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**THERMOMECHANICS OF MARTENSITIC PHASE TRANSITIONS IN
SHAPE MEMORY ALLOYS
I. CONSTITUTIVE THEORIES FOR SMALL AND LARGE
DEFORMATIONS**

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THERMOMECHANICS OF MARTENSITIC PHASE TRANSITIONS IN SHAPE MEMORY ALLOYS

I. CONSTITUTIVE THEORIES FOR SMALL AND LARGE DEFORMATIONS

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This article deals with the geometrically linear and nonlinear modeling of martensitic phase transitions in shape memory alloys. A geometrically nonlinear theory is required for the thermomechanical simulation of complex structures like endoscopic devices and stents. However, in certain situations like the simulation of pipe couplers, it is sufficient to apply a geometrically linear theory. In both cases, a free energy function is introduced, evolution equations for internal variables are postulated, and the dependence of the fraction of oriented martensite on the transformation strains is represented by a novel constitutive equation. In all, the developed constitutive theories are able to depict the thermomechanically coupled behavior of shape memory alloys. This is demonstrated in Part II of this article (to appear in this journal, in coauthorship with M. Schäfers). For this purpose, the theories are numerically treated in the framework of the finite element method in order to solve initial-boundary-value problems. These illustrate the main features of the constitutive theories by means of numerical test calculations. The results are compared with experimental data.

1. Introduction

The exceptional material behavior of shape memory alloys is based on martensitic phase transitions, which can be initiated and propagated by thermomechanical processes. In contrast to other kinds of phase changes, martensitic phase transitions take place without diffusion processes. These phase transitions are the result of cooperative movements of atomic layers until the crystal structure of the product phase is reached. The underlying physical processes on the micro scale are well understood [Funakubo 1987; Otsuka and Ren 1999; Otsuka and Wayman 1998; Patoor et al. 2006]. During the last decades, the material behavior including the fatigue properties of different shape memory alloys like NiTi and CuAlNi has been elaborately investigated in uniaxial tests; see, for example, [Funakubo 1987; Huo and Müller 1993; Otsuka and Wayman 1998; Shaw and Kyriakides 1995; Eggeler et al. 2004]. Moreover, the material properties under combined tension-torsion loads were studied by [Rogueda et al. 1996; Lim and McDowell 1999; Helm and Haupt 2001; Raniecki et al. 2001; McNaney et al. 2003]. Above the so-called austenite finish temperature A_f , martensitic phase transitions from austenite into oriented (detwinned) martensite occur at a certain stress level. Due to the involved crystal structure of the austenite and martensite phase, the occurring phase transitions are dominated by shear deformations and lead to macroscopic inelastic deformations. If the material is unloaded, the material returns back to its parent

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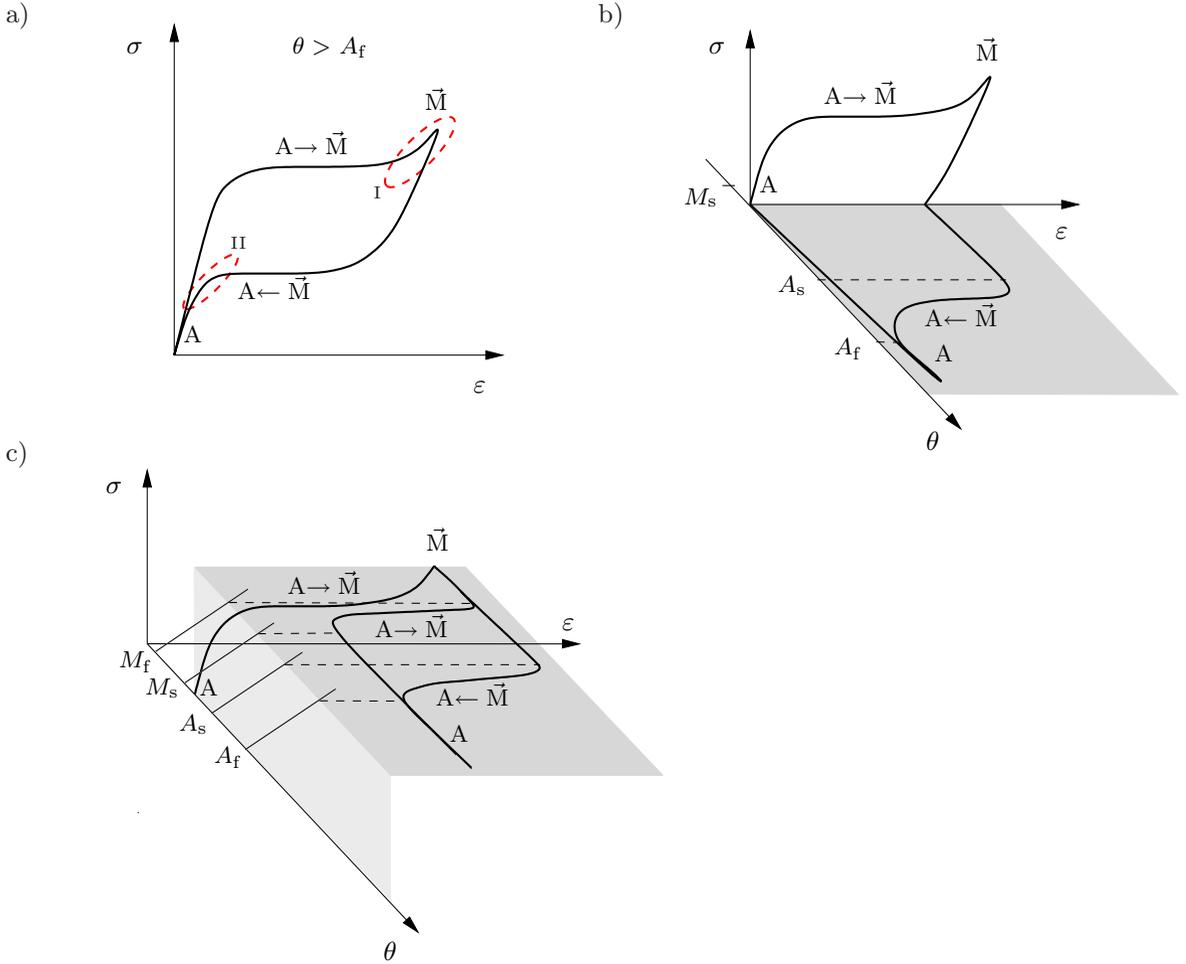


Figure 1. Sketch of the pseudoelasticity and the shape memory effects. A: austenite; \vec{M} : oriented (detwinned) martensite.

phase (austenite) and initial shape. This behavior is called pseudoelasticity or superelasticity, and is illustrated in Figure 1a. In the case of polycrystalline nickel-titanium shape memory alloys, the pseudoelastic deformations are in the magnitude of about 5–10% engineering strain.

On condition that the austenitic material is loaded below the austenite finish temperature A_f but above the martensite start temperature M_s (see Figure 1b and c), martensitic phase transitions occur during mechanical loading, but after unloading inelastic deformations remain in the shape memory alloy, because the detwinned martensite still exists (see Figure 1b). This effect is called pseudoplasticity due to martensitic phase transitions. Of course, the pseudoplastic behavior (r-pseudoplasticity) is also observed below M_f : in this situation, the shape memory alloy consists of martensite twins in the stress-free state, which can be oriented and reoriented by appropriate mechanical loads. In the present study, this effect is not regarded in the model, but the basic structure of the constitutive theory [Helm 2001; Helm and Haupt 2003] also includes the description of this phenomenon.

In addition to the pseudoelastic and pseudoplastic behavior, appropriate thermomechanical processes lead to one-way and two-way shape memory effects. The one-way shape memory effect takes place if the detwinned martensite is heated at sufficient small mechanical loads. Between the A_s - and A_f -temperature, the oriented martensite transforms back into austenite (see Figure 1b), the inelastic deformations disappear, and the material regains its original shape. Therefore, this material behavior is called one-way shape memory effect.

Under certain circumstances, shape memory alloys exhibit a two-way shape memory effect. Therefore, oriented martensite must be produced by an appropriate stress field in the microstructure, which can be the result of residual stresses or external forces. This stress field must be affected on the microstructure during a subsequent heating and cooling process between the A_f - and M_f -temperature (see Figure 1c). In analogy to the one way-shape memory effect, the material regains approximately its undeformed shape during heating. However, the required temperature to initiate and propagate the martensitic phase transitions is higher than in the case of the one-way shape memory effect, because the existing stress state increases the characteristic phase transition temperatures. In contrast to the one-way shape memory effect, the induced stress state during the cooling process leads to phase transitions from austenite into oriented martensite. Consequently, the material regains its deformed shape. In the used definition of the two-way shape memory effect, which is advantageously for the modeling of the material behavior, the two-way shape memory effect is released by a suitable stress field, which interacts with the microstructure, and an appropriate variation in the temperature field. This usage of the term two-way shape memory effect differs from the classical definition (see the explanations in [Funakubo 1987; Otsuka and Wayman 1998]): in the classical definition, the two-way shape memory effect is only released by residual stress fields. The other phenomenon is called two-way behavior of a shape memory alloy with a one-way characteristic [Funakubo 1987].

More than twenty years ago, the first constitutive theories for shape memory alloys were published [Achenbach and Müller 1982; Bertram 1982; Tanaka and Nagaki 1982; Falk 1983]. Since these pioneering studies, many different constitutive theories have been developed, and a number of models are able to predict the uniaxial behavior of shape memory alloys; see, for example, [Liang and Rogers 1990; Khan and Lagoudas 2002; Seelecke 2002; Paiva et al. 2005]. Such theories are well applicable to simulate the behavior of one-dimensional structures like the usage of wires in actuator applications. However, the simulation of applications like stents or pipe couplers requires three-dimensional formulated constitutive theories. For this purpose, a large number of phenomenological models were suggested: for example, Bertram [1982] and Graesser and Cozzarelli [1994] developed constitutive theories, which are not discussed in a thermodynamic framework. In contrast to these concepts, constitutive theories in the framework of continuum thermomechanics have been proposed in [Boyd and Lagoudas 1994; Raniecki et al. 1992; Raniecki and Lexcellent 1994; Leclercq and Lexcellent 1996; Souza et al. 1998; Juhász et al. 2000; Entchev and Lagoudas 2002; Helm and Haupt 2003; Lexcellent et al. 2006]. These models consist of a thermodynamic function for the free energy (Helmholtz free energy) or the free enthalpy (Gibbs free energy), which depends on state and internal variables. Moreover, evolution equations for certain internal variables are introduced to represent the history dependent material behavior as well as dissipation phenomena. An elaborate review about the phenomenological modeling of shape memory alloys was recently published in [Lagoudas et al. 2006]. In addition to the discussions in that paper, it should be mentioned that a part of the phenomenological models subdivide the evolution of the phase

transition strains into an evolution equation for the forward phase transition and an evolution equation for the reverse phase transition; see, for example, [Bondaryev and Wayman 1988; Boyd and Lagoudas 1994; Auricchio et al. 1997; Helm 2001; Lagoudas et al. 2006]. In contrast to this, the approaches in [Graesser and Cozzarelli 1994; Delobelle and Lexcellent 1996; Souza et al. 1998; Juhász et al. 2000; Helm and Haupt 2003; Auricchio and Stefanelli 2004] utilize only one evolution equation for both directions of phase transitions. In addition to these phenomenological concepts, different types of micromechanically motivated theories have also been proposed in the literature; see, for instance, [Patoor et al. 1994; Lexcellent et al. 1996; Huang et al. 2000; Lim and McDowell 2002; Tanaka et al. 2002; Anand and Gurtin 2003; Thamburaja and Anand 2003; Jung et al. 2004; Novák and Sittner 2004; Patoor et al. 2006], which are able to model the influence of the microstructure on the macroscopic behavior. Most of the proposed constitutive theories are formulated in the framework of a geometrically linear theory. However, the simulation of certain problems like stents or endoscopic devices requires a geometrically nonlinear theory. Referring to this, only a few geometrically nonlinear concepts have been proposed in the common literature: on the one hand, phenomenological theories were published in [Auricchio and Taylor 1997; Qidwai and Lagoudas 2000; Helm 2001; Müller and Bruhns 2004]. On the other hand, in [Anand and Gurtin 2003; Thamburaja and Anand 2003; Jung et al. 2004], the focus has been on micromechanical models at finite deformations.

