Shape memory alloy composites – modelling of the one-way effect and the fatigue behaviour

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Summary

In this paper, we present a computationally efficient implementation of a continuum mechanical model for shape memory alloys into a finite element code. The model covers several thermomechanically-coupled effects typical for the material behaviour of shape memory alloys, e. g. pseudo-elasticity, the one-way shape memory effect and the two-way shape memory effect due to external loads. Additionally the fatigue behaviour is investigated. Via the use of a finite element formulation based on only one Gauss point, the computational effort is reduced enormously [12].

Introduction

An efficient design of smart structures including shape memory alloys is based on a reliable simulation of the structural behaviour. Due to its general applicability the finite element method has become the most widely used simulation tool. It is therefore desirable to implement constitutive models for shape memory alloys into such a framework. Moreover, shape memory alloys interact in smart structures with further materials (i.e. polymers) which leads to a more complex response of the structure.

In the past years, the number of continuum mechanical models for shape memory alloys has increased noticeably. Some are derived in order to describe mainly the effect of pseudo-elasticity (see [1], [2]). Other authors focus on the behaviour of SMA composites ([3], [4]), where then also the shape memory effect has to be taken into account. But most of the models consider only the behaviour of shape memory alloys under uniaxial loading. One of the few models which includes at the continuum mechanical level both, pseudoelasticity and the shape memory effect, has been developed by Helm & Haupt ([5], [6]). One of its advantages is the fact that it is formulated analogously to classical models of metal plasticity. As such, the approach can be efficiently embedded in finite element formulations which include already a suitable integration scheme for internal variable-based models of inelasticity.

Another branch of the literature focuses on micromechanically based approaches ([7], [8]), where the microstructure in arbitrary boundary problems can be determined by means of recently developed relaxation techniques. The latter works are, however, usually restricted to pseudo-elasticity. Micromechanical concepts of this kind are promising, but involve, especially in the context of practical applications, a rather high computational effort.

Only a few publications in the literature focus on the finite element implementation itself, see e.g. [1], [2], [9], [10] and [11]. To the knowledge of the authors, none of

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these works includes the modelling of shape memory alloys in composite structures. Also the fatigue behaviour is not discussed. Besides we put special emphasis on a new finite element technology which allows us to circumvent numerical instabilities and to reduce the numerical effort noticeably.

Continnum mechanical model

The used material model is based on the concept proposed in [6]. We work with an additive decomposition of the linearized strain tensor ε into elastic (ε_e) and inelastic (ε_i) parts. The inelastic part ε_i considers the stress-induced martensitic phase transition in case of pseudo-elasticity as well as the orientation and reorientation of the martensite twins. To be more variable in the modelling of the pseudo-elastic hysteresis, the inelastic strains are furthermore decomposed into two terms: $\varepsilon_i = \varepsilon_{i_e} + \varepsilon_{i_d}$. The total Helmholtz free energy can be expressed in the form $\Psi = \Psi_e(\varepsilon_e, \theta, z) + \Psi_i(\varepsilon_{i_e}, \theta)$ where Ψ is a function of the strains $\varepsilon_e = \varepsilon - \varepsilon_i, \varepsilon_{i_e}$, the martensitic volume fraction z and the absolute temperature θ . Note that the model presented in this paper does not include the influence of the deformation on the temperature. Therefore we do not solve the balance of internal energy but manually control the temperature "from the outside". The set of constitutively independent variables consists of the strain ε and the internal variables $\mathbf{Z}_1 = \varepsilon_i$, $\mathbf{Z}_2 = \varepsilon_{i_d}$ and $\mathbf{Z}_3 = z\mathbf{1}$. For the latter, we formulate evolution equations of the form $\dot{\mathbf{Z}}_i = \mathbf{f}_i(\varepsilon, \varepsilon_i, \varepsilon_{i_d}, z, a\dot{\varepsilon})$ (i = 1, 2, 3). The scalar (constant) factor a is equal to 1 if we look at rate-independent material behaviour, whereas it takes on the value 0 if rate-dependent processes are considered. Both situations will be discussed in what follows.

