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Phenomenological modeling of shape memory effect using the concept of orientational back stress

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Abstract. A derivation of constitutive equations in a general three–dimensional setting is described, based on an additive decomposition of the rate of deformation tensor. The rate of deformation tensor is assumed to consist of an elastic part, a thermoelastic part, a plastic part, and a part due to phase transformation. The thermoelastic part due to thermoelastic coupling accounts for the influence of temperature near phase transformation, while the plastic part is taken in the form of classical flow theory of plasticity with combined isotropic and kinematic hardening, where the back stress represents a tensor of orientational microstresses. It is assumed that the part due to the phase transformation depends on the first and the second invariant of the tensor of crystallographic distortion, on the deviatoric part of the stress tensor, and on a special evolution parameter describing the rate of forming of a new phase. The derived constitutive equation is given in an explicit form with the corresponding tensor generators of the representation together with the irreducible integrity basis of the relevant tensor functions.

1. INTRODUCTION

A description of a complex nature of internal crystalline transformations, which induce special mechanical properties of shape memory materials, requires a set of constitutive equations that are general enough to describe the dependence of internal transformations, which can take place in a parent crystal, on a stress, temperature, and a deformation history of the material, to name just a few. One of the main goals in proposing an adequate constitutive model for shape memory materials is a formulation of constitutive equations that include a set of internal variables, which are easy to identify, easy to observe, and easy to measure experimentally. Then the necessary internal variables can be incorporated in constitutive equations in a general three–dimensional context. Specialization to a particular state of stress, like uni–axial or simple shear, then follows directly from a general three–dimensional version of equations. One among possible derivations of constitutive equations in a general three–dimensional setting is based on an additive decomposition of the rate of deformation tensor. In this type of formulation the rate of deformation tensor is assumed to consist of an elastic part, a thermoelastic part, a plastic part, and a part due to phase transformation. To justify such a decomposition for constitutive description of shape memory alloys we take into account most frequently encountered characteristics of load–deformation behavior. Shape memory materials exhibit a strong dependence on temperature in load–deformation curves. At low temperatures the behavior is almost like the behavior of plastic body with an initial elastic branch, yield limit, and creep upon loading, and residual deformation upon unloading. The main difference from the usual plastic behavior is the existence of lateral elastic branches along which the body can be loaded beyond the yield limit. At higher temperatures the load–deformation curves change in the sense that there is no residual deformation upon unloading. This type of behavior is called pseudo–elastic, because there is a complete return to the origin in a loading–unloading cycle like in a classical linear or nonlinear elasticity, but the path of return takes on a form of hysteresis. Consequently, the elastic part of the rate of deformation tensor can be taken in a standard form of a generalized Hooke's law. For engineering and for some other types of practical applications it is permissible to consider an isotropic version of the Hooke's law. On the other hand, the thermoelastic part due to thermoelastic coupling with the temperature dependent material constants accounts for the influence of temperature near the phase transformation. The plastic part is taken in the form of classical flow theory of plasticity with combined isotropic and kinematic hardening where the back stress represents a tensor of orientational microstresses. Furthermore, it is postulated that the part due to phase transformation depends on the first and the second invariant of the tensor of crystallographic distortion of phase transformation, on the deviatoric part of the stress tensor, and on a special evolution parameter describing the rate of forming of a new phase. The elastic part of the rate of deformation tensor is connected with the objective rate of Cauchy stress through the tensor of elastic compliance. As a result, under the adopted assumptions, a general form of derived constitutive equations takes on a similar structure as constitutive relations in finite deformation thermoplasticity.

