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CONSTITUTIVE MODELLING OF SHAPE MEMORY ALLOYS BASED ON A FINITE STRAIN DESCRIPTION

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Abstract

This paper presents the shape memory phenomena, and their crystallographical background. Furthermore a new model which is able to reproduce the basic responses of shape memory materials on both micro- and macrostructural aspects is also presented. The model is based on a local finite strain continuum description. A multiplicative decomposition of the total deformation gradient is used which involves elastic, plastic and phase transitional parts. The latter is given from microstructural measurement. For the elastic behavior of the material a coupled hyper-hypoelastic model and an objective logarithmic rate developed recently are used. Finally a constitutive equation is presented which consists of the kinetics of phase change process given by thermodynamical basis.

Keywords: shape memory, martensitic transformation, finite strain, logarithmic rate.

1. Introduction

In the recent years there has been active research work in the field of shape memory alloys (SMA). A good review of the work in this area up to 1997 can be found in the paper by BIRMAN [3]. These types of materials show unusual but 'intelligent' material behaviour which is required by the new developing technologies.

Behind the shape memory effects (SME) there is a crystallographical reason, namely the martensitic phase transition. The research that focussed directly on the investigation and measurement of the transition itself carries out more and more results, which grounds the basis of the theoretical modelling.

This modelling has started in both micro- and macroscopical way: based on micromechanics (E. PATOOR, 1987; M. BERVEILLER, A. EBERHARDT, 1994), on statistical mechanics and kinetical methods (I. MÜLLER, 1980; M. ACHENBACH, 1980), and on nonequilibrium thermostatics (J.S. CORY, 1985; J.L. MCNICHOLS, 1987). The development of the numerical methods, like finite element method, induced to improve constitutive models based on continuum descriptions and often use internal variables: models based on the free energy of phases (L.D. LANDAU, M. FRÉMOND, 1989; F. FALK, 1983; P. COLLI, M. NIEZGÓDKA, K.-H. HOFFMANN, 1990), and models using martensite volume fraction as internal variable (K. TANAKA, 1990; C. LIANG and C.A. ROGERS, 1991; L.C. BRINSON, 1993), or models based on macroscopical similarities of plastic flow (A. Bertram, 1982 [2]; F. Trochu and Y.-Y. Qian, 1997 [17]; J. Lubliner and F. Auricchio, 1996 [8]). The latest developments are based on a finite strain description (V.I. Levitas, 1996 [6], 1998 [7], Masud et al., 1997 [9]). (Citations which are not given here can be found in [3].)

Most of the models mentioned above are restricted to one dimension, since the generalization for two or three dimensions yields great difficulties.

The object of the present study is to develop a more general constitutive model for the shape memory materials, based on micro-macro description.

The paper is organized as follows. In Section 2 the three types of shape memory effect will be introduced. The phenomena will be explained by a crystallographic way in Section 3. The model based on a continuum description, using some micromechanical properties will be shown in Section 4.

Throughout this paper the following notation will be used. Tensors are denoted by bold-face characters. If **a** and **b** are second-order tensors and **H** is a fourth-order tensor then $(\mathbf{ab})_{ij} = a_{ik}b_{kj}$, $\mathbf{a} : \mathbf{b} = a_{ij}b_{ij}$, $(\mathbf{a}\otimes\mathbf{b})_{ijkl} = a_{ij}b_{kl}$, $(\mathbf{a}\bar{\otimes}\mathbf{b})_{ijkl} = a_{ik}b_{jl}$, $\|\mathbf{a}\| = \sqrt{\mathbf{a} : \mathbf{a}}$, $(\mathbf{H} : \mathbf{a})_{ij} = H_{ijkl}a_{kl}$, $(\mathbf{a} : \mathbf{H})_{ij} = a_{kl}H_{klij}$. The superposed dot denotes the material time derivative. The superscripts T and -1 denote transverse and inverse, the subscripts s and a denote symmetric and antisymmetric parts. $\boldsymbol{\delta} = \delta_{ij}$ is the second-order unit tensor (Kronecker delta), $\mathbf{I} = I_{ijkl} = 1/2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ is the fourth-order unit tensor.

2. Shape Memory Phenomena

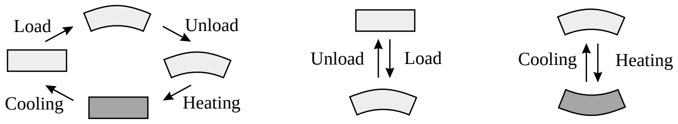
There are three groups of shape memory effects [13]. All of them have one common speciality, namely at least one shape (macroscopic state) of the material is recoverable.

