

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