For many applications, it is sufficient to apply a geometrically linear theory. However, a geometrically nonlinear constitutive theory is generally required, because different types of applications are characterized by large rotations. Therefore, the present work is concerned with the thermomechanical modeling in the case of small and also finite deformations. Our previous studies [Helm and Haupt 2003; Helm 2005] are geometrically linear theories and contain singularities in the phase transition function. Moreover, the concept of the former paper also contains a singularity in the phase transition rule. In certain cases, both types of singularities are removable if a simple von Mises phase transition function is applied. In contrast to these previous studies, the present constitutive theory does not contain such types of singularities, because the dependence of the fraction of oriented martensite on the transformation strains is modeled by a novel constitutive equation. In addition to this mathematical improvement, the modified constitutive relation leads also to a more precise depiction of the observed material behavior: e.g., the modeling of residual martensite after unloading at temperatures above A_f .

The first part of the article is organized as follows: in Section 2, the kinematics for representing inelasticity with respect to small and finite deformations are outlined. Thereafter, the basic structure of the constitutive theories to model the multiaxial behavior of shape memory alloys in the framework of continuum thermomechanics is developed (geometrically linear theory: Section 3; geometrically nonlinear theory: Section 4). In both cases, a free energy function and two evolution equations for internal variables are introduced. Both models are able to represent the basic phenomena of shape memory alloys due to martensitic phase transitions: i.e. pseudoelasticity and pseudoplasticity as well as one-way and two-way shape memory effect. Moreover, the representation of other effects like tension-compression asymmetries or the cyclic behavior of shape memory alloys is possible, if certain parts of the model are slightly changed. A second part of this article ([Helm and Schäfers 2006]) will deal with the numerical treatment of these constitutive theories in the framework of the finite element method. For this purpose, the system of differential equations is numerically integrated to obtain the stress state as well as the

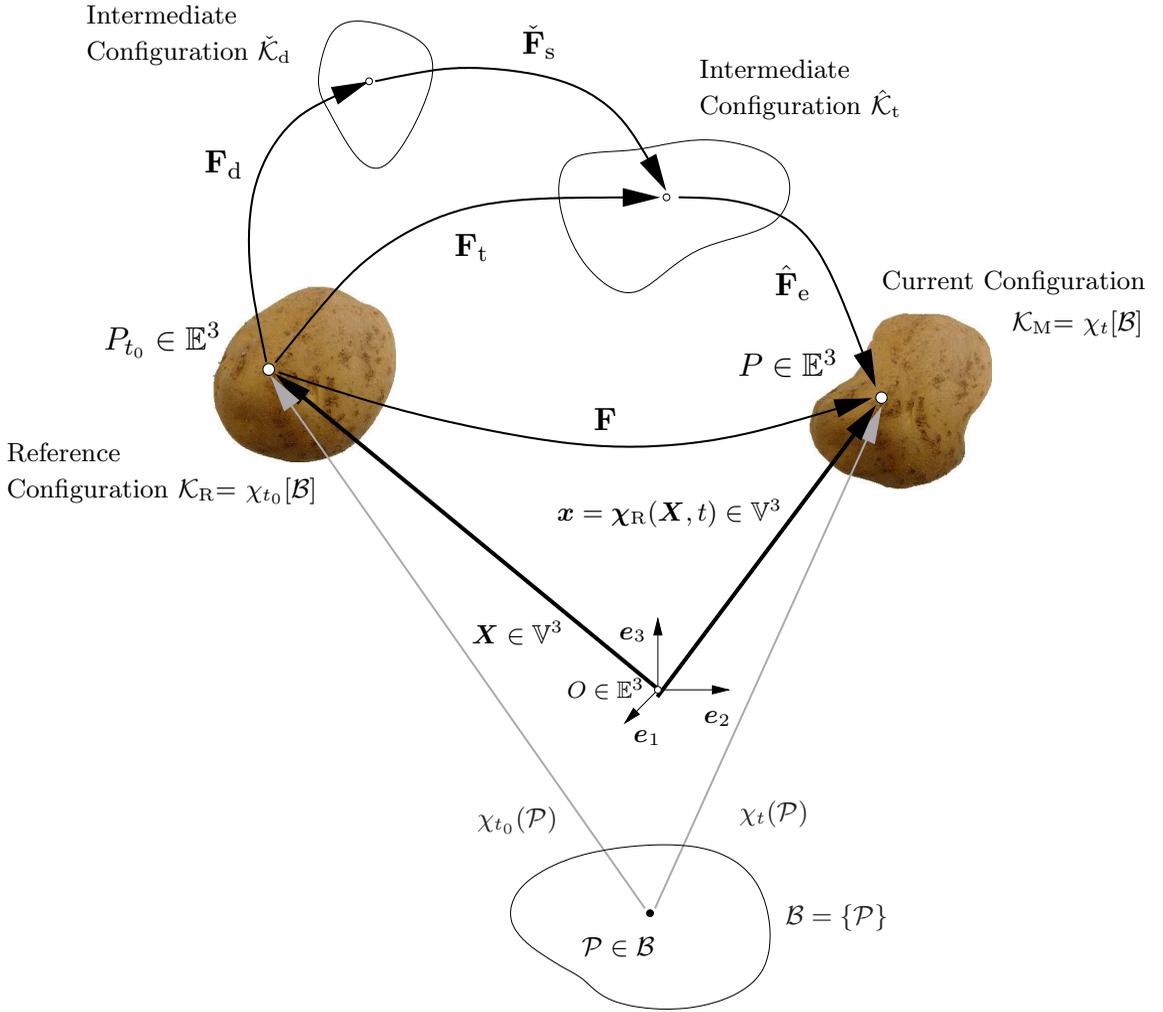


Figure 2. Reference, current, and intermediate configuration.

accompanying heat production. The capabilities of these constitutive theories are demonstrated with illustrative examples and the results of the constitutive theories are compared to experimental data.

2. Kinematics

The continuum mechanics is based on the assumption that a material body \mathcal{B} consists of material points \mathcal{P} and its motion is depicted by a continuous sequence of configurations (see Figure 2). If a reference configuration is selected, the motion is representable by the one-to-one mapping: $\mathbf{x} = \chi_{\mathbf{R}}(\mathbf{X}, t)$. The local changes in space of the motion are depicted by the deformation gradient $\mathbf{F}(\mathbf{X}, t) = \text{Grad } \chi_{\mathbf{R}}(\mathbf{X}, t)$, which is the Fréchet-derivative of the motion $\mathbf{x} = \chi_{\mathbf{R}}(\mathbf{X}, t)$. The deformation gradient transforms material line elements $d\mathbf{X}$ of the reference configuration $\mathcal{K}_{\mathbf{R}}$ into material line elements of the current configuration $\mathcal{K}_{\mathbf{M}}$: i.e., $d\mathbf{x} = \mathbf{F}d\mathbf{X}$.

The following theory for finite deformations makes use of the multiplicative split $\mathbf{F} = \mathbf{F}^* \bar{\mathbf{F}}$, which can be traced back to [Flory 1961]: in this multiplicative split, the deformation gradient \mathbf{F} is decomposed into a volumetric part \mathbf{F}^* and an isochoric part $\bar{\mathbf{F}}$ if the operators

$$(\cdot)^* : \mathbf{F} \mapsto \mathbf{F}^* = (\det \mathbf{F})^{1/3} \mathbf{1} \quad \text{and} \quad (\bar{\cdot}) : \mathbf{F} \mapsto \bar{\mathbf{F}} = (\det \mathbf{F})^{-1/3} \mathbf{F} \quad (1)$$

are applied. Throughout the whole article, these operators are used in a more general sense: the tensor $\bar{\mathbf{A}} = (\det \mathbf{A})^{-1/3} \mathbf{A}$ is the unimodular part of \mathbf{A} and the remaining nonunimodular part of \mathbf{A} is denoted by $\mathbf{A}^* = (\det \mathbf{A})^{1/3} \mathbf{1}$.

2.1. Multiplicative decompositions of the deformation gradient. In finite deformation theories for modeling the inelastic behavior of different types of materials, the multiplicative decomposition of the deformation gradient $\mathbf{F} = \hat{\mathbf{F}}_e \mathbf{F}_i$ into an elastic part $\hat{\mathbf{F}}_e$ and an inelastic part \mathbf{F}_i is often applied (see [Kröner 1960; Lee 1969; Lee and Liu 1967; Lubliner 1985; Haupt 2002]). In the present framework, the related multiplicative decomposition $\mathbf{F} = \hat{\mathbf{F}}_e \mathbf{F}_t$ is used: therein, $\hat{\mathbf{F}}_e$ is the elastic part of the deformation gradient and \mathbf{F}_t represents the inelastic part of the deformation gradient resulting from martensitic phase transitions see [Auricchio and Taylor 1997; Helm 2001]. The multiplicative decomposition of the deformation gradient implies a stress-free intermediate configuration $\hat{\mathcal{K}}_t$ (see Figure 2). Already in [Eckart 1948] and [Kröner 1958], stress-free intermediate configurations were introduced to define inelastic states. It is common knowledge that the multiplicative decomposition $\mathbf{F} = \hat{\mathbf{F}}_e \mathbf{F}_t$ leads to an incompatible intermediate configuration; see [Eckart 1948; Lee 1969; Mandel 1972; Haupt 2002].

As a result of our previous studies [Helm and Haupt 2003; Helm 2005], the consideration of internal stress fields is a useful concept to model the material behavior of shape memory alloys. It is known from viscoplasticity [Lion 2000] that an additional multiplicative decomposition of the inelastic part is appropriate to model internal stress fields in a geometrically nonlinear theory. Therefore, this concept is transferred to the present study (see [Helm 2001]): the inelastic part $\mathbf{F}_t = \check{\mathbf{F}}_s \mathbf{F}_d$ of the deformation gradient is decomposed into two parts $\check{\mathbf{F}}_s$ and \mathbf{F}_d . In the present theory, the part $\check{\mathbf{F}}_s$ is used to model energy storage effects during the evolution of internal stress fields while the remainder part \mathbf{F}_d is introduced to account for the accompanied dissipative phenomena. In addition to the intermediate configuration $\hat{\mathcal{K}}_t$, the additional decomposition of $\mathbf{F}_t = \check{\mathbf{F}}_s \mathbf{F}_d$ formally results in a further intermediate configuration $\check{\mathcal{K}}_d$ (see Figure 2).

2.2. Strain tensors.

2.2.1. Finite strains. Provided that the multiplicative decomposition is used, the Green strain tensor $\mathbf{E} = [\mathbf{C} - \mathbf{1}] / 2$ cannot be separated into purely elastic and inelastic parts. Therein, the tensor $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ is the right Cauchy–Green tensor. However, the transformation of the Green strain tensor to the intermediate configuration $\hat{\mathcal{K}}_t$ leads to a strain measure (see [Haupt 1985])

$$\hat{\mathbf{\Gamma}} = \mathbf{F}_t^{-T} \mathbf{E} \mathbf{F}_t^{-1} = \hat{\mathbf{\Gamma}}_e + \hat{\mathbf{\Gamma}}_t \quad \text{with} \quad \hat{\mathbf{\Gamma}}_e = \frac{1}{2} (\hat{\mathbf{C}}_e - \mathbf{1}) \quad \text{and} \quad \hat{\mathbf{\Gamma}}_t = \frac{1}{2} (\mathbf{1} - \hat{\mathbf{B}}_t^{-1}), \quad (2)$$

which is additively decomposable into an elastic part $\hat{\mathbf{\Gamma}}_e$ and an inelastic part $\hat{\mathbf{\Gamma}}_t$. Therein, the tensors $\hat{\mathbf{C}}_e = \hat{\mathbf{F}}_e^T \hat{\mathbf{F}}_e$ and $\hat{\mathbf{B}}_t = \mathbf{F}_t \mathbf{F}_t^T$ are defined in analogy to the right and left Cauchy–Green tensors, $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ and $\mathbf{B} = \mathbf{F} \mathbf{F}^T$. If $\hat{\mathbf{\Gamma}}_e$ and $\hat{\mathbf{\Gamma}}_t$ are expressed in terms of the reference configuration \mathcal{K}_R ,

$$\mathbf{E}_e = \mathbf{F}_t^T \hat{\mathbf{\Gamma}}_e \mathbf{F}_t = \frac{1}{2} (\mathbf{F}_t^T \hat{\mathbf{C}}_e \mathbf{F}_t - \mathbf{F}_t^T \mathbf{F}_t) \quad \text{and} \quad \mathbf{E}_t = \mathbf{F}_t^T \hat{\mathbf{\Gamma}}_t \mathbf{F}_t = \frac{1}{2} (\mathbf{F}_t^T \mathbf{F}_t - \mathbf{1}), \quad (3)$$

it becomes clear that the transformation strain state \mathbf{E}_t depends only on \mathbf{F}_t , but the elastic strain state \mathbf{E}_e is a function of $\hat{\mathbf{F}}_e$ and \mathbf{F}_t .