In the case of *one-way effect* the material gets a permanent deformation by applying mechanical load in a relative cool temperature ($\vartheta < \vartheta_{Af}$). But this deformation can disappear by heating above ϑ_{Af} and it remains unchanged during the cooling to the start temperature (*Fig. 1.a*).

When the start temperature is above ϑ_{Af}, mechanical load can cause deformation, but it disappears during unload. It seems like an elastic behaviour, but the deformation can be unusually great. This effect is the *pseudoelasticity*, which does not concern only shape memory properties (*Fig. 1.b*).

The third effect is the *two-way effect* that requires only thermal load to change between two stable shapes. One of the shapes is stable above ϑ_{Af} and the other one is stable below a different temperature $\vartheta_{Mf} < \vartheta_{Af}$. It has to be mentioned that this effect can be produced only after a special treatment (*Fig. 1.c*).

It's important to know that the deformations which take place in the effects can be finite, and the temperature distance ($\vartheta_{Af} - \vartheta_{Mf}$) is usually very narrow (< 50 °K).



a, b, c,

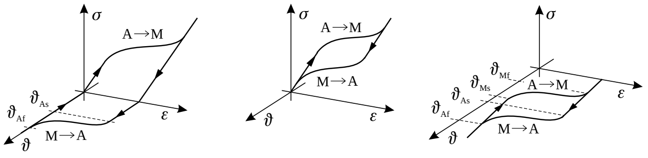
Fig. 1. Shape memory phenomena: a, one-way effect; b, pseudoelasticity; c, two-way effect

3. Crystallographical Background of Shape Memory Effects

Behind these effects there is a crystallographic transformation, namely the martensitic phase transition. The main properties of this phase change are as follows:

- non-equilibrium, diffusionless transition (the latter induces that the process is very quick),
- reversible in crystal structure, but not in general (in energetical respect, due to dissipation, see *Fig. 2*),
- it has a habit plane, which is invariant during the process,
- there is direct correspondence between the parent (austenit) and result (martensit) phases,
- the properties of transition depend strongly on the amount of alloying materials.

As it can be seen from the phenomena, the phase transitions can be induced by mechanical and thermal load. *Fig. 2* shows the effects in a stress-strain-temperature space. The forward (austenit to martensit, A → M) and backward (martensit to austenit, M → A) transitions and their temperatures are also illustrated. It is important to mention that twinning in the martensit phase and slip in both phases can occur beside the martensitic transition.



a, b, c,

Fig. 2. Shape memory phenomena in stress-strain-temperature space: a, one-way effect; b, pseudoelasticity; c, two-way effect

4. Theoretical Description and Constitutive Model

On the basis of the statements of the former sections, an elastoplastic model seems to be useful to extend for the description of the shape memory effects.

The new model has the following general features:

- local description,
- complex material behavior: elastic, plastic, phase transformational parts,
- finite strain description,
- direct connection between hypo- and hyperelasticity.

4.1. Kinematics

There is a lot of multiplicative decomposition of the total deformation gradient in the case of elastoplastic material. When phase transition can also occur in the material, a new part has to appear in the decomposition. The general extension is based on classical decomposition [5][18] and assumes that plastic flow occurs before or together with phase change [9][6][7]:

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^p \quad \longrightarrow \quad \mathbf{F} = \mathbf{F}^e\mathbf{F}^t\mathbf{F}^p \ . \tag{1}$$

The problem with the classic elastoplastic decomposition is that it is not a unique decomposition. But we can choose a different decomposition [18][1] which eliminates this problem, collecting the rotating part together [10][11]. This can be extended by taking a phase transitional part between the pure plastic deformation ($\mathbf{U}^p$) and the rotating tensor ($\mathbf{Q}$):

$$\mathbf{F} = \mathbf{V}^e\mathbf{Q}\mathbf{U}^p \quad \longrightarrow \quad \mathbf{F} = \underbrace{\mathbf{V}^e\mathbf{Q}}_{\bar{\mathbf{F}}^e}\ \mathbf{F}^t\mathbf{U}^p \ . \tag{2}$$

Here $\mathbf{V}^e$ is the elastic left stretch tensor, $\mathbf{U}^p$ is the plastic right stretch tensor and $\mathbf{Q} = \mathbf{R}^e\mathbf{R}^p$, where $\mathbf{R}^e$ is the elastic, $\mathbf{R}^p$ is the plastic rotation tensor, which can be got from the left and right polar decompositions of the elastic and plastic deformation gradient:

$$\mathbf{F}^e = \mathbf{V}^e\mathbf{R}^e \ , \ \mathbf{F}^p = \mathbf{R}^p\mathbf{U}^p \ . \tag{3}$$

