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Constitutive model for shape memory alloys including phase transformation, martensitic reorientation and twins accommodation

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ABSTRACT

This paper deals with the thermomechanical modeling of the macroscopic behavior of NiTi shape memory alloys (SMAs). A phenomenological 3D-model, based on thermodynamics of irreversible processes is presented. Three main physical mechanisms are considered: the martensitic transformation, the reorientation of martensite and the inelastic accommodation of twins in self-accommodated martensite. The description of such strain mechanisms allow an accurate analysis of SMA behavior under complex thermomechanical paths, especially when transformation occurs at low stress level. Moreover, some key characteristics such as tension–compression asymmetry and internal loops inside the major hysteresis loop are taken into account. Numerical simulations for various theromechanical loading paths are presented to illustrate the present model capability to capture the complex behavior of SMAs.

1. Introduction

Shape memory alloys are materials which present important reversible inelastic deformation, as a result of a thermoelastic martensitic transformation. Depending on testing temperature, strain which appears upon mechanical loading or cooling under stress are recovered after unloading and/or heating. Resulting effects, such as large recoverable strains, are widely used in innovative devices. Three main behaviors of the SMAs are utilized in most of the applications: the superelastic behavior, the constrained recovery and the thermal actuation (Otsuka and Wayman, 1998). To enhance applications using these alloys, there is a growing need to predict their response when a complex thermomechanical path is applied. An accurate model, which can predict these behavior is a valuable tool that have to be included in the design process.

From these last 30 years, several research teams have developed models to account for the behaviors observed in shape memory alloys. First models were phenomenological ones, describing superelastic 1D loadings (Tanaka, 1986; Liang and Rogers, 1990) or 3D loadings using a formulation derived from classical plasticity (Bertram, 1982). In the 90's, a new class of phenomenological models appeared, based on a phase diagram and developed within a thermodynamic framework. These models were able to simulate more complex thermomechanical paths like cooling under constant stress or shape memory effect (Liang and Rogers, 1992; Brinson, 1993; Raniecki and Lexcellent, 1994; Boyd and Lagoudas, 1996; Lexcellent and Leclercq, 1996; Brinson and Bekker, 1998; Bo and Lagoudas, 1999a). The latest models were implemented in FEA packages and used to design devices with complex shapes under thermomechanical paths (Qidwai and Lagoudas, 2000b; Bouvet et al., 2004; Peultier et al., 2006; Panico and Brinson, 2007; Popov and Lagoudas, 2007; Thiebaud et al., 2007; Zaki and Moumni, 2007; Peultier et al., 2008;

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SaintSulpice et al., 2009; Hartl et al., 2010a). Most of the models developed these last years are focused on different particular key points of SMA modeling like tension–compression asymmetry (Gillet et al., 1998; Raniecki and Lexcellent, 1998; Qidwai and Lagoudas, 2000a; Peultier et al., 2008), or the description of internal loops (Tanaka et al., 1995; Gillet et al., 1998; Bo and Lagoudas, 1999b; Bouvet et al., 2004; Peultier et al., 2006). It is also noted that the coupling between phase transformation and plasticity is also taken into account in some approaches (Lagoudas and Entchev, 2004; Hartl and Lagoudas, 2009), or between phase transformation and viscoplasticity in HTSMAs (Lagoudas et al., 2009; Hartl et al., 2010b). Some other models focus on cycling effects (Tanaka et al., 1995; Lagoudas and Entchev, 2004; SaintSulpice et al., 2009) Another class of models has to be mentioned for completeness. They are based on micromechanical considerations of the martensitic transformation and aim to predict the response of the bulk material from a local description of strain mechanisms and microstructure evolutions (Patoor et al., 1995, 1996; Huang and Brinson, 1998; Lu and Weng, 1998; Siredey et al., 1999; Gao et al., 2000; Huang et al., 2000). Despite their good predicting capabilities, implementation of these models into finite element softwares induces high computation costs due to the large amount of internal variables required to describe the macroscopic behavior of SMAs. Macroscopic phenomenological models are nowadays better fitted for the development of numerical tools for structure analysis. However, results from micromechanical simulations lead to a wise choice of simplifying assumptions useful for macroscopic models development.