2. FORMULATION OF PARTICULAR PARTS OF CONSTITUTIVE RELATION

From a continuum mechanics point of view we are dealing with macroscopic physical quantities. This notion is very important in defining the scale of formulation. Because the modeling region must be large enough it contains a large number of microrelated entities like grains in polycrystalline state or martensite plates in a single crystal state. These physical quantities, which can change quite rapidly on a scale of a larger subdomain, are then averaged over the chosen characteristic region $\mathscr{D}$ presumed to be representative enough to capture main characteristics of heterogeneous medium. To eliminate such a complicated spatial dependence, we average the local field variables over the representative domain using directional averaging over the complete solid angle ω. Such a procedure can be employed even if more general concept of directional averaging is needed. For example, by introducing an orientation distribution function $\mathscr{W}(\omega)$ in the formulation, the function $\mathscr{W}(\omega)$ can be considered as a weighting function of the integral relation of ensemble averaging, and the transition between micro and macroscale can be achieved by the volumetric average of local quantities employing the formula

$$(\cdot)_{global} = \langle\cdot\rangle = 1/V \int_{\mathscr{D}} [\mathscr{W}(\omega)(\cdot)]\, dV(\omega). \tag{1}$$

In what follows, we consider variables defined on a global level that are connected with the variables on a local level by Eq. (1).

We assume that the constitutive model admits an additive decomposition of the rate of deformation tensor $\boldsymbol{D}$ representing a symmetric part of velocity gradient evaluated at current configuration $\boldsymbol{L} = \partial \boldsymbol{v}/\partial \boldsymbol{x} = \boldsymbol{D} + \boldsymbol{W}$, where $\boldsymbol{x} = x_k \mathbf{e}_k$ is a position vector of the material point and $\mathbf{e}_k$ is the associated base vector of the 3D Euclidean space. The skew symmetric part of velocity gradient defines the corresponding spin tensor $\boldsymbol{W}$. Such an additive decomposition can be utilized by considering various thermo–mechanical effects that may take place during the process

$$\boldsymbol{D} = \boldsymbol{D}_{EL} + \boldsymbol{D}_{ET} + \boldsymbol{D}_{PT} + \boldsymbol{D}_{PD}. \tag{2}$$

Here $\boldsymbol{D}_{EL} = \mathcal{C}^{-1}\colon \overset{\nabla}{\boldsymbol{\sigma}}$ is the elastic part, $\mathcal{C}^{-1}$ is the fourth rank tensor of elastic compliances, $\overset{\nabla}{\boldsymbol{\sigma}}$ is an appropriate objective rate of the Cauchy stress. For example, the tensor of elastic moduli $\mathcal{C}$ expressed in terms of Lame constants λ and μ as well as the Jaumann co–rotational stress rate can be written as

$$\begin{gathered}
\overset{\nabla}{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\cdot\boldsymbol{W} - \boldsymbol{W}\cdot\boldsymbol{\sigma} = \dot{\boldsymbol{\sigma}} + \boldsymbol{\Omega}^{\sigma}\colon \boldsymbol{L}, \quad \boldsymbol{\Omega}^{\sigma} = \Omega^{\sigma}_{ijkl}\mathbf{e}_i\mathbf{e}_j\mathbf{e}_k\mathbf{e}_l, \\
\boldsymbol{\Omega}^{\sigma} = \tfrac{1}{2}(\sigma_{ik}\delta_{jl} - \sigma_{jl}\delta_{ik} + \sigma_{jk}\delta_{il} - \sigma_{il}\delta_{jk})\mathbf{e}_i\mathbf{e}_j\mathbf{e}_k\mathbf{e}_l, \quad \delta_{ij} = \mathbf{e}_i\cdot\mathbf{e}_j, \\
\mathcal{C} = (3\lambda + 2\mu)\mathcal{J} + 2\mu\mathcal{K} = [(3\lambda + 2\mu)\mathcal{J}_{ijkl} + 2\mu\mathcal{K}_{ijkl}]\mathbf{e}_i\mathbf{e}_j\mathbf{e}_k\mathbf{e}_l, \\
\mathcal{I}_{ijkl} = \mathcal{J}_{ijkl} + \mathcal{K}_{ijkl} = \tfrac{1}{3}\delta_{ij}\delta_{kl} + \tfrac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{jk}\delta_{il} - \tfrac{2}{3}\delta_{ij}\delta_{kl}\right).
\end{gathered} \tag{3}$$

2.1 The thermoelastic part

The thermoelastic part of rate of deformation tensor $\boldsymbol{D}_{ET}$ can be additionally split into two parts: the part due to volumetric thermal expansion with the corresponding tensor of thermoelastic expansion coefficients