From the phenomenological theory of martensitic transformations, it is known [16][12] that the martensitic transformation always consists of a lattice deformation (Bain distortion, $\mathbf{B}$), a lattice invariant shear ($\mathbf{S}$), and a lattice rotation ($\mathbf{R}$):

$$\mathbf{F}^t = \ \mathbf{R}\ \mathbf{B}\ \mathbf{S} \ . \tag{4}$$

According to Section 3, the main requirement for $\mathbf{F}^t$ is to be an invariant plane transformation. This can be realized in a different way by considering a simple shear along the habit plane ($\bar{\mathbf{S}}$) and a pure deformation orthogonal to habit plane $\bar{\mathbf{B}}$:

$$\mathbf{F}^t = \bar{\mathbf{B}}\,\bar{\mathbf{S}} = \mathbf{I} + \mathbf{k} \otimes \mathbf{n}\ , \tag{5}$$

where $\mathbf{n}$ is the outward unit normal vector of the habit plane and $\mathbf{k}$ is the displacement vector due to transformation [12].These vectors are known for a given material from experimental data. For the phase transformation process, we have to introduce a dimensionless internal (friction like) variable ξ, which varies between 0 and 1, indicating the state of transformation: for $\xi = 0$ there is no transformation and for $\xi = 1$ the transformation has finished [6][7]. This variable can be interpreted as a volume fraction of martensite phase in an infinitesimal volume. Using this variable, the transformational deformation gradient gets the form:

$$\mathbf{F}^t = \mathbf{I} + \xi\ \mathbf{k} \otimes \mathbf{n}\ . \tag{6}$$

From experimental observations it is known that a given material, with a given crystal structure has more than one habit plane (maximal value is 24). To choose the realizable one additional methods are needed, for example extremum principles [7] or direct microstructural calculations [15]. *Fig. 3* shows the decomposition (2) graphically. $\mathbf{n}_0$ is the initial unit normal vector to one slip plane and $\mathbf{s}_0$ is the initial unit vector in one slip direction in this slip plane. Under plastic stretching the crystal lattice retains its shape and orientations, so these vectors don't change with respect to the crystal structure. Martensitic transformation takes place along the habit plane, which is usually different from the slip plane. The $\mathbf{n}_t$ and $\mathbf{s}_t$ are the mentioned vectors after the phase change, while $\mathbf{n}_t^*$ and $\mathbf{s}_t^*$ are the same vectors after the rigid body rotation. Vectors in the current state are $\mathbf{n}$ and $\mathbf{s}$, which are finally deformed by an elastic stretching.

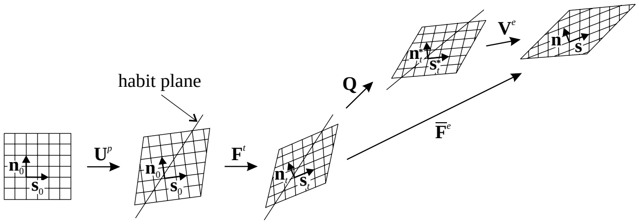


Fig. 3. Kinematics of the elastic-transformational-plastic deformation

The additive decomposition of the velocity gradient, based on (2) forms

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \dot{\bar{\mathbf{F}}}^e\bar{\mathbf{F}}^{e-1} + \bar{\mathbf{F}}^e\dot{\mathbf{F}}^t\mathbf{F}^{t\,-1}\bar{\mathbf{F}}^{e-1} + \bar{\mathbf{F}}^e\mathbf{F}^t\dot{\mathbf{U}}^p\mathbf{U}^{p\,-1}\mathbf{F}^{t\,-1}\bar{\mathbf{F}}^{e-1}\ , \tag{7}$$

$$\mathbf{L} = \mathbf{L}^e + \mathbf{L}^t + \mathbf{L}^p\ . \tag{8}$$

The rates of deformation and material spins defined by the symmetric and antisymmetric parts of the elastic, transformational and plastic velocity gradients respectively, are:

$$\mathbf{d}^e = (\mathbf{L}^e)_s \ , \ \mathbf{w}^e = (\mathbf{L}^e)_a \ , \tag{9}$$

$$\mathbf{d}^t = (\mathbf{L}^t)_s \ , \ \mathbf{w}^t = (\mathbf{L}^t)_a \ , \tag{10}$$

$$\mathbf{d}^p = (\mathbf{L}^p)_s \ , \ \mathbf{w}^p = (\mathbf{L}^p)_a \ . \tag{11}$$