On the basis of the foregoing discussion, an internal variable to represent internal stress fields can be introduced with respect to the intermediate configuration $\check{\mathcal{K}}_d$: the transformation of \mathbf{E}_t or $\hat{\mathbf{F}}_t$ to the intermediate configuration $\check{\mathcal{K}}_d$ leads to an internal variable $\check{\mathbf{Y}}$ of strain type,

$$\check{\mathbf{Y}} = \mathbf{F}_d^{-T} \mathbf{E}_t \mathbf{F}_d^{-1} = \check{\mathbf{F}}_s^T \hat{\mathbf{F}}_t \check{\mathbf{F}}_s = \check{\mathbf{Y}}_s + \check{\mathbf{Y}}_d, \quad (4)$$

which can be additively decomposed into $\check{\mathbf{Y}}_s$ and $\check{\mathbf{Y}}_d$:

$$\check{\mathbf{Y}}_s = \frac{1}{2}(\check{\mathbf{C}}_s - \mathbf{1}) \quad \text{and} \quad \check{\mathbf{Y}}_d = \frac{1}{2}(\mathbf{1} - \check{\mathbf{B}}_d^{-1}). \quad (5)$$

In analogy to the left and right Cauchy–Green tensors, the tensors $\check{\mathbf{C}}_s = \check{\mathbf{F}}_s^T \check{\mathbf{F}}_s$ and $\check{\mathbf{B}}_d = \mathbf{F}_d \mathbf{F}_d^T$ are defined.

Remark 1 (Notation). In order to distinguish between the different configurations the following terminology is applied (see Figure 2): Stress and strain tensors operating in the intermediate configuration $\hat{\mathcal{K}}_t$ are denoted by $(\hat{\cdot})$. In contrast to this, the stress and strain measures in the second intermediate configuration $\check{\mathcal{K}}_d$ are denoted by $(\check{\cdot})$. For the stress tensors in the reference configuration \mathcal{K}_R the notation $(\tilde{\cdot})$ is used and for the strain tensors the letters like \mathbf{E} and \mathbf{C} are applied. In the case of the theory for small deformations (see Eq.(6) and (7)), the distinction of different configurations is not required. Moreover, the quantities $\check{\mathbf{F}}_s$ and $\hat{\mathbf{F}}_e$ are denoted with $(\check{\cdot})$ and $(\hat{\cdot})$, because they transform material line elements from different intermediate configurations.

2.2.2. Small strains. The previously introduced strain measures on the basis of the multiplicative decompositions are not required in their exact forms if the special case of a theory for small deformations is considered: according to [Casey 1985], the multiplicative decomposition of the deformation gradient $\mathbf{F} = \hat{\mathbf{F}}_e \mathbf{F}_t$ corresponds in a geometrically linear theory to the additive decomposition of the linearized Green strain tensor,

$$\mathbf{E} = \mathbf{E}_e + \mathbf{E}_t, \quad (6)$$

into an elastic part \mathbf{E}_e and an inelastic part \mathbf{E}_t , which represent the transformation strain state. Finally, the other multiplicative decomposition $\mathbf{F}_t = \check{\mathbf{F}}_s \mathbf{F}_d$ merge into the additive decomposition

$$\mathbf{Y} = \mathbf{E}_t = \mathbf{Y}_s + \mathbf{Y}_d, \quad (7)$$

if the assumption of small deformations is applied. Consequently, the geometrically linear theory can be formulated on the basis of the additive decomposition (6) and (7).

3. Constitutive theory in relation to small deformations

3.1. Free energy. In shape memory alloys different types of energy storage mechanisms play an important role: for example the change in internal energy due to the thermoelasticity of a single-phase material, the energy change on account of the phase transitions, as well as energy storage phenomena resulting from internal stress fields. Consequently, it is assumed that the free energy of the proposed model depends on the elastic part of the linearized Green strain tensor \mathbf{E}_e (see Equation (6)), the absolute thermodynamic temperature θ , the fraction $z \in [0, 1]$ of oriented martensite, and the internal variable \mathbf{Y}_s :

$$\psi(\mathbf{E}_e, \theta, z, \mathbf{Y}_s) = \hat{\psi}_e(\mathbf{E}_e, \theta, z) + \hat{\psi}_s(\mathbf{Y}_s, \theta). \quad (8)$$

In this assumption, the thermoelastic part ψ_e represents the mixture of two thermoelastic single-phase materials (austenite (A) and martensite (M)):

$$\begin{aligned} \rho\psi_e &= \rho\hat{\psi}_e(\mathbf{E}_e, \theta, z) = z\rho\psi_e^M(\mathbf{E}_e, \theta) + (1-z)\rho\psi_e^A(\mathbf{E}_e, \theta) \\ &= \tilde{\mu}(\theta, z)\mathbf{E}_e^D \cdot \mathbf{E}_e^D + \frac{\tilde{\kappa}(\theta, z)}{2} (\text{tr } \mathbf{E}_e)^2 - 3\tilde{\alpha}(\theta, z) (\text{tr } \mathbf{E}_e) (\theta - \theta_0) \\ &\quad + z\rho \int_{\theta_0}^{\theta} c_{d_0}^M(\bar{\theta})d\bar{\theta} + (1-z)\rho \int_{\theta_0}^{\theta} c_{d_0}^A(\bar{\theta})d\bar{\theta} + \rho [u_0^A + z\Delta u_0] \\ &\quad - \theta \left[z\rho \int_{\theta_0}^{\theta} \frac{c_{d_0}^M(\bar{\theta})}{\bar{\theta}}d\bar{\theta} + (1-z)\rho \int_{\theta_0}^{\theta} \frac{c_{d_0}^A(\bar{\theta})}{\bar{\theta}}d\bar{\theta} + \rho [\eta_0^A + z\Delta\eta_0] \right]. \end{aligned} \quad (9)$$

Therein, the effective elasticity parameters

$$\tilde{\mu}(\theta, z) = z\mu^M(\theta) + (1-z)\mu^A(\theta), \quad (10)$$

$$\tilde{\kappa}(\theta, z) = z\kappa^M(\theta) + (1-z)\kappa^A(\theta), \quad \text{and} \quad (11)$$

$$\tilde{\alpha}(\theta, z) = z\alpha^M(\theta)\kappa^M(\theta) + (1-z)\alpha^A(\theta)\kappa^A(\theta) \quad (12)$$

contain the elasticity parameters of the different phases ($\omega = A, M$): μ^ω is the shear modulus, κ^ω the bulk modulus, and α^ω the linear expansion coefficient. Moreover, θ_0 represents the reference temperature, $c_{d_0}^\omega$ is a certain part of the specific heat at constant deformation, and the initial internal energy and the initial entropy are denoted by u_0^ω and η_0^ω . Furthermore the constants $\Delta u_0 = u_0^M - u_0^A$ and $\Delta\eta_0 = \eta_0^M - \eta_0^A$ are of special interest in the thermomechanical modeling of phase transitions (see [Huo and Müller 1993; Helm and Haupt 2003]): for instance, they play a dominant role in the description of latent heat effects. The thermomechanical interactions between the austenite and martensite phase in the microstructure of the material are strongly simplified due to the assumption of equal thermoelastic strain and temperature states in both phases.

The other part $\hat{\psi}_s(\mathbf{Y}_s)$ of the free energy models the energy storage due to the generation and variation of internal stresses. Each grain of a polycrystalline shape memory alloy contains a lot of imperfections like precipitations and impurities. Consequently, the martensitic phase transitions are obstructed by the imperfections and by the surrounding grains. As a macroscopical result of these microstructural phenomena, the associated part ψ_s of the free energy function is assumed to be

$$\rho\psi_s = \rho\hat{\psi}_s(\theta, \mathbf{Y}_s) = \frac{c(\theta)}{2} \mathbf{Y}_s \cdot \mathbf{Y}_s. \quad (13)$$

Therein, $c(\theta)$ is a nonnegative material function of temperature.

3.2. Evolution equations for internal variables. In order to develop a thermodynamically consistent theory, the basic structure of the free energy function according to Equation (8) is introduced into the internal dissipation inequality $\rho\delta_i = -\rho\dot{\psi} - \rho\dot{\theta}\eta + \mathbf{T} \cdot \dot{\mathbf{E}} \geq 0$ (for details see [Helm and Haupt 2003] or Section 4):

$$\rho\delta_i = \left[\mathbf{T} - \rho \frac{\partial \psi_e}{\partial \mathbf{E}_e} \right] \cdot \dot{\mathbf{E}}_e - \rho \left[\frac{\partial \psi}{\partial \theta} + \eta \right] \dot{\theta} - \rho \frac{\partial \psi_e}{\partial z} \dot{z} - \rho \frac{\partial \psi_s}{\partial \mathbf{Y}_s} \cdot \dot{\mathbf{Y}}_s + \mathbf{T} \cdot \dot{\mathbf{E}}_t \geq 0. \quad (14)$$

Therein, η is the entropy and the material density is denoted by ρ . For arbitrary rates of \mathbf{E}_e , θ , z , \mathbf{Y}_s , and $\dot{\mathbf{E}}_t$, this inequality implies potential relations for the stress tensor \mathbf{T} ,

$$\mathbf{T} = \rho \frac{\partial \psi_e}{\partial \mathbf{E}_e} = 2\tilde{\mu}(\theta, z)\mathbf{E}_e^D + \tilde{\kappa}(\theta, z)(\text{tr } \mathbf{E}_e)\mathbf{1} - 3\tilde{\alpha}(\theta, z)(\theta - \theta_0)\mathbf{1}, \quad (15)$$

and the entropy $\eta = -\partial\psi/\partial\theta$, if \dot{z} , $\dot{\mathbf{Y}}_s$, and $\dot{\mathbf{E}}_t$ do not depend on $\dot{\mathbf{E}}_e$ and $\dot{\theta}$ (see [Coleman and Gurtin 1967]). Furthermore, the remaining dissipation inequality motivates the definition of the thermodynamic quantity $\Xi = \rho\partial\psi_e/\partial z$,

$$\begin{aligned} \Xi = & \frac{\partial \tilde{\mu}(\theta, z)}{\partial z} \mathbf{E}_e^D \cdot \mathbf{E}_e^D + \frac{1}{2} \frac{\partial \tilde{\kappa}(\theta, z)}{\partial z} (\text{tr } \mathbf{E}_e)^2 - 3 \frac{\partial \tilde{\alpha}(\theta, z)}{\partial z} (\text{tr } \mathbf{E}_e)(\theta - \theta_0) \\ & + \rho \left[\int_{\theta_0}^{\theta} [c_{d_0}^M(\bar{\theta}) - c_{d_0}^A(\bar{\theta})] d\bar{\theta} + \Delta u_0 \right] - \rho\theta \left[\int_{\theta_0}^{\theta} \frac{c_{d_0}^M(\bar{\theta}) - c_{d_0}^A(\bar{\theta})}{\bar{\theta}} d\bar{\theta} + \Delta \eta_0 \right], \quad (16) \end{aligned}$$

and the internal stress field \mathbf{X}_ε :

$$\mathbf{X}_\varepsilon = \rho \frac{\partial \psi_s}{\partial \mathbf{Y}_s} = c(\theta) \mathbf{Y}_s = c(\theta) [\mathbf{E}_t - \mathbf{Y}_d]. \quad (17)$$

The thermodynamic quantity Ξ plays an important role in view of the depiction of the stress state, which is required to initiate and propagate the martensitic phase transitions. The other internal variable \mathbf{X}_ε incorporates the fact that the cooperative motion of the atoms during the martensitic phase transitions is limited by defects in the microstructure like impurities and precipitations. In classical theories of plasticity, \mathbf{X}_ε is denoted as back stress.