A first category of phenomenological models implemented in FEA packages describes the evolution of transformation strain with a unique martensitic volume fraction, and considers a proportional relationship between the evolution of transformation strain and the evolution of the martensitic volume fraction (Jaber et al., 2008; SaintSulpice et al., 2009; Arghavani et al., 2010). Other models are using a dependency of the transformation strain magnitude with respect to the applied stress to meet the need for straightforward experimental calibration (Hartl et al., 2010a). A second category of models (Panico and Brinson, 2007; Thiebaud et al., 2007) describes the material state considering two martensitic phases: self-accommodated, or thermal martensite (M^T), which is thermally induced, and stress-oriented martensite (M^σ), which is stress-induced. This decomposition was first proposed by Brinson (1993). A last description of the evolution of transformation strain was introduced by Peultier et al. (2006), where the martensite volume fraction and the mean transformation strain of martensite were considered as internal variables. This decomposition was also further used by Zaki and Moumni (2007). Most of these phenomenological models consider, in a direct or indirect fashion, that the magnitude of transformation strain is only dependent on the applied stress. However, martensite formed during a stress-free cooling adopts a characteristic self-accommodated structure. In shape memory alloys, this typical microstructure is easily deformed by an orientation mechanism when a macroscopic stress is applied. But it is important to consider that such an orientation process cannot be completed due to the presence of incompatible variant interfaces within grains and existence of strain incompatibilities between grains. On the other hand, the stress-induced martensite present a higher transformation strain magnitude, as it can be seen in isothermal experiments performed at different temperatures (Otsuka and Ren, 2005). Thus, the observable transformation is strongly dependent on the microstructure of martensite initially formed (i.e. self-accommodated or stress-oriented). To describe accurately the resulting transformation strain at a certain stress–temperature state, it is therefore important to describe the transformation strain magnitude as a function of the loading path followed.

Another characteristic of the SMAs behavior, though specific for NiTi material, is the additional strain mechanism observed at low stress level in self-accommodated martensite. When cooled down sufficiently low, in the absence of applied stress, a NiTi SMA sample presents a typical self-accommodated martensitic microstructure with twinned martensite variants. Mechanical response observed after performing an isothermal loading exhibits four deformation stages, according to Liu et al. (1999) observations: The first stage is related to the inelastic accommodation of twins which are present in self-accommodated martensite variants. Liu et al. (1999) had observed that these variants are not perfectly twin-related to each other in the self-accommodated state. Thus, when an external stress is applied, a strain mechanism occurs to form twin related interfaces between twinned martensite variants. Considering this unique strain mechanism is important to accurately describe the isothermal loading path starting from a self-accommodated martensitic state. To the author's knowledge there is no models that considers this mechanism, and it is one of the motivation of this work.

The model presented in this paper is motivated by the work of Peultier et al. (2006, 2008). A third macroscopic internal variable is added to account for the strain mechanism related to the accommodation of related to twins accommodation in NiTi alloys. The evolution of the microstructure of martensite is tracked by considering the evolution of a fourth internal variable. The expression of the Gibbs free energy is defined to describe the two key features described above, which are the introduction of a path-dependent transformation strain and the description of the twin accommodation mechanisms. Note that this model development focuses on NiTi behavior, because NiTi SMAs are nowadays widely used in several fields like biomedical and aerospace applications. Nevertheless, the proposed model can also be applied to describe the behavior of other class of SMAs like Cu-based alloys (e.g., CuAlBe or CuAlZn) with an appropriate model parameter identification. Also, the modeling of the partial loading, which lead to the generation of minor loops inside the full transformation loop is considered and generalizes the approach of Gillet et al. (1998). Finally, the effect of tension–compression asymmetry of the transformation strain magnitude is considered, and it is shown how this unique feature induces a significant change in the behavior of the SMA between tension and compression.