ELSEVIER

Materials Science and Engineering A 481–482 (2008) 343–346

MATERIALS SCIENCE & ENGINEERING A

www.elsevier.com/locate/msea

Finite-element modelling of shape memory alloys—A comparison between small-strain and large-strain formulations

D. Christ*, S. Reese

Institute of Solid Mechanics, Braunschweig University of Technology, Schleinitzstr. 20, 38106 Braunschweig, Germany

Received 6 July 2006; received in revised form 3 November 2006; accepted 22 November 2006

Abstract

In this contribution, we present a finite deformation material model for shape memory alloys (SMAs) which includes the effect of pseudoelasticity and pseudoplasticity. A special algorithm has been developed to incorporate the concept into a finite-element (FE) code. The final aim of the research work is to investigate whether FE simulations of SMA applications should be based on large-strain formulations as the transformation strain during the phase transition can reach up to 10%. If such a large-strain model was not necessary the computational cost of the numerical investigations could be reduced significantly.

Keywords: Shape memory alloys; Material modelling; Large strains; FE simulation

1. Introduction

Shape memory alloys (SMAs) can undergo diffusionless and reversible phase transformations between a higher ordered austenite phase and a lower ordered martensite phase as a result of changes in temperature and/or the state of stress. Consequently, SMAs exhibit several macroscopic phenomena not present in traditional materials (e.g. pseudoelasticity and shape memory effect). These unique features of SMAs have found numerous applications in automotive and aerospace industries as well as in the field of medical technology. The increasing use in commercially valuable applications has motivated a vivid interest in the development of accurate constitutive models to describe the behaviour of SMAs. Meanwhile, a large number of material models have been developed to describe the complex behaviour of SMAs, particularly the effect of pseudoelasticity. These models follow three different approaches depending on whether a formulation at the micro-, the meso- or the macro-scale is used. The micro-level models are generally based on the description of micro-scale effects such as nucleation, interface motion or twin growth. They consider phase volume fraction as a consequence of interface movements (e.g. [1,2]). The meso-level models combine micro-mechanical aspects (such as habit planes, martensite variants, etc.) and macro-scale thermodynamics. The constitutive equations are defined at the micro-scale. The response on the macro-level is obtained due to the use of proper homogenization techniques (e.g. [3,4]). The macro-level models deal with macroscopic quantities, which lead to a description of the global mechanical behaviour [5–7]. One of the advantages of the latter type of models is their convenient implementation into a finite-element (FE) code. Therefore, they are widely used in structural engineering applications. Although a lot of these material models have been implemented into the finite-element method, only a few of them are derived in the framework of finite deformation [8–10]. The goal of this work is to propose a three-dimensional material model which is able to reproduce the pseudoelastic behaviour within the large-strain regime. The model has been compared to the corresponding small deformation model to investigate, whether the effect of pseudoelasticity can be realistically represented by means of small-strain formulations.

2. Macro-mechanical model

2.1. Kinematic assumptions

At the continuum mechanical level we introduce the deformation gradient

$$\mathbf{F} := \mathbf{F}_e\mathbf{F}_t \Rightarrow \mathbf{F}_e = \mathbf{F}\mathbf{F}_t^{-1} \tag{1}$$

* Corresponding author. Tel.: +49 531 391 7054; fax: +49 531 391 7053.
E-mail address: d.christ@tu-bs.de (D. Christ).

0921-5093/$ – see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.msea.2006.11.174

and its decomposition into an elastic part $\mathbf{F}_e$ and a "transformation" part $\mathbf{F}_t$ which describes the transition from the austenitic to the martensitic phase. This multiplicative split of the deformation gradient $\mathbf{F}$ is known from crystal plasticity (e.g. [11]). In the same manner we decompose the transition part $\mathbf{F}_t$ according to

$$\mathbf{F}_t := \mathbf{F}_{t_e}\mathbf{F}_{t_d} \Rightarrow \mathbf{F}_{t_e} = \mathbf{F}_t\mathbf{F}_{t_d}^{-1} \tag{2}$$

where $\mathbf{F}_{t_e}$ is used to model the energy storage and the second term $\mathbf{F}_{t_d}$ expresses in conjunction with the Helmholtz free energy the physical dissipation during the phase transition.