With these definitions, the remaining dissipation inequality takes the following form:

$$\rho \delta_i = -\Xi \dot{z} + \mathbf{T} \cdot \dot{\mathbf{E}}_t - \mathbf{X}_\varepsilon \cdot \dot{\mathbf{Y}}_s \geq 0. \quad (18)$$

To complete the material model, constitutive equations for the internal variables z , \mathbf{E}_t , and $\mathbf{Y}_d = \mathbf{E}_t - \mathbf{Y}_s$ have to be defined. On account of the physical understanding of the deformation mechanisms (see [Miyazaki and Otsuka 1989], for instance) and also based on experimental studies, the martensitic phase transitions between austenite and oriented martensite are accompanied by inelastic deformations. In polycrystalline materials, the required constitutive relation between the oriented martensite fraction z and the transformation strain tensor \mathbf{E}_t is quite difficult to identify. However, the following physical aspects should be considered in a constitutive theory for shape memory alloys: if the material is completely in the austenite phase, the transformation strains must vanish, i.e. $\mathbf{E}_t = \mathbf{0}$. Moreover, if a complex deformation path is performed, which starts and ends at $\mathbf{E}_t = \mathbf{0}$, it must be guaranteed that the fraction of oriented martensite is always zero if $\mathbf{E}_t = \mathbf{0}$. Both $z = \hat{z}(\mathbf{E}_t)$ with the restriction $\hat{z}(\mathbf{0}) = 0$ and $\mathbf{E}_t = \bar{\mathbf{E}}_t(z)$ with the constraint $\bar{\mathbf{E}}_t(0) = \mathbf{0}$ are appropriate strategies to model the observations. In the present concept the fraction of oriented martensite $z = \hat{z}(\mathbf{E}_t)$ is depicted as function of \mathbf{E}_t . It should be emphasized that such a relation is only meaningful between the fraction of detwinned martensite and the inelastic strain state, because the fraction of twinned martensite does not depend on the inelastic strain state.

Remark 2. Instead of a function $z = \hat{z}(\mathbf{E}_t)$, it is possible to apply an evolution equation for z , namely $\dot{z} = Z(\mathbf{E}_t) \cdot \dot{\mathbf{E}}_t$. Then, the relation

$$z = \oint Z(\mathbf{E}_t) \cdot d\mathbf{E}_t = 0 \quad (19)$$

must be fulfilled if an arbitrary deformation process starts at $\mathbf{E}_t = \mathbf{0}$. This relation guarantees that z vanishes after an arbitrary multiaxial process, which starts and ends at $\mathbf{E}_t = \mathbf{0}$. Of course, Equation (19) is fulfilled, if and only if $Z(\mathbf{E}_t)$ is equal to $dz/d\mathbf{E}_t$.

For an isotropic material, the fraction z of oriented martensite depends on the basic invariants ($J_{t1} = \text{tr } \mathbf{E}_t$, $J_{t2} = \text{tr } \mathbf{E}_t^2$, and $J_{t3} = \text{tr } \mathbf{E}_t^3$): $z = \hat{z}(\mathbf{E}_t) = \tilde{z}(J_{t1}, J_{t2}, J_{t3})$. In the remaining dissipation inequality, the material time derivative of $z = \tilde{z}(J_{t1}, J_{t2}, J_{t3})$ is required:

$$\dot{z} = \frac{d\hat{z}}{d\mathbf{E}_t} \cdot \dot{\mathbf{E}}_t \quad \text{with} \quad \frac{\partial \hat{z}}{\partial \mathbf{E}_t} = \frac{\partial \tilde{z}}{\partial J_{t1}} \mathbf{1} + 2 \frac{\partial \tilde{z}}{\partial J_{t2}} \mathbf{E}_t + 3 \frac{\partial \tilde{z}}{\partial J_{t3}} \mathbf{E}_t^2. \quad (20)$$

Martensitic phase transitions are accompanied by small volume changes (see [Shimizu and Tadaki 1987], for instance), which may be neglected. For example, in NiTi the volume change by phase transitions between austenite and martensite amounts 0.34%. Consequently, the underlying deformation mechanism is nearly volume preserving. As a result of this material property, the influence of the first invariant J_{t1} in the function of z can be omitted. Furthermore, the transformation strains are small and dominated by shear deformations. Therefore, the influence of the second invariant is much more important than that of the third invariant. However, for the modeling of tension-compression asymmetries in the strain space, the first and third invariants may be important quantities. Ignoring these possibilities, the fraction of oriented martensite is introduced to be a function of the second invariant J_{t2} : $z = \tilde{z}(J_{t2})$. In phenomenological theories for shape memory alloys; see, for example, [Levitas 1998; Juhász et al. 2000; Helm and Haupt 2003], the fraction of oriented martensite is commonly depicted in the following form:

$$z = \hat{z}(\mathbf{E}_t) = \tilde{z}(J_{t2}) = \frac{\|\mathbf{E}_t\|}{\sqrt{\frac{3}{2}} \gamma_t} \quad \Rightarrow \quad \dot{z} = \frac{\mathbf{E}_t \cdot \dot{\mathbf{E}}_t}{\sqrt{\frac{3}{2}} \gamma_t \|\mathbf{E}_t\|}. \quad (21)$$

Therein, the norm of \mathbf{E}_t is given by $\|\mathbf{E}_t\| = \sqrt{\mathbf{E}_t \cdot \mathbf{E}_t}$ and γ_t represents the maximum transformation strain, which can be measured in a uniaxial test. It should be mentioned that a similar relation was suggested by Bertram [1982] in terms of the so-called limit function. As pointed out in [Helm and Haupt 2003], the evolution equation (phase transition rule) for the transformation strains incorporates the time derivative of z according to Equation (21)₂. Therefore, the applied phase transition rule (see Equation (27) and the internal variable \mathbf{X}_θ according to Equation (24) for $\gamma_0 = 0$) and likewise the introduced phase transition function are singular, if a process starts at $\mathbf{E}_t = \mathbf{0}$. In certain cases, these singularities are removable, but difficulties in numerical implementation still remain. Similar problems exist in the theories of Souza et al. [1998], Juhász et al. [2000], and Auricchio and Stefanelli [2004]. In order to avoid this problem, Auricchio and Petri [2004] introduce a regularized norm operator. Moreover, the shape memory materials often show a smooth transition from the retransformation plateau into the elastic region (see region II in Figure 1a): in previous models, such as that of [Helm and Haupt 2003], this smooth transition cannot be described. Therefore, an improved constitutive equation for representing the fraction

of oriented martensite as a function of the transformation strain tensor is proposed in the present article:

$$z = \hat{z}(\mathbf{E}_t) = \tilde{z}(J_{t2}) = \frac{\sqrt{\frac{2}{3}\mathbf{E}_t \cdot \mathbf{E}_t + \gamma_0^2}}{\gamma_t} - z_0. \quad (22)$$

In this constitutive relation, γ_t is still the maximum transformation strain. In contrast to the constitutive relation (21), the positive parameters γ_0 and z_0 are additionally introduced. The parameter z_0 is pre-determined, because the physical understanding of the occurring martensitic phase transitions between austenite and oriented martensite requires $z = \hat{z}(\mathbf{0}) = 0$. Consequently, this condition leads to $z_0 = \gamma_0/\gamma_t$. The parameter γ_0 has an important influence on the rate of z (Equation (22)),

$$\dot{z} = \frac{\mathbf{E}_t \cdot \dot{\mathbf{E}}_t}{\sqrt{\frac{3}{2}\gamma_t \sqrt{\mathbf{E}_t \cdot \mathbf{E}_t + \frac{3}{2}\gamma_0^2}}}, \quad (23)$$

because the influence of γ_0 on z is only negligible if $\|\mathbf{E}_t\| \gg \gamma_0$. In order to obtain the final form of the internal dissipation inequality (18), the time derivative of z according to Equation (23) is inserted, the time derivative of $\mathbf{Y}_s = \mathbf{E}_t - \mathbf{Y}_d$ is replaced by usage of Equation (7), and the internal variable \mathbf{X}_θ of stress type (see the discussion in [Helm and Haupt 2003]):

$$\mathbf{X}_\theta = \Xi \frac{d\hat{z}}{d\mathbf{E}_t} = \frac{\Xi \mathbf{E}_t}{\sqrt{\frac{3}{2}\gamma_t \sqrt{\mathbf{E}_t \cdot \mathbf{E}_t + \frac{3}{2}\gamma_0^2}}}, \quad (24)$$

as well as $\mathbf{X} = \mathbf{X}_\varepsilon + \mathbf{X}_\theta$ is considered:

$$\rho \delta_i = [\mathbf{T} - \mathbf{X}] \cdot \dot{\mathbf{E}}_t + \mathbf{X}_\varepsilon \cdot \dot{\mathbf{Y}}_d \geq 0. \quad (25)$$

The introduced internal variable \mathbf{X}_θ has a physical meaning, because \mathbf{X}_θ is responsible for the depiction of the temperature-dependence of the required stress state to initiate and progress the martensitic phase transitions. Due to the applied thermoelastic mixture, the thermodynamic quantity Ξ strongly depends on temperature. The most important term in Ξ is given by $\rho(\Delta u_0 - \theta \Delta \eta_0)$. Therefore, if suitable material parameters are used, the model predicts a nearly linear temperature-dependence of the required phase transition stress over a certain temperature range. This is the stress state, which is necessary to initiate and progress the martensitic phase transitions. In contrast to [Helm 2001; Helm and Haupt 2003], the internal variable \mathbf{X}_θ is a continuous function of \mathbf{E}_t . For a simple tension-compression load, the 11-component of \mathbf{X}_θ is proportional to

$$\frac{\varepsilon_t}{\sqrt{\varepsilon_t^2 + \gamma_0^2}}.$$

This function is plotted in Figure 3 for different values of γ_0 .

The final inequality (25) is an excellent basis to introduce a phase transition function

$$f = \|\mathbf{T}^D - \mathbf{X}^D\| - \sqrt{\frac{2}{3}}k(\theta) \quad (26)$$

and the evolution equations for the internal variables \mathbf{E}_t and \mathbf{Y}_d . In the phase transition function, the quantity $k(\theta)$ is the radius of the phase transition surface. In general, it is also possible to introduce the phase transition radius as function of the fraction of oriented martensite in order to model isotropic

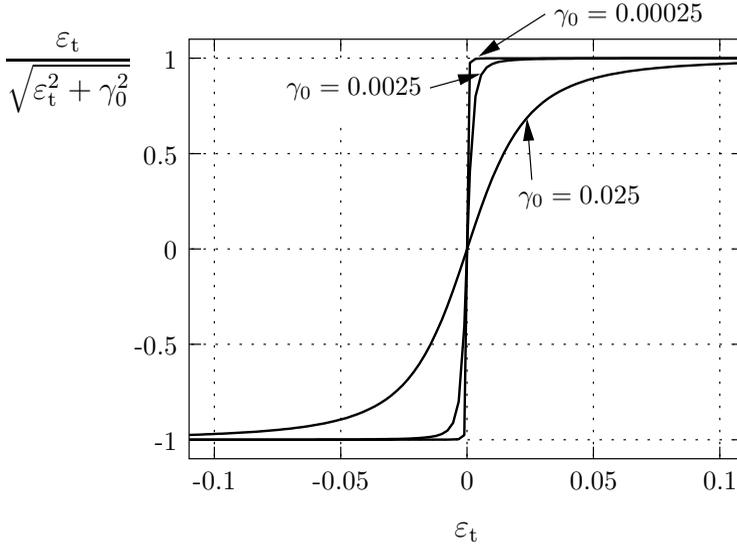


Figure 3. Illustration of $\mathbf{e}_1 \cdot \mathbf{X}_\theta \mathbf{e}_1 \sim \varepsilon_t / \sqrt{\varepsilon_t^2 + \gamma_0^2}$ for uniaxial tension-compression load.

transformation hardening. Such transformation hardening functions are commonly used in the modeling of shape memory alloys (see discussions in [Lagoudas et al. 2006]). Moreover, it is assumed that only deviatoric stress states influence the value of the phase transition function: $\mathbf{T}^D = \mathbf{T} - (\text{tr } \mathbf{T})/3 \mathbf{1}$. Due to the fact that phase transition function f depends on the internal variable \mathbf{X}_θ according to Equation (24), the model is restricted to a temperature range, which implies $\Xi \geq 0$ at $\mathbf{E}_e = \mathbf{0}$.