For the finite element computations it is certainly necessary to specify Ψ_e further. It is common to assume a linear dependence on z: $\Psi_e = z\Psi_e^M + (1-z)\Psi_e^A$ where Ψ_e^M and Ψ_e^A characterize the contributions of the martensitic phase and the austenitic phase, respectively. Based on the assumption that the material is isotropic, we can assume that Ψ_e^M has the same form as the Helmholtz free energy function of a linear-elastic material: $\Psi_e^M = \mu^M \varepsilon_e^D \cdot \varepsilon_e^D + (\kappa^M/2) (\mathrm{tr} \varepsilon_e)^2 - 3\kappa^M \alpha^M (\theta - \theta_0) \mathrm{tr} \varepsilon_e$. The above form can be analogously used for Ψ_e^A . The notation A^D refers to the deviatoric part of a second order tensor **A**, whereas the symbol tr **A** denotes its trace. The parameters $\mu^M (\mu^A)$ and $\kappa^M (\kappa^A)$ are the elastic material constants of the martensitic (austenitic) phase evaluated at the initial temperature θ_0 . $\alpha^M (\alpha^A)$ denotes the thermal expansion coefficient of the martensitic (austenitic) phase. A reasonable choice for Ψ_i is $\Psi_i = \frac{1}{2}\mu_i \varepsilon_{i_e}^D \cdot \varepsilon_{i_e}^D$ where μ_i controls the slope of the pseudo-elastic stress-strain hysteresis. This part is not influenced by the fact, whether the material is in its martensitic or austenic phase (see for a discussion about this issue [6]).

In the field of continuum mechanics it is desirable to derive the constitutive equations from the second law of thermodynamics, e.g. given in the Clausius-Duhem form, where the positiveness of the entropy production is postulated. After exploiting the constitutive relation $\sigma = \partial \Psi_e / \partial \varepsilon_e$ we arrive at the residual inequality $(\sigma - \mathbf{X}_i) : \dot{\varepsilon}_i + \mathbf{X}_i : \dot{\varepsilon}_{i_d} - \Delta \Psi \dot{z} \ge 0$ where the definitions $\mathbf{X}_i := \partial \Psi_i / \partial \varepsilon_{i_e}$ and $\Delta \Psi := \Psi_e^{\mathsf{M}} - \Psi_e^{\mathsf{A}}$ have been introduced. The fact that $\Delta \Psi$ depends on the deformation will be neglected in what follows. The tensor \mathbf{X}_i is usually termed back stress.

(a) One-way effect

To exploit the shape memory effect (e.g. in form of the one-way effect) one usually needs a pseudo-plastic load cycle to transform unoriented (z_u) into oriented martensite (z_0) . During such a pseudo-plastic transformation the total amount of z remains constant: $\dot{z} = 0$. The residual inequality reduces to the requirement $(\sigma - \mathbf{X}_i) \cdot \dot{\varepsilon}_i + \mathbf{X}_i \cdot \dot{\varepsilon}_{i_d} \ge 0$ which is fulfilled with

$$\dot{\mathbf{\varepsilon}}_i = \dot{\lambda} \mathbf{N}_{\bar{T}}, \ \dot{\mathbf{\varepsilon}}_{i_d} = \frac{b}{2\mu_i} \dot{\lambda} \mathbf{X}_i, \ \dot{z}_{\mathsf{u}} = \dot{\lambda} \frac{1}{\beta} = -\dot{z}_{\mathsf{o}}$$
(1)