This gives also an additive decomposition of the deformation rate and material spin:

$$\mathbf{d} = \mathbf{d}^e + \mathbf{d}^t + \mathbf{d}^p \quad , \quad \mathbf{w} = \mathbf{w}^e + \mathbf{w}^t + \mathbf{w}^p \ . \tag{12}$$

Using (6), (7) and Sherman-Morrison's inverse formulation, (10) can be expressed by

$$\mathbf{d}^t \ = \ \frac{\dot{\xi}}{1+\xi \ \mathbf{n} \ \mathbf{k}} \left(\bar{\mathbf{F}}^e(\mathbf{k}\otimes\mathbf{n})\bar{\mathbf{F}}^{e-1}\right)_s \ = \ \dot{\xi} \ \bar{\mathbf{d}}^t \ , \tag{13}$$

$$\mathbf{w}^t \ = \ \frac{\dot{\xi}}{1+\xi \ \mathbf{n} \ \mathbf{k}} \left(\bar{\mathbf{F}}^e(\mathbf{k}\otimes\mathbf{n})\bar{\mathbf{F}}^{e-1}\right)_a \ = \ \dot{\xi} \ \bar{\mathbf{w}}^t \ . \tag{14}$$

It can be mentioned now, that the advantage of the chosen decomposition (2) is that $\mathbf{w}^p$ can be explained as the function of $\mathbf{d}^p$ [14]:

$$\mathbf{w}^p = \mathbf{H} : \mathbf{d}^p \ , \tag{15}$$

in which

$$\mathbf{H} = \mu_1^p(\bar{\mathbf{U}}^p\bar{\otimes}\boldsymbol{\delta}-\boldsymbol{\delta}\bar{\otimes}\bar{\mathbf{U}}^p) \ + \ \mu_2^p(\bar{\mathbf{U}}^{p2}\bar{\otimes}\boldsymbol{\delta}-\boldsymbol{\delta}\bar{\otimes}\bar{\mathbf{U}}^{p2})+\mu_3^p(\bar{\mathbf{U}}^{p2}\bar{\otimes}\bar{\mathbf{U}}^p-\bar{\mathbf{U}}^p\bar{\otimes}\bar{\mathbf{U}}^{p2}), \tag{16}$$

where $\bar{\mathbf{U}}^p = \bar{\mathbf{F}}^e\mathbf{F}^t\mathbf{U}^p\mathbf{F}^{t\,T}\bar{\mathbf{F}}^{eT}$ and the coefficients are the functions of the first, second and third scalar invariants of $\bar{\mathbf{U}}^p$

$$\mu_1^p = \frac{I^{p2}}{I^pII^p - III^p} \ , \ \mu_2^p = -\frac{I^p}{I^pII^p - III^p} \ , \ \mu_3^p = \frac{1}{I^pII^p - III^p} \ . \tag{17}$$

4.2. *Objective Rates*

For the description of the elastic behavior of the material a logarithmic strain $\ln \mathbf{V}^e$ was chosen because it was proved that the logarithmic strain is the only strain measure whose corotational rate can give the deformation rate [19]. Two corotational objective derivatives are used for the description of rate type equations. The first is the recently developed logarithmic rate [19][20], the second is its modification namely the elastic logarithmic rate [14]. The logarithmic derivative of the Kirchhoff stress tensor can be expressed by:

$$\overset{\circ}{\boldsymbol{\tau}}{}^{log} = \dot{\boldsymbol{\tau}} + \boldsymbol{\tau}\boldsymbol{\Omega}^{log} - \boldsymbol{\Omega}^{log}\boldsymbol{\tau} \ , \tag{18}$$

where the logarithmic spin tensor

$$\boldsymbol{\Omega}^{log} = \mathbf{w} + \mathbf{A} : \mathbf{d} \tag{19}$$

with

$$\mathbf{A} = \nu_1(\mathbf{V}\bar{\otimes}\boldsymbol{\delta} - \boldsymbol{\delta}\bar{\otimes}\mathbf{V}) + \nu_2(\mathbf{V}^2\bar{\otimes}\boldsymbol{\delta} - \boldsymbol{\delta}\bar{\otimes}\mathbf{V}^2) + \nu_3(\mathbf{V}^2\bar{\otimes}\mathbf{V} - \mathbf{V}\bar{\otimes}\mathbf{V}^2), \tag{20}$$