It should be mentioned that the simple v. Mises-type phase transition function leads initially to a symmetric tension-compression behavior. Such a behavior is almost observable for the first cycle in the uniaxial tension-compression experiments of Lim and McDowell [1995] on NiTi. In the case of a polycrystalline NiTi shape memory alloy without texture, the micromechanical studies of Gall and Sehitoglu [1999] lead to the result that, at the macroscopic level, merely a small tension-compression asymmetry is observable. In contrast to these results, a tension-compression asymmetry is experimentally observed and theoretically investigated in different types of shape memory alloys: see [Patoor et al. 1996; Gall and Sehitoglu 1999; Lim and McDowell 1999; Qidwai and Lagoudas 2000; Raniecki et al. 2001; Lexcellent et al. 2006]. Both the induced set of active martensite variants by the applied stress state and the texture of the material influence the tension-compression asymmetry. Consequently, depending on the underlying shape memory alloy and its microstructure, an appropriate phase transition function should be applied; see [Patoor et al. 1996; Qidwai and Lagoudas 2000].

Finally, the evolution equations for the internal variables \mathbf{E}_t and \mathbf{Y}_d are postulated.

- It is assumed that the transformation strain state \mathbf{E}_t evolves according to the phase transition rule

$$\dot{\mathbf{E}}_t = \lambda_t \mathbf{N} \quad \text{with the normal} \quad \mathbf{N} = \frac{\partial f}{\partial \mathbf{T}} = \frac{\mathbf{T}^D - \mathbf{X}^D}{\|\mathbf{T}^D - \mathbf{X}^D\|}. \quad (27)$$

In analogy to [Helm and Haupt 2003] and [Helm 2005], a nonnegative inelastic multiplier

$$\lambda_t = \begin{cases} \frac{1}{\eta_t(\theta)} \left\langle \frac{f}{r_t} \right\rangle^{m_t(\theta)} & \text{A} \rightarrow \vec{\text{M}} \text{ if } z < 1 \text{ and } \mathbf{E}_t \cdot \mathbf{N} \geq 0, \\ \frac{1}{\eta_t(\theta)} \left\langle \frac{f}{r_t} \right\rangle^{m_t(\theta)} & \vec{\text{M}} \rightarrow \text{A} \text{ if } z > 0 \text{ and } \mathbf{E}_t \cdot \mathbf{N} < 0, \\ 0 & \text{in all other cases} \end{cases} \quad (28)$$

of Perzyna-type is assumed [Perzyna 1963; Hohenemser and Prager 1932]. Therein, $\eta_t(\theta) > 0$ and $m_t(\theta)$ are temperature-dependent material functions and r_t is introduced to obtain a dimensionless argument to the operator: $\langle x \rangle = (|x| + x)/2$. The introduced inelastic multiplier leads to a rate-dependent theory. However, if $\eta_t(\theta) \rightarrow 0$ (but always $\eta_t(\theta) > 0$) or if sufficiently slow processes are considered, the material model approximates a rate-independent theory in the sense of an asymptotic limit. This property is well known in thermoviscoplasticity [Haupt et al. 1992; Haupt 2002].

For representing the history-dependent material behavior of shape memory alloys, a few case distinctions are introduced: the phase transition from austenite to oriented martensite takes place if the phase transition function f is positive, austenite is available ($z < 1$), and the fraction of oriented martensite increases ($dz \sim \mathbf{E}_t \cdot \mathbf{N} \geq 0$). In contrast to the forward transition, the retransformation occurs if oriented martensite is available ($z > 0$) and the fraction of oriented martensite decreases ($dz \sim \mathbf{E}_t \cdot \mathbf{N} < 0$). In comparison with the magnitude of the isochoric deformations, the occurring volume changes during the martensitic phase transitions are negligible. Therefore, a deviatoric evolution of \mathbf{E}_t is assumed; that is,

$$\mathbf{E}_t^D = \mathbf{E}_t - (\text{tr } \mathbf{E}_t)/3 \mathbf{1}.$$

As pointed out in [Helm and Haupt 2003], the applied evolution equation (27) is able to predict the direction of the transformation strain-rate in accordance with the experimental studies of [Lim and McDowell 1999]. The main reason for this result is that the internal variable \mathbf{X}_θ significantly influences the direction of the transformation strain-rate.

- Furthermore, the evolution of \mathbf{Y}_d is proposed to be proportional to the internal stress tensor \mathbf{X}_ε :

$$\dot{\mathbf{Y}}_d = \zeta_d \mathbf{X}_\varepsilon. \quad (29)$$

The introduced proportional factor $\zeta_d \geq 0$ is assumed to be

$$\zeta_d = \frac{B(\theta, z, \dot{z})}{c(\theta)} \dot{s}_t \quad \text{with} \quad \dot{s}_t = \sqrt{\frac{2}{3}} \|\dot{\mathbf{E}}_t\| \quad (30)$$

and the function

$$B(\theta, z, \dot{z}) = \begin{cases} \frac{1}{2} (\tanh[-\beta(\theta)(z - \gamma(\theta))] + 1) b(\theta) & \text{if } \dot{z} > 0, \\ b(\theta) & \text{if } \dot{z} < 0. \end{cases} \quad (31)$$

Here, \dot{s}_t is the rate of the accumulated phase transition strain s_t . Therein, b , β , and γ are nonnegative and generally temperature-dependent material functions. The constitutive model for the evolution of the internal stress fields (Equation (13), (30), and (31)) is a modification of a classical Armstrong–Frederick type approach: thus the strong stress slope as well as the different slope in the loading and unloading paths at the end of the phase transition plateau (see region I in Figure 1a and the experiments in [Huo and

Müller 1993; Shaw and Kyriakides 1995; Helm and Haupt 2001]) are all incorporated in the suggested constitutive theory.

On account of the internal stress tensor \mathbf{X}_ε (Equation (17)) and the accompanying evolution equation for the internal variable \mathbf{Y}_d (Equation (29)), the evolution of the internal stress state \mathbf{X}_ε depends on the deformation history and leads to an anisotropic behavior of the model, because the value of the phase transition function f (Equation (26)) depends on \mathbf{X}_ε . Therefore, the characteristic phase transition stresses and temperatures depends also on the deformation history.

If both evolution equations are introduced into the remaining dissipation inequality (25),

$$\rho \delta_i = \lambda_t \|\mathbf{T}^D - \mathbf{X}^D\| + \zeta_d \|\mathbf{X}_\varepsilon\|^2 \geq 0, \quad (32)$$

it is discernible that the proposed constitutive theory is thermodynamically consistent, because of $\lambda_t \geq 0$ and $\zeta_d \geq 0$ according to Equation (28) and (30).

4. Constitutive theory in relation to finite deformations

In the foregoing section, a small strain theory has been constructed to model the thermomechanical behavior of shape memory alloys due to martensitic phase transitions. To formulate a relation between the fraction of oriented martensite and the transformation strain tensor, a new constitutive equation in form of Equation (22) was introduced. In this section, the developed constitutive theory is enhanced on the basis of [Helm 2001] to a finite strain theory. In that work we introduced a basic concept for shape memory alloys at finite deformations. This concept is based on a twofold multiplicative decomposition of the deformation gradient in order to distinguish between elastic and inelastic deformations as well as to incorporate the influences of internal stress states. Furthermore, the theory contains two evolution equations for the phase transition strain: one evolution equation models the phase transition from austenite into oriented martensite and the other evolution equation represents the retransformation. In the present section, the finite deformation theory of our earlier work is revised in order to obtain a constitutive theory, which requires only one simple constitutive equation to describe the evolution of the phase transition strains, which is valid for the forward and the reverse phase transition as well.

4.1. Free energy. According to [Helm 2001] and in analogy to the proposed geometrically linear theory in the foregoing section, the main energy storage phenomena are describable if the free energy is introduced as a function of the elastic strain state $\hat{\mathbf{\Gamma}}_e$, the absolute thermodynamic temperature θ , and the fraction of martensite z as well as an internal variable $\check{\mathbf{Y}}_s$:

$$\psi = \hat{\psi}(\hat{\mathbf{\Gamma}}_e, \theta, z, \check{\mathbf{Y}}_s) = \hat{\psi}_e(\hat{\mathbf{\Gamma}}_e, \theta, z) + \hat{\psi}_s(\check{\mathbf{Y}}_s, \theta). \quad (33)$$

In analogy to the small strain theory, the thermoelastic part ψ_e of the free energy results from the simple mixture of two single phase materials:

$$\psi_e(\theta, \hat{\mathbf{\Gamma}}_e, z) = z \psi_e^M(\theta, \hat{\mathbf{\Gamma}}_e) + (1 - z) \psi_e^A(\theta, \hat{\mathbf{\Gamma}}_e). \quad (34)$$

Here, it is assumed that the elastic strains in the austenite and martensite phase are equal. Each single phase material is depicted by a finite thermoelasticity relation (see [Helm 2001; 2006]):

$$\begin{aligned} \psi_e^\omega &= \frac{1}{2\rho_R} \kappa^\omega(\theta) \left(\ln(\det \hat{\mathbf{C}}_e)^{1/2} \right)^2 + \frac{1}{2\rho_R} \mu^\omega(\theta) (\text{tr} \bar{\hat{\mathbf{C}}}_e - 3) \\ &- \frac{1}{\rho_R} \kappa^\omega(\theta) \ln(1 + \alpha^\omega(\theta) [\theta - \theta_0])^3 \ln(\det \hat{\mathbf{C}}_e)^{1/2} + \int_{\theta_0}^{\theta} c_d^\omega(\bar{\theta}) d\bar{\theta} + u_0^\omega - \theta \left[\int_{\theta_0}^{\theta} \frac{c_d^\omega(\bar{\theta})}{\bar{\theta}} d\bar{\theta} + \eta_0^\omega \right]. \end{aligned} \quad (35)$$

Therein, the first part describes the energy storage due to volumetric deformations (see [Simo and Pister 1984]), and the free energy contribution of isochoric deformations is given by the second term (see [Simo 1985; 1988]), which is of neo-Hooke type. Moreover, the third term represents the thermoelastic coupling phenomena. Applying the useful assumption of small thermoelastic strains $\alpha^\omega(\theta) [\theta - \theta_0]$, this term can be written in its approximation $\kappa^\omega(\theta) \ln[(1 + \alpha^\omega(\theta) [\theta - \theta_0])^3] \approx 3\kappa^\omega(\theta) \alpha^\omega(\theta) [\theta - \theta_0]$. The last term in Equation (34) models the energy storage due to caloric effects. The meaning of the material parameters in the free energy function of a single-phase material are already known from the small strain theory (see Section 3.1).

If the free energy of the single phase material (35) is inserted into the mixture relation (34), the free energy of the two-phase material is given by

$$\begin{aligned} \rho_R \psi_e &= \frac{\tilde{\kappa}(\theta, z)}{2} \left(\ln(\det \hat{\mathbf{C}}_e)^{1/2} \right)^2 + \frac{1}{2} \tilde{\mu}(\theta, z) (\text{tr} \bar{\hat{\mathbf{C}}}_e - 3) - 3\tilde{\alpha}(\theta, z) (\theta - \theta_0) \ln(\det \hat{\mathbf{C}}_e)^{1/2} \\ &+ z\rho_R \int_{\theta_0}^{\theta} c_{d_0}^M(\bar{\theta}) d\bar{\theta} + (1-z)\rho_R \int_{\theta_0}^{\theta} c_{d_0}^A(\bar{\theta}) d\bar{\theta} + \rho_R [u_0^A + z\Delta u_0] \\ &- \theta \left[z\rho_R \int_{\theta_0}^{\theta} \frac{c_{d_0}^M(\bar{\theta})}{\bar{\theta}} d\bar{\theta} + (1-z)\rho_R \int_{\theta_0}^{\theta} \frac{c_{d_0}^A(\bar{\theta})}{\bar{\theta}} d\bar{\theta} + \rho_R [\eta_0^A + z\Delta\eta_0] \right]. \end{aligned} \quad (36)$$

According to Equation (10)–(12), the material functions $\tilde{\kappa}(\theta, z)$, $\tilde{\mu}(\theta, z)$, and $\tilde{\alpha}(\theta, z)$ are already known. Altogether, the main thermoelastic effects are representable by the proposed finite thermoelasticity relation.

