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A finite element model for shape memory alloys considering thermomechanical couplings at large strains

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ABSTRACT

In the present work we propose a new thermomechanically coupled material model for shape memory alloys (SMA) which describes two important phenomena typical for the material behaviour of shape memory alloys: pseudoelasticity as well as the shape memory effect. The constitutive equations are derived in the framework of large strains since the martensitic phase transformation involves inelastic deformations up to 8%, or even up to 20% if the plastic deformation after the phase transformation is taken into account. Therefore, we apply a multiplicative split of the deformation gradient into elastic and inelastic parts, the latter concerning the martensitic phase transformation. An extended phase transformation function has been considered to include the tension–compression asymmetry particularly typical for textured SMA samples. In order to apply the concept in the simulation of complex structures, it is implemented into a finite element code. This implementation is based on an innovative integration scheme for the existing evolution equations and a monolithic solution algorithm for the coupled mechanical and thermal fields. The coupling effect is accurately investigated in several numerical examples including pseudoelasticity as well as the free and the suppressed shape memory effect. Finally, the model is used to simulate the shape memory effect in a medical foot staple which interacts with a bone segment.

1. Introduction

In the last years smart materials have attracted much attention, especially because of their versatile application in smart structures, medical devices and actuator systems (e.g. Van Humbeeck, 2001; Fu et al., 2004; Morgan, 2004). Among these materials, shape memory alloys, particularly Nickel–Titanium (NiTi) belong to the most established. In comparison to other metallic materials they exhibit large inelastic recoverable strains (of the order of 8%) resulting from the transformation between austenitic and martensitic phases (see Otsuka and Wayman, 1999). This transformation may be induced by a change either in the applied stress, the temperature, or in a combination of both.

From the macroscopic point of view, the behaviour of shape memory alloys exhibits two major phenomena. The first one is known as pseudoelasticity which is characterised by nonlinearly elastic behaviour. Here, very large strains upon loading occur but full recovery is achieved in a hysteresis loop upon unloading. The shape memory effect, on the other hand, is accompanied by large residual strains after loading and subsequent unloading. These strains are due to the orientation of martensite twins (pseudoplasticity). They may be fully recovered simply by raising the temperature of the body. Additionally, these materials exhibit full thermomechanical coupling. Thus, the temperature of the alloy changes upon applied force, and the mechanical response changes upon temperature deviation.

During the last decade the area of constitutive modelling of shape memory alloys (SMA) has been the topic of many research publications. The majority of the published material models can be classified into three different groups: micromechanically based approaches, concepts based on statistical thermodynamics and phenomenological models. Since we already reviewed the three groups in detail (Reese and Christ, 2008), we now concentrate on a literature overview of phenomenological models for shape memory alloys. We subdivide them into models for the different phenomena pseudoelasticity and the shape memory effect as well as finally the tension–compression asymmetry. We also present existing models which are derived in the framework of large strains. After all, the implementation of the material models into a finite element code is surveyed. If the reader is interested in further research on this topic we recommend Roubicek (2005) and Patoor et al. (2006) who give a detailed overview of micromechanical modelling of shape memory alloys. Lagoudas et al. (2006) provide a survey of constitutive formulations for polycrystalline shape memory alloys where a distinction between the micromechanical and the phenomenological approach is made.

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The most common material laws for shape memory alloys are able to describe the effect of pseudoelasticity. In the 1980s (e.g. Tanaka, 1986) and in the 1990s (e.g. Raniecki et al., 1992; Brinson, 1993) one-dimensional constitutive models were already proposed to describe the hysteretical behaviour of shape memory alloys during the phase transformation from austenite to martensite. From the late 1990s three-dimensional concepts were developed. Most of these approaches are structured similarly. They are based on a macroscopic free energy function (either Gibbs free energy or Helmholtz free energy) which includes internal variables to describe the phase transformation. In general, one scalar variable, the martensitic volume fraction, defines the progress of the phase transformation and determines its end. Raniecki et al. (1992) among others derived a relation between the martensitic volume fraction and the inelastic strain occurring during the phase transformation. By defining the martensitic volume fraction via a norm of the transformation strain tensor, the three-dimensional character of the phase transformation is considered (e.g. Raniecki and Lexcellent, 1994; Boyd and Lagoudas, 1996).

Patoor et al. (1987) and Achenbach (1989) were the first to suggest an additive decomposition of the martensitic volume fraction into different variants. Brinson (1993) has introduced this concept into the phenomenological material modelling. The motivation for this idea was to introduce the so-called temperature induced martensite (also known as self-accommodated martensite) which serves to include the shape memory effect into the material model. The idea of the additive split of the martensitic volume fraction was further developed by, for example, Leclercq and Lexcellent (1996), Lexcellent et al. (2002), Souza et al. (1998), Helm and Haupt (2003), Christ et al. (2004), Auricchio and Petrini (2004a), Paiva et al. (2005) and Popov and Lagoudas (2007).