and the coefficients ν_i are given with the eigenvalues ($\lambda_{i,i=1..3}$) of the left stretch tensor **V**:

$$\left.\nu_1 = \nu_2 = \nu_3 = 0 \right\} \quad \text{if} \quad \lambda_1 = \lambda_2 = \lambda_3$$

$$\left.\nu_1 = \frac{1}{\lambda_1 - \lambda_2} h\left(\frac{\lambda_1}{\lambda_2}\right), \ \nu_2 = \nu_3 = 0 \right\} \quad \text{if} \quad \lambda_1 \neq \lambda_2 = \lambda_3$$

$$\left.\begin{aligned} \nu_k &= \frac{(-1)^k}{\Delta} \sum_{i=1}^{3} \lambda_i^{3-k} h\left(\varepsilon_i\right), \ k = 1, 2, 3 \\ \Delta &= (\lambda_1 - \lambda_2)(\lambda_2 - \lambda_3)(\lambda_3 - \lambda_1), \\ \varepsilon_1 &= \frac{\lambda_2}{\lambda_3}, \quad \varepsilon_2 = \frac{\lambda_3}{\lambda_1}, \quad \varepsilon_3 = \frac{\lambda_1}{\lambda_2}, \end{aligned}\right\} \quad \text{if} \quad \lambda_1 \neq \lambda_2 \neq \lambda_3 \neq \lambda_1 \tag{21}$$

where h is the logarithmic spin function:

$$h(z) = \frac{1 + z^2}{1 - z^2} + \frac{1}{\ln z} \ . \tag{22}$$

The elastic logarithmic rate has the same form with change of $\mathbf{d}$, $\mathbf{w}$, $\mathbf{V}$, λ_i to $\mathbf{d}^e$, $\mathbf{w}^e$, $\mathbf{V}^e$, λ_i^e:

$$\overset{\circ}{\boldsymbol{\tau}}{}^{log\text{-}e} = \dot{\boldsymbol{\tau}} + \boldsymbol{\tau}\boldsymbol{\Omega}^{log\text{-}e} - \boldsymbol{\Omega}^{log\text{-}e}\boldsymbol{\tau} \ , \tag{23}$$

$$\boldsymbol{\Omega}^{log\text{-}e} = \mathbf{w}^e + \mathbf{A}^e : \mathbf{d}^e \ , \tag{24}$$

$$\begin{aligned} \mathbf{A}^e \ = \ & \nu_1^e(\mathbf{V}^e\bar{\otimes}\boldsymbol{\delta} - \boldsymbol{\delta}\bar{\otimes}\mathbf{V}^e) \ + \ \nu_2^e(\mathbf{V}^{e2}\bar{\otimes}\boldsymbol{\delta} - \boldsymbol{\delta}\bar{\otimes}\mathbf{V}^{e2}) \\ + \ & \nu_3^e(\mathbf{V}^{e2}\bar{\otimes}\mathbf{V}^e - \mathbf{V}^e\bar{\otimes}\mathbf{V}^{e2}). \end{aligned} \tag{25}$$

The advantage of these rates is that applying them for the total and elastic logarithmic strains they can only give the total and elastic rates of deformation [19] [14]:

$$(\ln \overset{\circ}{\mathbf{V}})^{log} = \mathbf{d} \quad \longrightarrow \quad (\ln \overset{\circ}{\mathbf{V}}{}^e)^{log\text{-}e} = \mathbf{d}^e \ . \tag{26}$$

By means of these properties a direct connection between the hyper and hypoelastic equations can be established.

4.3. Thermodynamics

The second law of thermodynamics in the form of the local Planck inequality is as follows [4]:

$$\rho_0 \mathcal{D} = \boldsymbol{\tau} : \mathbf{d} - \rho_0 \dot{\psi} - \rho_0 s \dot{\vartheta} \ \geq 0 \ , \tag{27}$$

where ρ_0 is the mass density in the reference configuration, $\mathcal{D}$ is the rate of dissipation per unit mass, $\boldsymbol{\tau}$ is the Kirchhoff stress tensor, ψ is the specific Helmholtz free energy per unit mass, s is the entropy and ϑ is the temperature. It is assumed that

$$\psi = \psi \left(\ln \mathbf{V}^e, \vartheta, \xi \right) \ . \tag{28}$$

Inserting the total derivative of (28) to (27), then using (12) and (26), the rate of dissipation leads to:

$$\begin{aligned} \mathcal{D} \ &= \ \left(\frac{1}{\rho_0}\, \boldsymbol{\tau} - \frac{\partial \psi}{\partial (\ln \mathbf{V}^e)} \right) : (\ln \overset{\circ}{\mathbf{V}}{}^e)^{log\text{-}e} \ - \ \left(\frac{\partial \psi}{\partial \vartheta} + s \right) \dot{\vartheta} \\ &+ \ \frac{1}{\rho_0}\, \boldsymbol{\tau} : \mathbf{d}^p \ + \frac{1}{\rho_0}\, \boldsymbol{\tau} : \mathbf{d}^t - \frac{\partial \psi}{\partial \xi}\, \dot{\xi} \ \geq 0 \ . \end{aligned} \tag{29}$$

In elastic processes there is no dissipation and $\dot{\vartheta}$ can be both positive and negative due to heating or cooling. This gives the hyperelasticity law and the expression for entropy:

$$\boldsymbol{\tau} \ = \ \rho_0 \, \frac{\partial \psi}{\partial (\ln \mathbf{V}^e)} \ , \tag{30}$$

$$s \ = \ - \, \frac{\partial \psi}{\partial \vartheta} \ . \tag{31}$$

The rest of the dissipation rate consists of the plastic and phase transformational parts:

$$\mathcal{D} = \frac{1}{\rho_0}\, \boldsymbol{\tau} : \mathbf{d}^p + X^{\xi} \dot{\xi} \ \geq 0 \ , \tag{32}$$

where X^{ξ} is the dissipative force conjugated to $\dot{\xi}$. Using (13) for the relation of $\mathbf{d}^t$ and $\bar{\mathbf{d}}^t$,

$$X^{\xi} = \frac{1}{\rho_0}\, \boldsymbol{\tau} : \bar{\mathbf{d}}^t - \frac{\partial \psi}{\partial \xi} \ . \tag{33}$$

One simple assumption that each rate depends on its conjugate force and the internal variable leads to evolution equations [7]

$$\mathbf{d}^p = \mathbf{f}^p(\boldsymbol{\tau}, \xi) \ \ , \ \ \dot{\xi} = f^{\xi}(X^{\xi}, \xi) \ , \tag{34}$$

which are known as flow rule and kinetic equation of phase transition.

4.4. Phase Kinetics

It can be seen that the conjugated force X^{ξ} drives the phase transformation process. In the dissipation free case the threshold value is 0 for both the forward and reverse transition and no hysteresis has appeared. But from the mentioned phenomena it is known that there is dissipation in the shape memory effects. So the phase transformation criteria can be expressed by

$$\begin{array}{llllll} \text{if} & X^{\xi} \geq k_{\mathrm{A}\rightarrow\mathrm{M}} > 0 & \text{and} \ \dot{X}^{\xi} > 0 & \text{and} \ \xi < 1 & \text{then} & \dot{\xi} > 0, \\ \text{if} & X^{\xi} \leq k_{\mathrm{M}\rightarrow\mathrm{A}} < 0 & \text{and} \ \dot{X}^{\xi} < 0 & \text{and} \ \xi > 0 & \text{then} & \dot{\xi} < 0, \\ & & & & \text{else} & \dot{\xi} = 0. \end{array} \tag{35}$$

Here $k_{\mathrm{A}\rightarrow\mathrm{M}}$ and $k_{\mathrm{M}\rightarrow\mathrm{A}}$ are the threshold values of force X^{ξ}, which is experimentally determined and can depend on some parameters, for example on ϑ and $\mathbf{F}^{p}$. The simplest assumption for $\dot{\xi}$ is the linear dependence on X_{ξ}. Then the phase kinetic equation consisting of the conditions gets the following form

$$\begin{aligned} \dot{\xi} \ &= \ \mathrm{H}(\dot{X}^{\xi})\ \mathrm{H}(1-\xi)\ \big(1-\mathrm{H}(k_{\mathrm{A}\rightarrow\mathrm{M}}-X^{\xi})\big)\, C_{\mathrm{A}\rightarrow\mathrm{M}} X^{\xi} \\ &+ \ \mathrm{H}(-\dot{X}^{\xi})\ \mathrm{H}(\xi)\ \big(1-\mathrm{H}(X^{\xi}-k_{\mathrm{M}\rightarrow\mathrm{A}})\big)\, C_{\mathrm{M}\rightarrow\mathrm{A}} X^{\xi}\ , \end{aligned} \tag{36}$$

where $C_{\mathrm{A}\rightarrow\mathrm{M}}$ and $C_{\mathrm{M}\rightarrow\mathrm{A}}$ are positive constants and $\mathrm{H}(.)$ is the Heaviside function: $\mathrm{H}(x) = 1$ if $x > 0$ and $\mathrm{H}(x) = 0$ if $x \leq 0$.