$\boldsymbol{H}_0$ as in standard thermoelasticity, e.g., in isotropic case we have $\boldsymbol{H}_0 = -\beta \boldsymbol{I}$ where β is the coefficient of volumetric temperature expansion, and the part due to pseudoelasticity with the tensor $\boldsymbol{H}_1$ characterizing thermal softening effects

$$\boldsymbol{D}_{ET} = (\boldsymbol{H}_0 + \boldsymbol{H}_1)\,\dot{\theta} = \left(\boldsymbol{H}_0 - \frac{\mathrm{Tr}\boldsymbol{\sigma}}{9K}\frac{\partial \ln K(\theta)}{\partial \theta}\boldsymbol{I} - \frac{1}{2G}\frac{\partial \ln G(\theta)}{\partial \theta}\mathrm{Dev}\boldsymbol{\sigma}\right)\dot{\theta}, \tag{4}$$

where $\mathrm{Tr}(\cdot)$ is the trace operator, $\mathrm{Dev}(\cdot)$ designates a deviatoric part of the operator, $K(\theta)$ and $G(\theta)$ are temperature dependent bulk and shear moduli, respectively. Even with this two simple types of constitutive relationship various reversible thermoelastic and pseudoelastic phenomena can be described [8–11].

2.2 The phase transformation part

In the process of transformation the alloy can be viewed as a mixture of a parent austenite phase and the product martensite phase. By employing the volume fraction of martensite as an internal variable, the transformation kinetics is given as an evolution equation of the internal variables. The evolution equation for the product phase $\xi = V_2/V$ is postulated as

$$\dot{\xi} = X_\theta(I_\sigma, II_\sigma, \theta, \xi)\,\dot{\theta} + \boldsymbol{X}_{\boldsymbol{\sigma}}(I_\sigma, II_\sigma, \theta, \xi) : \dot{\boldsymbol{\sigma}}, \quad \text{where} \quad I_\sigma = \mathrm{Tr}\boldsymbol{\sigma}, \;\; II_\sigma = \tfrac{1}{2}\mathrm{Dev}\boldsymbol{\sigma} : \mathrm{Dev}\boldsymbol{\sigma} = \tfrac{1}{3}\bar{\sigma}^2, \tag{5}$$

which is a generalization of a standard 1D–evolution equations as described in [1] and [4]. One among possible generalizations is to consider a material time derivative of an effective–equivalent stress $\dot{\bar{\sigma}}$ as a substitute for uni–axial stress in original 1D equations. This yields $\boldsymbol{X}_{\boldsymbol{\sigma}} = X\,\mathrm{Dev}\boldsymbol{\sigma}$ where $X = X(I_\sigma, II_\sigma, \theta, \xi)$ is the corresponding constitutive function. However, such an approach may not always lead to the satisfactory results as pointed out in [12]. Therefore, in the course of further development, the general form of the evolution law (5) will be used. For example, we can use one of the simplest relations describing the kinetics of transformation the so–called the Koistinen–Marburger and the Magee–type of kinetics

$$\xi = 1 - \exp\left[-k_0 \boldsymbol{E}^* : \boldsymbol{\sigma} + k_0 \rho_0 \left|\frac{\partial \Delta\phi_{CH}}{\partial \theta}\right| (\theta - \theta_{MS})\right], \tag{6}$$

where $\Delta\phi_{CH}(\theta)$ represents the chemical driving force as a difference between the specific chemical energy in both phases, $\boldsymbol{E}^*$ is the transformation strain, θ_{MS} the martensite start temperature, k_0 is the material constant, and ρ_0 material density referring to the reference configuration. Further details of the transformation kinetics together with a comprehensive discussion of its implications in transformation induced plasticity can be found in [3],[4] and [6]. As a result, the equation (6) which is an extended three–dimensional version of the Koistinen–Marburger and the Magee–type kinetics leads to the postulated form of phase kinetics evolution law (5) with

$$\log(1 - \xi) = -k_0 \boldsymbol{E}^* : \boldsymbol{\sigma} + k_0 \rho_0 \left|\frac{\partial \Delta\phi_{CH}}{\partial \theta}\right| (\theta - \theta_{MS}),$$

$$\boldsymbol{X}_{\boldsymbol{\sigma}} = k_0(1 - \xi)\boldsymbol{E}^*, \quad X_\theta = k_0 \rho_0 (1 - \xi)\left|\frac{\partial \Delta\phi_{CH}}{\partial \theta}\right|.$$