2.2. Free energy

The Helmholtz free energy is defined as

$$\Psi = \Psi_e(\mathbf{C}_e, z) + \Psi_t(\mathbf{C}_{t_e}). \tag{3}$$

The first term Ψ_e includes the energy storage in the material at elastic deformations due to mechanical loading and Ψ_t represents the energy storage during the phase transition. Exploiting the principle of material objectivity the Helmholtz free energy depends only on the "elastic" Cauchy–Green tensors

$$\mathbf{C}_e = \mathbf{F}_e^T\mathbf{F}_e = \mathbf{F}_t^{-T}\mathbf{C}\mathbf{F}_t^{-1}, \tag{4}$$

$$\mathbf{C}_{t_e} = \mathbf{F}_{t_e}^T\mathbf{F}_{t_e} = \mathbf{F}_{t_d}^{-T}\mathbf{C}_t\mathbf{F}_{t_d}^{-1}. \tag{5}$$

Due to the use of the martensitic volume fraction z it is considered that two different phases coexist during the phase transition. z has always a value between 0 and 1 whereby $z = 0$ denotes pure austenite and $z = 1$ pure martensite. Certainly the material behaviour of shape memory alloys is strongly temperature dependent so that in general the temperature should be considered as an additional independent variable. However, in the present contribution we focus mainly on the effect of pseudoelasticity which may be displayed under approximately isothermal conditions. Therefore, we choose to treat the temperature as a constant.

2.3. Thermodynamical framework

Assuming isothermal conditions the Clausius–Duhem form of the entropy inequality takes the form $\mathbf{S} \cdot \frac{1}{2}\dot{\mathbf{C}} - \dot{\Psi} \geq 0$ where $\mathbf{S}$ denotes the second Piola–Kirchhoff stress tensor. We insert (3) into the inequality and obtain the form

$$\mathbf{S} \cdot \frac{1}{2}\dot{\mathbf{C}} - \frac{\partial\Psi_e}{\partial\mathbf{C}_e} \cdot \dot{\mathbf{C}}_e - \frac{\partial\Psi_e}{\partial z}\dot{z} - \frac{\partial\Psi_t}{\partial\mathbf{C}_{t_e}} \cdot \dot{\mathbf{C}}_{t_e} \geq 0. \tag{6}$$

In analogy to former publications [5,7] the martensitic volume fraction z can be expressed in terms of the Green–Lagrange strain $\mathbf{E}_t := \frac{1}{2}(\mathbf{C}_t - \mathbf{1})$:

$$z := \omega_\gamma ||\mathbf{E}_t|| \tag{7}$$

Here, ω_γ is a material parameter which describes the length of the stress–strain hysteresis. The material time derivative of z is then computed by means of the relation

$$\dot{z} = \omega_\gamma \frac{\mathbf{E}_t}{||\mathbf{E}_t||} \cdot \frac{1}{2}\dot{\mathbf{C}}_t = \omega_\gamma \left(\mathbf{F}_t \frac{\mathbf{E}_t}{||\mathbf{E}_t||}\mathbf{F}_t^T\right) \cdot \mathbf{d}_t \tag{8}$$

where the symmetric part of the deformation rate tensor $\mathbf{d}_t$ is defined by $\mathbf{d}_t := \frac{1}{2}\mathbf{F}_t^{-T}\dot{\mathbf{C}}_t\mathbf{F}_t^{-1}$. We further rewrite the deformation rates $\dot{\mathbf{C}}_e$ and $\dot{\mathbf{C}}_{t_e}$ in the format

$$\dot{\mathbf{C}}_e = -\mathbf{l}_t^T\mathbf{C}_e + \mathbf{F}_t^{-T}\dot{\mathbf{C}}\mathbf{F}_t^{-1} - \mathbf{C}_e\mathbf{l}_t, \tag{9}$$

$$\dot{\mathbf{C}}_{t_e} = -\mathbf{l}_{t_d}^T\mathbf{C}_{t_e} + \mathbf{F}_{t_d}^{-T}\dot{\mathbf{C}}_t\mathbf{F}_{t_d}^{-1} - \mathbf{C}_{t_e}\mathbf{l}_{t_d}. \tag{10}$$