It's important to mention that the chosen phase kinetic equation (36) always satisfies the non-negative restriction for the rate of dissipation given by (32).

4.5. Constitutive Equation

Let us consider the Helmholtz free energy as

$$\psi(\ln \mathbf{V}^{e}, \vartheta, \xi) = \frac{(\ln \mathbf{V}^{e}) : \mathbf{D}^{e} : (\ln \mathbf{V}^{e})}{2\rho} + \psi^{\vartheta}(\vartheta, \xi)\ , \tag{37}$$

then the hyperelastic law (30) becomes the following form

$$\boldsymbol{\tau} = \mathbf{D}^{e} : \ln \mathbf{V}^{e}\ . \tag{38}$$

Here $\mathbf{D}^{e}$ is the fourth order elastic stiffness tensor, which is assumed not depending on ξ. Applying the elastic logarithmic rate for (38), it changes to the hypoelastic law:

$$\overset{\circ}{\boldsymbol{\tau}}{}^{\mathit{log\text{-}e}} = \mathbf{D}^{e} : \mathbf{d}^{e}\ . \tag{39}$$

The connection between the logarithmic and elastic logarithmic rates comes out from its definitions

$$\overset{\circ}{\boldsymbol{\tau}}{}^{\mathit{log}} \ = \ \overset{\circ}{\boldsymbol{\tau}}{}^{\mathit{log\text{-}e}} \ - \ \boldsymbol{\tau}\boldsymbol{\Omega}^{\mathit{log\text{-}e}} \ + \ \boldsymbol{\Omega}^{\mathit{log\text{-}e}}\boldsymbol{\tau} \ + \ \boldsymbol{\tau}\boldsymbol{\Omega}^{\mathit{log}} \ - \ \boldsymbol{\Omega}^{\mathit{log}}\boldsymbol{\tau}\ . \tag{40}$$

By applying (39) and (24) for (40), we have

$$\begin{aligned} \overset{\circ}{\boldsymbol{\tau}}^{log} &= \mathbf{D}^e : \mathbf{d}^e \;-\; \boldsymbol{\tau}(\mathbf{w}^e + \mathbf{A}^e : \mathbf{d}^e) \;+\; (\mathbf{w}^e + \mathbf{A}^e : \mathbf{d}^e)\boldsymbol{\tau} \\ &+ \;\; \boldsymbol{\tau}(\mathbf{w} + \mathbf{A} : \mathbf{d}) \;-\; (\mathbf{w} + \mathbf{A} : \mathbf{d})\boldsymbol{\tau} \ , \end{aligned} \tag{41}$$

then by considering the additive decomposition of deformation rate and spin of (12) we can obtain

$$\begin{aligned} \overset{\circ}{\boldsymbol{\tau}}^{log} &= \mathbf{D}^e : (\mathbf{d} - \mathbf{d}^t - \mathbf{d}^p) + \boldsymbol{\tau}\left[\mathbf{w}^t + \mathbf{w}^p + (\mathbf{A} - \mathbf{A}^e) : \mathbf{d} + \mathbf{A}^e : (\mathbf{d}^t + \mathbf{d}^p)\right] \\ &- \;\left[\mathbf{w}^t + \mathbf{w}^p + (\mathbf{A} - \mathbf{A}^e) : \mathbf{d} + \mathbf{A}^e : (\mathbf{d}^t + \mathbf{d}^p)\right]\boldsymbol{\tau} \ . \end{aligned} \tag{42}$$

Finally by using equation (15) for plastic material spin, (13) and (14) for phase transformational parts yield

$$\overset{\circ}{\boldsymbol{\tau}}^{log} = (\mathbf{D}^e + \mathbf{B}) : \mathbf{d} - (\mathbf{D}^e - \mathbf{C}) : \mathbf{d}^p - \mathbf{e}\,\dot{\xi} \ , \tag{43}$$

where **B**, **C** and **e** are given in the following way:

$$B_{ijkl} = \tau_{in}(A_{njkl} - A^e_{njkl}) - (A_{imkl} - A^e_{imkl})\tau_{mj} \ , \tag{44}$$

$$C_{ijkl} = \tau_{in}(H_{njkl} + A^e_{njkl}) - (H_{imkl} + A^e_{imkl})\tau_{mj} \ , \tag{45}$$

$$\mathbf{e} = \mathbf{D}^e : \bar{\mathbf{d}}^t - \boldsymbol{\tau}(\bar{\mathbf{w}}^t + \mathbf{A}^e : \bar{\mathbf{d}}^t) + (\bar{\mathbf{w}}^t + \mathbf{A}^e : \bar{\mathbf{d}}^t)\boldsymbol{\tau} \ . \tag{46}$$