Since the shape memory effect originates from stress orientation of the martensite twins and subsequent heating, the temperature plays an important role. The simplest way to include the temperature in the modelling is to hold it fixed at each point of the structure and to assume a homogeneous temperature field. This would result in a one-sided thermomechanical coupling where only the influence of the temperature on the deformation is taken into account. But important physical effects as heat conduction and heat generation due to energy dissipation during the phase transformation, can only be considered if full thermomechanical coupling (including the solution of the first law of thermodynamics) is incorporated. The finite element implementation of thermomechanically coupled models were accomplished by Lim and McDowell (2002), Auricchio and Petrini (2004b), Migliavacca et al. (2004), Iadicola and Shaw (2004), Popov and Lagoudas (2007) and Helm (2007b). However, all publications mentioned are limited to small strains.

Phenomenological large strain concepts were proposed by Levitas (1998), Auricchio and Taylor (1997), Masud et al. (1997), Idesman et al. (1999), Auricchio (2001), Anand and Gurtin (2003), Müller and Bruhns (2006), Vieille et al. (2007), Ziolkowski (2007), Helm (2007a) and Reese and Christ (2008). Thermomechanical coupling is additionally included in the models of Müller and Bruhns (2006) and Ziolkowski (2007). Particularly the concepts of Auricchio and Taylor (1997), Auricchio (2001), Vieille et al. (2007) and Reese and Christ (2008) focus on the finite element implementation of the constitutive model. The above mentioned articles do not focus on the shape memory effect. Hence, it seems that none of the presented models is fully capable of combining all important features as pseudoelasticity, the shape memory effect, thermomechanical coupling and finite deformations in only one model and additionally offers an efficient and robust finite element implementation.

In the present work we seek to make another step forward on this way. For this purpose, we enhance the model proposed in Reese and Christ (2008) by an additive split of the martensitic volume fraction z into an oriented martensite fraction z_o and an unoriented martensite z_u, also known as self-accommodated martensite. The split allows us to describe the martensite orientation below the martensite finish temperature as well as the thermally driven phase transformation from oriented martensite to austenite by heating above the austenite start temperature A_s. Additionally, we extend the approach to thermomechanical coupling by applying the balance of internal energy. Hence, an interaction between the mechanical and the thermal quantities is enabled. The model is derived in the framework of large strains based on the multiplicative decomposition of the deformation gradient into an elastic part and a transformation part where the latter stands for the inelastic deformation produced during the phase transformation or the orientation of martensite twins, respectively. The numerical implementation of this model is carried out by means of an integration algorithm based on the exponential map which preserves the volume during the phase transformation.

2. Kinematic framework

2.1. Deformation gradients

The proposed material model is derived in the framework of finite deformations. This implies the use of the deformation gradient $\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}$, where the vector $\mathbf{x} = \hat{\mathbf{x}}(\mathbf{X}, t)$ (t: time) denotes the position of a point in the current configuration and $\mathbf{X}$ the position of the same point in the reference configuration. The determinant of the deformation gradient $J = \det \mathbf{F}$ describes the volume change of the material during the deformation. As in classical plasticity, we assume an intermediate state which is stress free and decouples the elastic deformation from the deformation during the martensitic phase transformation $\mathbf{F}_t = \mathbf{F}_e^{-1}\mathbf{F}$. The subscript e stands for the elastic deformation and t for the transformation part. As shown in earlier investigations (e.g. Fu et al., 1992) the phase transformation in polycrystalline shape memory alloys does not emerge spontaneously. During the forward transformation the stress is slightly increasing whereas during the backward transformation the stress is decreasing. This characteristic can be described phenomenologically by introducing an additional deformation gradient $\mathbf{F}_{t_d} = \mathbf{F}_{t_e}^{-1}\mathbf{F}_t$ which is multiplicatively coupled to the deformation during the phase transformation. Since the phase transformation in NiTi approximately proceeds without a volume change (see Bhattacharya, 1992), the determinant of the transformation deformation gradient $J_t = \det \mathbf{F}_t$ has to remain unchanged so that $J_t \equiv 1$ holds.

It should be emphasised that the triple multiplicative split $\mathbf{F} = \mathbf{F}_e\mathbf{F}_{t_e}\mathbf{F}_{t_d}$ has been used already several times, for the first time probably in the work of Lion (2000) to model kinematic hardening, see also Dettmer and Reese (2004), Vladimirov et al. (2008). According to Lion (2000) the elastic part of the inelastic deformation (in the present contribution denoted by $\mathbf{F}_{t_e}$) results from dislocation-induced lattice rotations and stretches on the microscale, whereas the inelastic part (here defined by $\mathbf{F}_{t_d}$) relates to local plastic deformations coming from inelastic slip on crystallographic slip systems. Helm (2007a) suggests to transfer the idea of the triple multiplicative split on phase transformations. The same approach is taken by Reese and Christ (2008).

2.2. Strain tensors and its time derivatives

Since the deformation gradient $\mathbf{F}$ is not a suitable strain measure we use the Green–Lagrange strain tensor $\mathbf{E} = (\mathbf{C} - \mathbf{1})/2$, where $\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}$ denotes the right Cauchy–Green tensor. In the same manner we introduce the transformation strain tensor