In this context the definitions $\mathbf{l}_t := \dot{\mathbf{F}}_t\mathbf{F}_t^{-1}$ and $\mathbf{l}_{t_d} := \dot{\mathbf{F}}_{t_d}\mathbf{F}_{t_d}^{-1}$ have been used. After the application of several rules from tensor calculus and the exploitation of the symmetry of $\partial\Psi_e/\partial\mathbf{C}_e$ and $\partial\Psi_t/\partial\mathbf{C}_{t_e}$ the Clausius–Duhem inequality (6) is transformed into the relation

$$\begin{aligned}&\left(\mathbf{S} - 2\,\mathbf{F}_t^{-1}\frac{\partial\Psi_e}{\partial\mathbf{C}_e}\mathbf{F}_t^{-T}\right) \cdot \frac{1}{2}\dot{\mathbf{C}}\\ &- \left(2\,\mathbf{F}_{t_e}\frac{\partial\Psi_t}{\partial\mathbf{C}_{t_e}}\mathbf{F}_{t_e}^T + \omega_\gamma\,\Delta\Psi\,\mathbf{F}_t\frac{\mathbf{E}_t}{||\mathbf{E}_t||}\mathbf{F}_t^T\right) \cdot \mathbf{d}_t\\ &+ \left(2\,\mathbf{C}_e\frac{\partial\Psi_e}{\partial\mathbf{C}_e}\right) \cdot \mathbf{l}_t + \left(2\,\mathbf{C}_{t_e}\frac{\partial\Psi_t}{\partial\mathbf{C}_{t_e}}\right) \geq 0.\end{aligned} \tag{11}$$

The introduced material parameter $\Delta\Psi$ considers the difference of the internal energy and the entropy between the austenitic and the martensitic phase [7]. At this point we assume that Ψ_e and Ψ_t are isotropic functions of $\mathbf{C}_e$ and $\mathbf{C}_{t_e}$, respectively. One consequence of this specialisation is the coaxiality of $\mathbf{C}_e$ and $\partial\Psi_e/\partial\mathbf{C}_e$ as well as of $\mathbf{C}_{t_e}$ and $\partial\Psi_t/\partial\mathbf{C}_{t_e}$. Therefore, also the Mandel stress tensors

$$\mathbf{M} := 2\,\mathbf{C}_e\frac{\partial\Psi}{\partial\mathbf{C}_e} \quad \text{and} \quad \mathbf{M}_t := 2\,\mathbf{C}_{t_e}\frac{\partial\Psi}{\partial\mathbf{C}_{t_e}} \tag{12}$$

are symmetric reducing the inequality to

$$\left(\mathbf{S} - 2\,\mathbf{F}_t^{-1}\frac{\partial\Psi}{\partial\mathbf{C}_e}\mathbf{F}_t^{-T}\right) \cdot \frac{1}{2}\dot{\mathbf{C}} + (\mathbf{M} - \mathcal{X}) \cdot \mathbf{d}_t + \mathbf{M}_t \cdot \mathbf{d}_{t_d} \geq 0 \tag{13}$$

where the back stress

$$\mathcal{X} := 2\,\mathbf{F}_{t_e}\frac{\partial\Psi_t}{\partial\mathbf{C}_{t_e}}\mathbf{F}_{t_e}^T + \omega_\gamma\,\Delta\Psi\,\mathbf{F}_t\frac{\mathbf{E}_t}{||\mathbf{E}_t||}\mathbf{F}_t^T \tag{14}$$

has been introduced.

2.4. Constitutive equations

The final form of the Clausius–Duhem inequality is sufficiently satisfied by the relation

$$\mathbf{S} = 2\,\mathbf{F}_t^{-1}\frac{\partial\Psi_e}{\partial\mathbf{C}_e}\mathbf{F}_t^{-T} \tag{15}$$

for the second Piola–Kirchhoff stress tensor $\mathbf{S}$ and the evolution equations

$$\mathbf{d}_t = \dot{\lambda}\frac{\mathbf{M}^D - \mathcal{X}^D}{||\mathbf{M}^D - \mathcal{X}^D||} = \frac{\partial\Phi_{SMA}}{\partial\mathbf{M}} \tag{16}$$