In addition to the thermoelastic part of the free energy, a constitutive equation for the inelastic part is assumed to be (see [Helm 2001])

$$\psi_s = \frac{1}{4\rho_R} c(\theta) (\text{tr} \bar{\hat{\mathbf{C}}}_s - 3). \quad (37)$$

Therein, the tensor $\bar{\hat{\mathbf{C}}}_s$ is the unimodular part of $\check{\hat{\mathbf{C}}}_s$.

4.2. Evolution equations for internal variables. In a finite deformation theory it is important to introduce conjugate variables and associated time derivatives. The concept of dual variables [Haupt and Tsakmakis 1989; Haupt 2002] implies that the variables $\tilde{\mathbf{T}}$ (second Piola–Kirchhoff stress tensor) and \mathbf{E} are not only conjugate but also dual variables. Other dual variables result from the postulate that the invariance of the following physically significant inner products is fulfilled: the scalar product between the second Piola–Kirchhoff stress tensor $\tilde{\mathbf{T}}$ and the Green strain tensor \mathbf{E} ($\tilde{\mathbf{T}} \cdot \mathbf{E}$), the stress power $\dot{\tilde{\mathbf{T}}} \cdot \dot{\mathbf{E}}$, the complementary stress power $\dot{\hat{\mathbf{T}}} \cdot \dot{\mathbf{E}}$, and finally the incremental stress power $\dot{\hat{\mathbf{T}}} \cdot \dot{\hat{\mathbf{E}}}$. In relation to the

intermediate configuration $\hat{\mathcal{K}}_t$, the stress tensor $\hat{\mathbf{S}} = \mathbf{F}_t \tilde{\mathbf{T}} \mathbf{F}_t^T$ and the strain tensor $\hat{\mathbf{\Gamma}}$ (see Equation (2)) are dual variables, because this pair does not influence, for example, $\tilde{\mathbf{T}} \cdot \dot{\mathbf{E}} = \hat{\mathbf{S}} \cdot \hat{\mathbf{\Gamma}}$ and

$$\tilde{\mathbf{T}} \cdot \dot{\mathbf{E}} = \text{tr} \left(\underbrace{\mathbf{F}_t \tilde{\mathbf{T}} \mathbf{F}_t^T}_{\hat{\mathbf{S}}} \underbrace{\mathbf{F}_t^{-T} \dot{\mathbf{E}} \mathbf{F}_t^{-1}}_{\hat{\mathbf{\Gamma}}} \right) = \hat{\mathbf{S}} \cdot \hat{\mathbf{\Gamma}}. \quad (38)$$

Therein, $\hat{\mathbf{\Gamma}}$ represents the Oldroyd derivative of $\hat{\mathbf{\Gamma}}$,

$$\hat{\mathbf{\Gamma}} = \dot{\hat{\mathbf{\Gamma}}} + \hat{\mathbf{L}}_t^T \hat{\mathbf{\Gamma}} + \hat{\mathbf{\Gamma}} \hat{\mathbf{L}}_t \quad \text{with} \quad (\hat{\cdot}) = (\dot{\cdot}) + \hat{\mathbf{L}}_t^T (\dot{\cdot}) + (\dot{\cdot}) \hat{\mathbf{L}}_t, \quad (39)$$

which is an associated time derivative, formulated relative to the intermediate configuration $\hat{\mathcal{K}}_t$. This Oldroyd derivative of $\hat{\mathbf{\Gamma}}$ is calculated on the basis of the inelastic deformation rate $\hat{\mathbf{L}}_t = \dot{\mathbf{F}}_t \mathbf{F}_t^{-1}$. Furthermore, the relation

$$\hat{\mathbf{\Gamma}} = \hat{\mathbf{\Gamma}}_e + \hat{\mathbf{\Gamma}}_t, \quad \text{with} \quad \hat{\mathbf{\Gamma}}_e = \dot{\hat{\mathbf{\Gamma}}}_e + \hat{\mathbf{L}}_t^T \hat{\mathbf{\Gamma}}_e + \hat{\mathbf{\Gamma}}_e \hat{\mathbf{L}}_t \quad \text{and} \quad \hat{\mathbf{\Gamma}}_t = \dot{\hat{\mathbf{\Gamma}}}_t + \hat{\mathbf{L}}_t^T \hat{\mathbf{\Gamma}}_t + \hat{\mathbf{\Gamma}}_t \hat{\mathbf{L}}_t \quad (40)$$

is valid, because the Oldroyd derivative is a linear operator. It should be mentioned that the relation

$$\hat{\mathbf{\Gamma}}_t = \frac{1}{2} [\hat{\mathbf{L}}_t + \hat{\mathbf{L}}_t^T] = \hat{\mathbf{D}}_t \quad (41)$$

is valid for the Oldroyd derivative of $\hat{\mathbf{\Gamma}}_t$. This relation underlines that the Oldroyd rate of $\hat{\mathbf{\Gamma}}_t$ depends only on \mathbf{F}_t and its material time derivative. In contrast to this, the Oldroyd derivative of $\hat{\mathbf{\Gamma}}_e$ is influenced by $\hat{\mathbf{\Gamma}}_e$, \mathbf{F}_t and their material time derivatives.

In analogy to Section 3.2, the basic structure of the constitutive theory is developed on the basis of the internal dissipation inequality, given by $\rho_R \delta_i = -\rho_R \dot{\psi} - \rho_R \dot{\theta} \eta + \tilde{\mathbf{T}} \cdot \dot{\mathbf{E}} \geq 0$. Here, ρ_R is the mass density with respect to the reference configuration. Inserting the free energy function (33), the identity (38), and the relation (40) into the internal dissipation inequality, the resulting inequality is given by

$$\delta_i = -\frac{\partial \hat{\psi}_e}{\partial \hat{\mathbf{\Gamma}}_e} \cdot \dot{\hat{\mathbf{\Gamma}}}_e - \frac{\partial \hat{\psi}_e}{\partial z} \dot{z} - \left[\eta + \frac{\partial \hat{\psi}}{\partial \theta} \right] \dot{\theta} - \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \cdot \dot{\check{\mathbf{Y}}}_s + \frac{1}{\rho_R} \hat{\mathbf{S}} \cdot \hat{\mathbf{\Gamma}}_e + \frac{1}{\rho_R} \hat{\mathbf{S}} \cdot \hat{\mathbf{\Gamma}}_t. \quad (42)$$

In the next step, $\dot{\hat{\mathbf{\Gamma}}}_e$ is replaced by its Oldroyd derivative according to Equation (40)₂. In the same way, $\dot{\check{\mathbf{Y}}}_s$ is substituted by an associated time derivative: with respect to the intermediate configuration $\check{\mathcal{K}}_d$, an internal stress tensor $\check{\mathbf{X}}_\varepsilon = \mathbf{F}_t \tilde{\mathbf{X}}_\varepsilon \mathbf{F}_t^T$ is defined, which represents the transformation of the internal stress state $\tilde{\mathbf{X}}_\varepsilon$ from the reference configuration to the intermediate configuration $\check{\mathcal{K}}_d$. Its dual strain tensor in the reference configuration is named as $\check{\mathbf{Y}}$ and the variable $\check{\mathbf{Y}}$ is the associated strain tensor in the intermediate configuration $\check{\mathcal{K}}_d$. The analysis of the stress power,

$$\check{\mathbf{X}}_\varepsilon \cdot \dot{\check{\mathbf{Y}}} = \text{tr} \left(\underbrace{\mathbf{F}_d \tilde{\mathbf{X}}_\varepsilon \mathbf{F}_d^T}_{\check{\mathbf{X}}_\varepsilon} \underbrace{\mathbf{F}_d^{-T} \dot{\check{\mathbf{Y}}} \mathbf{F}_d^{-1}}_{\hat{\mathbf{Y}}} \right) = \check{\mathbf{X}}_\varepsilon \cdot \hat{\mathbf{Y}}, \quad (43)$$

leads to the associated time derivative:

$$\hat{\mathbf{Y}} = \dot{\check{\mathbf{Y}}} + \check{\mathbf{L}}_d^T \check{\mathbf{Y}} + \check{\mathbf{Y}} \check{\mathbf{L}}_d, \quad (\hat{\cdot}) = (\dot{\cdot}) + \check{\mathbf{L}}_d^T (\dot{\cdot}) + (\dot{\cdot}) \check{\mathbf{L}}_d, \quad (44)$$

with $\check{\mathbf{L}}_d = \dot{\mathbf{F}}_d \mathbf{F}_d^{-1}$. Consequently, $\hat{\mathbf{Y}}$ represents an Oldroyd derivative relative to the intermediate configuration $\check{\mathcal{K}}_d$. Since this Oldroyd derivative is also a linear operator, the relation

$$\hat{\mathbf{Y}} = \hat{\mathbf{Y}}_s + \hat{\mathbf{Y}}_d \quad \text{with} \quad \hat{\mathbf{Y}}_s = \dot{\mathbf{Y}}_s + \check{\mathbf{L}}_d^T \check{\mathbf{Y}}_s + \check{\mathbf{Y}}_s \check{\mathbf{L}}_d \quad \text{and} \quad \hat{\mathbf{Y}}_d = \dot{\mathbf{Y}}_d + \check{\mathbf{L}}_d^T \check{\mathbf{Y}}_d + \check{\mathbf{Y}}_d \check{\mathbf{L}}_d \quad (45)$$

is likewise valid. In analogy to Equation (41), the Oldroyd derivative of $\check{\mathbf{Y}}_d$ is representable as

$$\hat{\mathbf{Y}}_d = \frac{1}{2} [\check{\mathbf{L}}_d + \check{\mathbf{L}}_d^T] = \check{\mathbf{D}}_d. \quad (46)$$

Consequently, the identities according to Equation (40)₂ and also Equation (45)₂ are used to replace in Equation (42) the material time derivative of $\hat{\mathbf{\Gamma}}_e$ and $\check{\mathbf{Y}}_s$ by their Oldroyd derivatives. Additionally, the additive relation according to Equation (45)₁ is applied in Equation (42):

$$\begin{aligned} \delta_i = & \frac{1}{\rho_R} \left[\hat{\mathbf{S}} - \rho_R \frac{\partial \hat{\psi}_e}{\partial \hat{\mathbf{\Gamma}}_e} \right] \cdot \hat{\mathbf{\Gamma}}_e - \left[\eta + \frac{\partial \hat{\psi}}{\partial \theta} \right] \dot{\theta} - \frac{\partial \hat{\psi}_e}{\partial z} \dot{z} - \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \cdot \hat{\mathbf{Y}} + \frac{1}{\rho_R} \hat{\mathbf{S}} \cdot \hat{\mathbf{\Gamma}}_t \\ & + \underbrace{\frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \cdot \left[\hat{\mathbf{Y}}_d + \check{\mathbf{L}}_d^T \check{\mathbf{Y}}_s + \check{\mathbf{Y}}_s \check{\mathbf{L}}_d \right]}_{\left[\check{\mathbf{C}}_s \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \right] \cdot \hat{\mathbf{Y}}_d} + \underbrace{\frac{\partial \hat{\psi}_e}{\partial \hat{\mathbf{\Gamma}}_e} \cdot \left[\hat{\mathbf{L}}_t^T \hat{\mathbf{\Gamma}}_e + \hat{\mathbf{\Gamma}}_e \hat{\mathbf{L}}_t \right]}_{\left[\hat{\mathbf{C}}_e \frac{\partial \hat{\psi}_e}{\partial \hat{\mathbf{\Gamma}}_e} \right] \cdot \hat{\mathbf{\Gamma}}_t} \geq 0. \quad (47) \end{aligned}$$