Here $\mathbf{N}_{\bar{T}}$ is given by $\mathbf{N}_{\bar{T}} = \partial \bar{\Phi} / \partial \sigma$, where $\bar{\Phi}$ is assumed to have von Mises form: $\bar{\Phi} = ||\mathbf{T}^D|| - k^{\mathsf{M}\mathsf{M}}(\theta)$. The tensor \mathbf{T} is given by $\mathbf{T} = \sigma - \mathbf{X}_i$. The quantity $\mathbf{N}_{\bar{T}}$ reads $\mathbf{N}_{\bar{T}} = \mathbf{T}^D / ||\mathbf{T}^D||$. The scalar λ denotes the slip rate. Additionally the Kuhn-Tucker conditions $\lambda \geq 0$, $\bar{\Phi} \leq 0$, $\lambda \bar{\Phi} = 0$ have to be fulfilled. The parameters *b* and $\beta = \sqrt{3/2}\gamma$ (γ width of hysteresis) are material constants. The temperature-dependent parameter $k^{\mathsf{M}\mathsf{M}}$ is something like a yield stress in classical elasto-plasticity. The pseudo-plastic phase transformation can only take place if θ lies below the martensite finish temperature M_f . Further the conditions $z_{\mathsf{u}} > 0$ and $z_{\mathsf{o}} < 1$ have to be fulfilled.

Of high practical importance is the situation, where the temperature controls the phase transformation process (*temperature-induced* phase transformation). If the specimen can deform freely (at a given stress state), a temperature cycle of heating and cooling leads to a decrease (transformation of martensite into austenite: MA) and increase (transformation of austenite into martensite: AM) of the deformation. On the other hand, if the deformation is fixed, the leading stress component in the specimen increases (MA) and decreases (AM). These two phenomena should be described by the model.

Several authors describe the evolution of the oriented martensitic volume (for the temperature-induced phase transformation) by means of the evolution laws $\dot{z}_0 = -|\dot{\theta}|/(M_s - M_f) \operatorname{sign} \Delta \Psi > 0$, $\dot{z}_0 = -|\dot{\theta}|/(A_f - A_s) \operatorname{sign} \Delta \Psi < 0$ where the first one holds for $\dot{\theta} < 0$, $\theta \leq M_s$ (M_s martensite start temperature, i. e. $\Delta \Psi < 0$) and z < 1. The second evolution equation is used if the conditions $\dot{\theta} > 0$, $\theta \geq A_s$ (A_s austenite start temperature, i. e. $\Delta \Psi > 0$) and z > 0 are fulfilled.

We modify these equations in the way that we replace $-\operatorname{sign}\Delta\Psi$ by means of the product $P = \mathbf{N}_{\varepsilon} \cdot \mathbf{N}_{T}$. Here the tensor \mathbf{N}_{ε} is defined with $\mathbf{N}_{\varepsilon} = \varepsilon/||\varepsilon||$. \mathbf{N}_{T} is constructed analogously to $\mathbf{N}_{\overline{\tau}}$, however on the basis of $\mathbf{T} := \sigma - \mathbf{X}_{i} - \Delta\Psi/\beta \mathbf{N}_{\varepsilon}$:

$$\dot{z}_{o} = |\dot{\theta}| / (M_{s} - M_{f}) P > 0, \ \dot{z}_{o} = |\dot{\theta}| / (A_{f} - A_{s}) P < 0$$
(2)

We also state the conditions

$$\dot{\varepsilon}_{i} = \dot{\lambda} \mathbf{N}_{T} = \frac{\dot{z}_{o}}{P} \beta \mathbf{N}_{T}, \quad \dot{\varepsilon}_{i_{d}} = \dot{\lambda} \frac{b}{2\mu_{i}} \mathbf{X}_{i} = \frac{\dot{z}_{o}}{P} \beta \frac{b}{2\mu_{i}} \mathbf{X}_{i}$$
(3)

where, in contrast to the pseudo-plastic case, $\dot{\lambda} = (\dot{z}_o/P)\beta$ is a given quantity. It can be easily shown that the residual inequality is satisfied.