Let assume isotrop hardening with non-associated flow law. Then the yield function and the plastic potential depend on the Kirchhoff stress tensor $\boldsymbol{\tau}$, on the hardening parameter κ and on the internal variable ξ

$$F(\boldsymbol{\tau}, \kappa, \xi) \;\; \leq \;\; 0 \ , \tag{47}$$

$$f(\boldsymbol{\tau}, \kappa, \xi) \quad . \tag{48}$$

The consistency condition, applying the equivalence between the corotational rate and the material time rate of F, takes the form

$$\dot{F} = \overset{\circ}{F}^{log} = \frac{\partial F}{\partial \boldsymbol{\tau}} : \overset{\circ}{\boldsymbol{\tau}}^{log} + \frac{\partial F}{\partial \kappa}\dot{\kappa} + \frac{\partial F}{\partial \xi}\dot{\xi} = 0 \ . \tag{49}$$

The flow rule (34) in a direct form can be expressed by

$$\mathbf{d}^p = \lambda \mathbf{Q} \ , \tag{50}$$

where λ is the plastic multiplier and **Q** is the unit gradient of plastic potential. The rate of the hardening parameter is in general form:

$$\dot{\kappa} = \lambda a \ . \tag{51}$$

With the use of (43), (49), (50) and (51), the plastic multiplier can be expressed by which applying it in (43), the final form of the constitutive equation (39) can be found

$$\begin{aligned}\overset{\circ}{\boldsymbol{\tau}}{}^{log} &= \left[\mathbf{D}^e + \mathbf{B} - \frac{(\mathbf{D}^e - \mathbf{C}) : \mathbf{Q} \otimes \mathbf{P} : (\mathbf{D}^e + \mathbf{B})}{\mathrm{H} + \mathbf{P} : (\mathbf{D}^e - \mathbf{C}) : \mathbf{Q}}\right] : \mathbf{d} \\ &- \left[\frac{\mathbf{P} : \mathbf{e} + \mathrm{L}}{\mathrm{H} + \mathbf{P} : (\mathbf{D}^e - \mathbf{C}) : \mathbf{Q}} (\mathbf{D}^e - \mathbf{C}) : \mathbf{Q} \ + \ \mathbf{e}\right] \dot{\xi} \ .\end{aligned} \tag{52}$$

Here **P** is the unit gradient of yield surface while the plastic hardening modulus H and L are given by

$$\mathrm{H} = -\frac{1}{\|\frac{\partial F}{\partial \boldsymbol{\tau}}\|}\frac{\partial F}{\partial \kappa} a \ , \quad \mathrm{L} = \frac{1}{\|\frac{\partial F}{\partial \boldsymbol{\tau}}\|}\frac{\partial F}{\partial \xi} \ . \tag{53}$$

The constitutive equation (52) together with the phase kinetical equation (36) can be used in any numerical solution, for example in a modified finite element method, to solve a boundary-value problem. The numerical solution leads generally to a Newton–Raphson iteration process based on the tangent constitutive operator. The present paper aimed to extend the elastic-plastic constitutive operator to the case of shape memory phase transformations, based on finite strains. This process also can solve the following reorientation problem. The material point is in martensitic phase and the direction of the applied load changes that another martensit variant reaches the realizable position. The possibility to change variants makes the model more realistic in description of the shape deformation of the material.

5. Concluding Remarks

The presented model extends a finite strain elasto-plastic description to phase transition case. It can be used for the parallel appearance of plastic and phase transformational processes. The first thing in every calculation step is to choose the most favorable martensite variant in every point, to determine the kinematic parameters. In the final constitutive operator a new part has appeared, which is used for the description of phase transition. The model can be applied for the forward and reverse martensitic transformation and for the reorientation and martensit twinning process.

Beside these good properties, the model has some missing parts. It is unable to describe that the phase transition can occur only in a finite volume whose size is a critical nucleus size. Furthermore it does not consider the interface propagation. The next step is to develop the model for these microstructural processes, and to make some analytical calculations with the model.

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