As shown in the last line of Equation (47), these terms can be replaced if $\partial \hat{\psi}_s / \partial \check{\mathbf{Y}}_s$ is an isotropic tensor function of $\check{\mathbf{Y}}_s$ and if $\partial \hat{\psi}_e / \partial \hat{\mathbf{\Gamma}}_e$ is an isotropic tensor function of $\hat{\mathbf{\Gamma}}_e$ [Mandel 1972; Haupt 2002]. Furthermore, the relation

$$\frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \cdot \hat{\mathbf{Y}} = \check{\mathbf{F}}_s \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \check{\mathbf{F}}_s^T \cdot \check{\mathbf{F}}_s^{-T} \hat{\mathbf{Y}} \check{\mathbf{F}}_s^{-1} = \check{\mathbf{F}}_s \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \check{\mathbf{F}}_s^T \cdot \hat{\mathbf{\Gamma}}_t. \quad (48)$$

is valid for the last term in the first line of the inequality (47). Considering these identities into the internal dissipation inequality (47), the resulting inequality

$$\begin{aligned} \rho_R \delta_i = & \left[\hat{\mathbf{S}} - \rho_R \frac{\partial \hat{\psi}_e}{\partial \hat{\mathbf{\Gamma}}_e} \right] \cdot \hat{\mathbf{\Gamma}}_e - \rho_R \left[\eta + \frac{\partial \hat{\psi}}{\partial \theta} \right] \dot{\theta} - \rho_R \frac{\partial \hat{\psi}_e}{\partial z} \dot{z} + \left[\check{\mathbf{C}}_s \rho_R \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \right] \cdot \hat{\mathbf{Y}}_d + \left[\hat{\mathbf{C}}_e \hat{\mathbf{S}} - \check{\mathbf{F}}_s \rho_R \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \check{\mathbf{F}}_s^T \right] \cdot \hat{\mathbf{\Gamma}}_t \\ & \geq 0 \quad (49) \end{aligned}$$

implies a potential relation for the stress tensor

$$\begin{aligned} \hat{\mathbf{S}} = \rho_R \frac{\partial \hat{\psi}_e}{\partial \hat{\mathbf{\Gamma}}_e} = 2 \rho_R \frac{\partial \hat{\psi}_e}{\partial \hat{\mathbf{C}}_e} = & \tilde{\mu}(\theta, z) (\det \hat{\mathbf{C}}_e)^{-1/3} \left[\mathbf{1} - \frac{1}{3} (\text{tr} \hat{\mathbf{C}}_e) \hat{\mathbf{C}}_e^{-1} \right] \\ & + \left[\tilde{\kappa}(\theta, z) \ln (\det \hat{\mathbf{C}}_e)^{1/2} - 3 \tilde{\alpha}(\theta, z) (\theta - \theta_0) \right] \hat{\mathbf{C}}_e^{-1}, \quad (50) \end{aligned}$$

which is related to the intermediate configuration $\hat{\mathcal{K}}_t$, and the entropy $\eta = -\partial \hat{\psi} / \partial \theta$, if \dot{z} , $\hat{\mathbf{Y}}_d$, and $\hat{\mathbf{\Gamma}}_t$ do

not depend on $\hat{\Gamma}_e^\Delta$ and $\dot{\theta}$ [Coleman and Gurtin 1967]. Furthermore, the remaining internal dissipation inequality

$$\rho_R \delta_i = - \underbrace{\rho_R \frac{\partial \hat{\psi}_e}{\partial z}}_{\Xi} \dot{z} + \left[\check{\mathbf{C}}_s \rho_R \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \right] \cdot \hat{\mathbf{Y}}_d + \left[\underbrace{\hat{\mathbf{C}}_e \hat{\mathbf{S}}}_{\hat{\mathbf{P}}} - \underbrace{\check{\mathbf{F}}_s \rho_R \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} \check{\mathbf{F}}_s^T}_{\hat{\mathbf{P}}_{X_\varepsilon}} \right] \cdot \hat{\Gamma}_t \quad (51)$$

motivates the introduction of four definitions: the partial derivative in the first term is interpretable as a thermodynamic force $\Xi = \rho_R \partial \psi_e / \partial z$,

$$\Xi = \frac{1}{2} \frac{\partial \tilde{\mu}}{\partial z} (\text{tr } \bar{\mathbf{C}}_e - 3) + \frac{1}{2} \frac{\partial \tilde{\kappa}}{\partial z} \left(\ln (\det \hat{\mathbf{C}}_e)^{1/2} \right)^2 - 3 \frac{\partial \tilde{\alpha}}{\partial z} (\theta - \theta_0) \ln (\det \hat{\mathbf{C}}_e)^{1/2} + \rho_R \left[\int_{\theta_0}^{\theta} [c_{d_0}^M(\bar{\theta}) - c_{d_0}^A(\bar{\theta})] d\bar{\theta} + \Delta u_0 \right] - \rho_R \theta \left[\int_{\theta_0}^{\theta} \frac{c_{d_0}^M(\bar{\theta}) - c_{d_0}^A(\bar{\theta})}{\bar{\theta}} d\bar{\theta} + \Delta \eta_0 \right], \quad (52)$$

which is already known from the geometrically linear theory. Furthermore, the partial derivative in the second term,

$$\check{\mathbf{X}}_\varepsilon = \rho_R \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{Y}}_s} = 2\rho_R \frac{\partial \hat{\psi}_s}{\partial \check{\mathbf{C}}_s} = \frac{c(\theta)}{2} (\det \check{\mathbf{C}}_s)^{-1/3} \left[\mathbf{1} - \frac{1}{3} (\text{tr } \check{\mathbf{C}}_s) \check{\mathbf{C}}_s^{-1} \right], \quad (53)$$

can be understood as the internal stress tensor (back stress tensor) on the intermediate configuration $\check{\mathcal{K}}_d$. The stress tensor

$$\hat{\mathbf{P}} = \hat{\mathbf{C}}_e \hat{\mathbf{S}} = \tilde{\kappa}(\theta, z) \ln (\det \hat{\mathbf{C}}_e)^{1/2} \mathbf{1} + \tilde{\mu}(\theta, z) \bar{\mathbf{C}}_e^D - 3\tilde{\alpha}(\theta, z) (\theta - \theta_0) \mathbf{1} \quad (54)$$

is known as the Mandel stress tensor [1972] (see also [Lublinter 1990]). Due to the assumption that $\partial \hat{\psi}_e / \partial \hat{\Gamma}_e$ is an isotropic tensor function of $\hat{\Gamma}_e$, the Mandel-stress tensor $\hat{\mathbf{P}}$ is symmetric. In contrast to this, the stress tensor

$$\check{\mathbf{M}}_{X_\varepsilon} = \check{\mathbf{C}}_s \check{\mathbf{X}}_\varepsilon = \frac{c(\theta)}{2} \bar{\mathbf{C}}_s^D \quad (55)$$

has the structure of a Mandel stress tensor and the stress tensor

$$\hat{\mathbf{P}}_{X_\varepsilon} = \check{\mathbf{F}}_s \check{\mathbf{M}}_{X_\varepsilon} \check{\mathbf{F}}_s^T = \frac{c(\theta)}{2} \bar{\mathbf{B}}_s^D \quad (56)$$

is the transformation of $\check{\mathbf{X}}_\varepsilon$ from the intermediate configuration $\check{\mathcal{K}}_d$ onto $\hat{\mathcal{K}}_t$. The stress tensor $\hat{\mathbf{P}}_{X_\varepsilon}$ is of Mandel-type, too.

Using these definitions, the remaining dissipation inequality (see [Helm 2001]) is given by

$$\rho_R \delta_i = -\Xi \dot{z} + \check{\mathbf{M}}_{X_\varepsilon} \cdot \hat{\mathbf{Y}}_d + [\hat{\mathbf{P}} - \hat{\mathbf{P}}_{X_\varepsilon}] \cdot \hat{\Gamma}_t \geq 0. \quad (57)$$

In shape memory alloys, the martensitic phase transitions between austenite and oriented martensite result from a cooperative movement of the atomic lattice. In analogy to Equation (22), a constitutive equation is required for incorporating this coupling phenomenon between the fraction of oriented martensite and the transformation strain. Already in [Helm 2001] the coupling between the fraction z of oriented martensite

and the inelastic Cauchy–Green tensor \mathbf{C}_t was represented in a finite-strain concept by the constitutive relation

$$z = \frac{1}{\sqrt{3}\gamma_t} \sqrt{\text{tr} [\bar{\mathbf{C}}_t] - 3}. \quad (58)$$

According to the definition in Equation (1), the tensor $\bar{\mathbf{C}}_t$ is the unimodular part of $\mathbf{C}_t = \mathbf{F}_t^T \mathbf{F}_t$. However, if the relation (58) was applied in the present context, the model would contain a phase transition criterion and a phase transition rule, which would be singular at $\bar{\mathbf{C}}_t = \mathbf{1}$ (see the discussions in [Helm 2001; Helm and Haupt 2003]). Moreover, the smooth transition from the retransformation plateau into the elastic region (see region II in Figure 1a) cannot be depicted. Therefore, a new constitutive equation is suggested in analogy to Equation (22):

$$z = \frac{1}{\sqrt{3}\gamma_t} \sqrt{\text{tr} [\bar{\mathbf{C}}_t] - 3(1 - \gamma_0^2)} - z_0. \quad (59)$$

Therein, γ_0 is a positive material parameter and $z_0 = \gamma_0/\gamma_t$ follows from the condition $\hat{z}(\bar{\mathbf{C}}_t = \mathbf{1}) = 0$. On account of the introduced material parameter $\gamma_0 > 0$, the resulting model does not contain any singularity.

In the dissipation inequality (57), the material time derivative of z is required:

$$\dot{z} = \frac{(\det \mathbf{C}_t)^{-1/3} \left[\mathbf{1} - \frac{1}{3} \text{tr} (\mathbf{C}_t) \mathbf{C}_t^{-1} \right]}{\sqrt{3}\gamma_t \sqrt{\text{tr} \bar{\mathbf{C}}_t - 3(1 - \gamma_0^2)}} \cdot \frac{1}{2} \dot{\bar{\mathbf{C}}}_t. \quad (60)$$

Multiplying the time derivative of z with the thermodynamic quantity Ξ and transforming the participated variables from the reference configuration \mathcal{K}_R to the intermediate configuration $\hat{\mathcal{K}}_t$, the resulting relation ($\hat{\mathbf{B}}_t = \mathbf{F}_t \mathbf{F}_t^T$)

$$\Xi \dot{z} = \frac{\Xi \bar{\mathbf{B}}_t^D \cdot \hat{\mathbf{F}}_t}{\sqrt{3}\gamma_t \sqrt{\text{tr} \hat{\mathbf{B}}_t - 3(1 - \gamma_0^2)}} = \hat{\mathbf{P}}_{\mathbf{X}_\theta} \cdot \hat{\mathbf{F}}_t, \quad (61)$$

motivates the definition of an internal variable $\hat{\mathbf{P}}_{\mathbf{X}_\theta}$ of stress type:

$$\hat{\mathbf{P}}_{\mathbf{X}_\theta} = \frac{\Xi \bar{\mathbf{B}}_t^D}{\sqrt{3}\gamma_t \sqrt{\text{tr} \hat{\mathbf{B}}_t - 3(1 - \gamma_0^2)}}. \quad (62)$$

Owing to $\hat{\mathbf{P}}_{\mathbf{X}_\theta}$, which is a continuous function of $\hat{\mathbf{B}}_t$, the present constitutive model is able to represent the temperature-dependence of the phase transition stress.