Another point which should be discussed is the evolution of the unoriented martensite. Usually the application of the shape memory effect is preceded by a pseudo-plastic phase transformation starting in the low temperature range. At the beginning only unoriented martensite is present. Due to the increase of the stress or the deformation, the unoriented martensite transforms into oriented martensite. In a structure with an inhomogeneous stress state the unoriented martensite is usually not fully transformed. Thus, when the temperature cycle starts, there is still unoriented martensite in the structure. During the heating process this kind of martensite can also be transformed into austenite. In order to take this behaviour into account we assume that the oriented martensite transforms according to the evolution equations discussed at the end of this Section. The evolution of z_u is modelled by the rate equation stated at the beginning of this Section. The latter processes is based on the assumption that the inelastic strains do *not* develop.

Figure 1 shows a grip element modelled by means of the described material law. At first a SMA layer is stretched whereupon a pseudo-plastic phase transition from unoriented into oriented martensite takes place. Subsequently the layer is sprayed with silicon. During the heating the SMA layer "remembers" its initial state and retransforms into martensite, i.e. the length of the SMA layer reduces. Due to the excentric position of the layer in the composite a bending deformation is enforced. After cooling down the layer goes back to the martensitic state, the bending is reversed.



Figure 1: Bending of a grip element

(b) Fatigue behaviour

Experimental investigations have shown that the number of load cycles to be achieved with one product is limited due to thermal fatigue. This undesirable effect reduces the grip force and generates a permanent strain. The deviation from the original behaviour increases with increasing number of cycles until the point where the grip is no longer usable. To include the effect of thermal fatigue into our model it is important to state that the temperature-dependent function $\Delta \Psi = \Delta e - \Theta \Delta \eta$ (where Δe and $\Delta \eta$ are usually assumed to be constant) varies with the transition temperatures M_f , M_s , A_s and A_f . On the other hand it is well-known that the thermal fatigue effect goes along with a change of the transition temperatures. From this observation we draw the conclusion that an appropriate variation of $\Delta \Psi$ should bring us in the position to model thermal fatigue realistically. A reasonable ansatz can be made in the following way:

$$\Delta e_n = \Delta e_0 f_{\mathsf{sat}}(n) f_{\mathsf{rup}}(n), \quad \lim_{n \to n_{\mathsf{sat}}} \Delta e_n = a_{\mathsf{sat}} \Delta e_0 \tag{4}$$

$$f_{sat}(n) = 1 + (a_{sat} - 1)(1 - \exp(-bn) \text{ for } n \le n_{sat}, \text{ otherwise } = 1$$

$$f_{rup}(n) = 1 + (n - n_{sat})^p \text{ for } n > n_{sat}, \text{ otherwise } = 1$$
(5)

Here *n* denotes the number of thermal cycles. a_{sat} and *b* are material parameters. The former one is defined by the limit stated in (4). The function f_{rup} is only needed if rupture occurs. The change of $\Delta \eta$ and k^{AM} with increasing number of cycles can be described analogously. Thermal fatigue is usually accompanied by a reduction of the grip force and a displacement of the grip point. This is taken into account by the stress-strain relation

$$\boldsymbol{\sigma} = E\left(1 - D\right)\left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{i} - \boldsymbol{\alpha}_{T}\left(\boldsymbol{\Theta} - \boldsymbol{\Theta}_{0}\right)\mathbf{1}\right),\tag{6}$$

where the damage parameter *D* is defined by $1 - D = f_{sat}(n) f_{rup}(n)$. The computation in Figure 2 has been made under the assumption that rupture does not occur ($n_{sat} = \infty$, $f_{rup} = 1$). We further use $a_{esat} = 0.95$, $a_{\eta sat} = 1$, $a_{ksat} = 0.5$ (the indices e, η, k referring to the change of the internal energy Δe_n , the entropy $\Delta \eta_n$ and the parameter k^{AM}) as well as $\beta = 0.07$. The transition temperatures decrease as it is also observed experimentally [13]: $A_{ssat} = A_{s0} - 21K$, $M_{ssat} = M_{s0} - 5K$.



Figure 2: Thermal fatigue

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