Remark 3 (Interpretation of $\hat{\mathbf{P}}_{\mathbf{X}_\theta}$). The internal variable $\hat{\mathbf{P}}_{\mathbf{X}_\theta}$ can be better understood if a simple inelastic shear deformation is regarded: $\mathbf{F}_t = \mathbf{1} + \gamma_{12} \mathbf{e}_1 \otimes \mathbf{e}_2$. On account of

$$\hat{\mathbf{B}}_t = \bar{\hat{\mathbf{B}}}_t = \mathbf{1} + \gamma_{12} (\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1) + \gamma_{12}^2 \mathbf{e}_1 \otimes \mathbf{e}_1, \quad (63)$$

the 12-component of $\hat{\mathbf{P}}_{\mathbf{X}_\theta}$ can be calculated:

$$\mathbf{e}_1 \cdot \hat{\mathbf{P}}_{\mathbf{X}_\theta} \mathbf{e}_2 = \frac{\Xi}{\sqrt{3}\gamma_t} \frac{\gamma_{12}}{\sqrt{\gamma_{12}^2 + 3\gamma_0^2}}. \quad (64)$$

For $\gamma_{12} \gg \gamma_0$, the value of this shear stress is given by $\Xi/(\sqrt{3}\gamma_t)$, because the other term is approximately ± 1 . Consequently, the effect of the introduced constitutive relation for $\hat{\mathbf{P}}_{\mathbf{X}_\theta}$ on the whole theory is similar to the influence of the internal variable \mathbf{X}_θ in the small strain theory (see Equation (24) and Figure 3).

Remark 4 (Trace of a unimodular tensor). The first invariant $I_{\mathbf{A}}$ of a unimodular tensor \mathbf{A} (i.e., $\text{III}_{\mathbf{A}} = \det \mathbf{A} = 1$ is valid) has a lower bound $I_{\mathbf{A}} = \text{tr } \mathbf{A} \geq 3$ [Haupt 2002, (9.91)]. Therefore, the term

$$f(\bar{\mathbf{B}}_t) = \sqrt{\text{tr } \bar{\mathbf{B}}_t - 3(1 - \gamma_0^2)} \geq \sqrt{3}\gamma_0 \quad (65)$$

in Equation (62) has likewise a lower bound and the ratio $1/f(\bar{\mathbf{B}}_t)$ is always defined, because $\gamma_0 > 0$ is required in the model.

If the important relation $\Xi \dot{z} = \hat{\mathbf{P}}_{\mathbf{X}_\theta} \cdot \hat{\mathbf{\Gamma}}_t$ according to Equation (61) is inserted into the remaining dissipation inequality (57), the resultant inequality (see [Helm 2001])

$$\rho_R \delta_i = \check{\mathbf{M}}_{\mathbf{X}_e} \cdot \hat{\mathbf{Y}}_d + [\hat{\mathbf{P}} - \hat{\mathbf{P}}_{\mathbf{X}}] \cdot \hat{\mathbf{\Gamma}}_t \geq 0 \quad (66)$$

with the definition $\hat{\mathbf{P}}_{\mathbf{X}} = \hat{\mathbf{P}}_{\mathbf{X}_e} + \hat{\mathbf{P}}_{\mathbf{X}_\theta}$, is a suitable basis to specify the phase transition function

$$f = \|\hat{\mathbf{P}}^D - \hat{\mathbf{P}}_{\mathbf{X}}^D\| - \sqrt{\frac{2}{3}}k(\theta) \quad (67)$$

and the required evolution equations for the internal variables $\hat{\mathbf{\Gamma}}_t$ and $\check{\mathbf{Y}}_d$.

- In the case of the transformation strain tensor $\hat{\mathbf{\Gamma}}_t$ the phase transition rule

$$\hat{\mathbf{\Gamma}}_t = \lambda_t \hat{\mathbf{P}}_{\mathbf{N}} \quad \text{with} \quad \hat{\mathbf{P}}_{\mathbf{N}} = \frac{\partial f}{\partial \hat{\mathbf{P}}} = \frac{\hat{\mathbf{P}}^D - \hat{\mathbf{P}}_{\mathbf{X}}^D}{\|\hat{\mathbf{P}}^D - \hat{\mathbf{P}}_{\mathbf{X}}^D\|} \quad (68)$$

is suggested. Therein, $\lambda_t \geq 0$ is the inelastic multiplier. This evolution equation states that $\hat{\mathbf{\Gamma}}_t$ is a deviatoric tensor. Consequently, the model incorporates the assumption of isochoric inelastic deformations: $\det \mathbf{F}_t = 1$.

In analogy to the inelastic multiplier of the small deformation theory, a Perzyna-type (see [Perzyna 1963; Hohenemser and Prager 1932]) multiplier λ_t is introduced:

$$\lambda_t = \begin{cases} \frac{1}{\eta_t(\theta)} \left\langle \frac{f}{r_t} \right\rangle^{m_t(\theta)} & \mathbf{A} \rightarrow \bar{\mathbf{M}} \text{ if } z < 1 \text{ and } \bar{\mathbf{B}}_t^D \cdot \hat{\mathbf{P}}_{\mathbf{N}} \geq 0, \\ \bar{\mathbf{M}} \rightarrow \mathbf{A} \text{ if } z > 0 \text{ and } \bar{\mathbf{B}}_t^D \cdot \hat{\mathbf{P}}_{\mathbf{N}} < 0, \\ 0 & \text{in all other cases.} \end{cases} \quad (69)$$

The material parameters and the case distinctions have the same meaning as in the small strain theory, but the condition of increasing martensite requires $dz \sim \bar{\mathbf{B}}_t^D \cdot \hat{\mathbf{P}}_{\mathbf{N}} \geq 0$ and the martensite decreases, if $dz \sim \bar{\mathbf{B}}_t^D \cdot \hat{\mathbf{P}}_{\mathbf{N}} < 0$ is fulfilled.

- For the internal variable $\check{\mathbf{Y}}_d$, the evolution equation

$$\hat{\Delta} \check{\mathbf{Y}}_d = \zeta_d \check{\mathbf{M}}_{\mathbf{X}_e} = \zeta_d \check{\mathbf{C}}_s \check{\mathbf{X}}_e, \quad (70)$$

is proposed. Likewise in the case of finite deformations, ζ_d is introduced in form of

$$\zeta_d = \frac{B(\theta, z, \dot{z})}{c(\theta)} \dot{s}_t \quad \text{with} \quad \dot{s}_t = \sqrt{\frac{2}{3}} \|\hat{\Delta} \hat{\mathbf{T}}_t\|. \quad (71)$$

Therein, $B(\theta, z, \dot{z})$ is given according to Equation (31) and s_t is the accumulated transformation strain.

It should be mentioned that no further constitutive equations are required to represent the evolution of the internal variables $\hat{\mathbf{T}}_t$ and $\check{\mathbf{Y}}_d$ according to (68) and (70), because it is not necessary to determine the orthogonal part \mathbf{R}_t of the polar decomposition $\mathbf{F}_t = \mathbf{R}_t \mathbf{U}_t$ and the orthogonal part \mathbf{R}_d of the polar decomposition $\mathbf{F}_d = \mathbf{R}_d \mathbf{U}_d$ in the proposed constitutive theory for an isotropic elastic material (see [Haupt 2002] or [Helm and Schäfers 2006], for example). Only the evolution of the stretch tensors \mathbf{U}_t and \mathbf{U}_d is represented by the evolution equations (68) and (70).

If the evolution equations (68) and (70) are inserted into the inequality (66) the internal dissipation is written in the following form:

$$\rho_R \delta_i = \zeta_d \|\check{\mathbf{M}}_{\mathbf{X}_e}\|^2 + \lambda_t \|\hat{\mathbf{P}}^D - \hat{\mathbf{P}}_{\mathbf{X}}^D\|. \quad (72)$$

Obviously ($\lambda_t \geq 0$ and $\zeta_d \geq 0$), the postulated geometrically nonlinear constitutive theory is thermodynamically consistent for arbitrary thermomechanical processes.

Remark 5 (Mandel stress tensors). In the context of a constitutive theory for viscoplastic materials, Mandel [1972] proposed to consider the stress tensor $\hat{\mathbf{P}} = \hat{\mathbf{C}}_e \hat{\mathbf{S}}$ in the yield function. Mandel's theory has been formulated on the basis of the multiplicative decomposition of the deformation gradient in an elastic and inelastic part. In order to describe the kinematic hardening behavior of metals in a finite deformation theory using continuum thermomechanics, Tsakmakis [1996] found out that the yield function should depend on a back stress tensor of Mandel-type.

5. Conclusions

In the present article, two basic concepts for modeling martensitic phase transitions in shape memory alloys are developed: the first model is based on the assumption of small deformations, and the second concept is formulated in the context of finite deformations. In both cases, the energy storage and release phenomena during thermomechanical processes are represented by a free energy function. Moreover, evolution equations for two internal variables are introduced in order to model the history-dependent material behavior and the dissipation phenomena. An essential element of the developed theories is that the deformation and the strain-like internal variables are decomposed into volumetric and isochoric parts. This leads to a simple representation of the occurring mechanisms. In contrast to other constitutive theories for shape memory alloys, the developed concept is formulated in the framework of thermoviscoplasticity. Therefore, the system of constitutive equations has a strong resemblance to classical models, which depict the viscoplastic behavior of metals by using the concept of kinematic hardening. The present approach of

finite thermoviscoplasticity is based on [Lion 2000], which introduces a multiple multiplicative decomposition of the deformation gradient for the modeling of kinematic hardening in the framework of finite deformations. In analogy to [Helm 2001], only a double multiplicative decomposition of the deformation gradient is introduced without any thermal intermediate configuration. Therefore, the entropy results immediately from the free energy function by means of a potential relation. Similar strategies for incorporating the kinematic hardening at finite strains were discussed in [Dettmer and Reese 2004; Tsakmakis and Willuweit 2004]. In the present constitutive theory, all energy storage phenomena due to isochoric deformations are depicted by modified neo-Hooke-type models. This strategy leads to a simple representation of the occurring energy storage mechanisms and the kinematic hardening behavior. In all, the developed concept can be easily transformed to give the thermoviscoplastic behavior of metals if only a few modifications are considered: e.g. $\gamma_t = \infty$, $\mathbf{X}_\theta = \mathbf{0}$ or $\hat{\mathbf{P}}_{\mathbf{X}_\theta} = \mathbf{0}$, and a single phase material is modeled.

It is important to mention that the number of material parameters or functions is identical for both theories. Provided that the material functions do not depend on temperature, the model includes 20 material parameters: the modeling of the thermoelastic material properties of a two-phase material requires eleven material parameters (μ^A , μ^M , κ^A , κ^M , α^A , α^M , $c_{d_0}^A$, $c_{d_0}^M$, ρ , Δu_0 , and $\Delta \eta_0$). The evolution of the transformation strain tensor is adjusted by the parameters η_t and m_t . The limit case $\eta_t \rightarrow 0$ results in a rate-independent theory. Moreover, the material parameters c (modulus for \mathbf{X}_ε), b (saturation value), γ (parameter in $B(\theta, z, \dot{z})$), and β (parameter in $B(\theta, z, \dot{z})$) are used to model the internal stress field \mathbf{X}_ε . The height of the hysteresis is influenced by the phase transition radius k and the relation between the fraction of oriented martensite and the transformation strain state is adjusted by γ_t (maximum transformation strain) and γ_0 . Of course, the identification of all these parameters is a challenge: e.g. the determination of all thermoelasticity parameters requires an elaborate testing equipment. In [Helm 2005] it is demonstrated that a certain part of the set of material parameters can be identified by common experiments in combination with the method of neural networks.

The present constitutive theory models only the material behavior of shape memory alloys due to martensitic phase transitions. For simplicity, the influence of the orientation and reorientation of martensite twins on the material behavior of shape memory alloys is not considered. However, it is possible to combine the current theory with the proposed strategy in [Helm and Haupt 2003] for the representation of the orientation and reorientation of martensite twins. To do this, it is necessary to separate the fraction of martensite into the fraction of self-accommodated martensite (twinned martensite) and the fraction of oriented martensite (detwinned martensite); compare the discussion in [Lagoudas et al. 2006].

From a mathematical point of view, the theories developed are particularly suitable for the numerical solution of initial-boundary value problems, because the introduced internal variables to describe the temperature-dependent phase transition stress are continuous functions of the transformation strain tensor. The numerical treatment of the proposed material models is discussed in the second part of this article [Helm and Schäfers 2006]. Moreover, the main features of the theories are demonstrated in numerical examples, which include the comparison to experimental data.

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