According to the theory of a single variant transformation, the tensor of crystallographic distortion $\mathcal{F}$ is defined by the transformation $d\boldsymbol{x}_{(2)} = \mathcal{F} \cdot d\boldsymbol{x}_{(1)}$ that defines the relationship between the parent phase (1) and the product phase (2). With the help of $\mathcal{F}$ the kinematics between both phases is completely defined. Consequently, the bulk effect of phase transformation due to the volumetric dilatation of the lattice attributed to the lattice distortion tensor $\mathcal{F}$ is related to the volumetric distortion rate, which is assumed proportional to the constitutive response function and to the rate of forming of a new phase. Similar reasoning applies for a deviatoric part that accounts for the extent of plastic accommodation during the phase transformation. Both parts combined yield the evolution equation for the rate of deformation tensor due to the phase transformation

$$\boldsymbol{D}_{PT} = \chi_0(I_{\mathcal{F}})\,\dot{\xi}\,\boldsymbol{I} + \chi_1(II_{\mathcal{F}})\,\dot{\xi}\,\mathrm{Dev}\boldsymbol{\sigma},$$

which by virtue of Eq. (5) can be put in a general form used in further development

$$\boldsymbol{D}_{PT} = \boldsymbol{H}_2(I_{\sigma\mathcal{F}}, II_{\sigma\mathcal{F}}, \theta, \xi)\,\dot{\theta} + \mathcal{S}_2(I_{\sigma\mathcal{F}}, II_{\sigma\mathcal{F}}, \theta, \xi) : \dot{\boldsymbol{\sigma}} = (H_{2ij}\,\dot{\theta} + \mathcal{S}_{2ijkl}\,\dot{\sigma}_{kl})\mathrm{e}_i\mathrm{e}_j. \tag{7}$$

Here the constitutive tensors $\boldsymbol{H}_2$ and $\mathcal{S}_2$ are given by

$$\begin{aligned} \boldsymbol{H}_2 &= \chi_0 X_\theta \boldsymbol{I} + \chi_1 X_\theta \mathrm{Dev}\boldsymbol{\sigma} = (\chi_0 X_\theta \delta_{ij} + \chi_1 X_\theta \mathrm{Dev}\sigma_{ij})\mathrm{e}_i\mathrm{e}_j, \\ \mathcal{S}_2 &= \chi_0 \boldsymbol{I} \otimes \boldsymbol{X}_{\boldsymbol{\sigma}} + \chi_1 \mathrm{Dev}\boldsymbol{\sigma} \otimes \boldsymbol{X}_{\boldsymbol{\sigma}} = (\chi_0 \delta_{ij} X^{\sigma}_{kl} + \chi_1 \mathrm{Dev}\sigma_{ij} X^{\sigma}_{kl})\mathrm{e}_i\mathrm{e}_j\mathrm{e}_k\mathrm{e}_l. \end{aligned} \tag{8}$$

2.3 Orientational back stress and plastic irreversibility

Most shape memory alloys exhibit some sort of quasi–plastic behavior at low temperatures, in some alloys this can happen near the room temperature, whereas at comparably higher temperatures the effect of pseudoelasticity sets in. To model the effect of plastic irreversibility at lower temperatures we use standard concepts from classical plasticity. The plastic part of the macroscopic rate of deformation tensor due to dislocation movement is determined by employing the well-known normality condition. Consequently, we define the plastic flow rule as

$$\boldsymbol{D}_{PD} = \dot{\lambda}\frac{\partial F}{\partial \boldsymbol{\sigma}}, \quad F(\boldsymbol{\sigma}, \boldsymbol{\alpha}, \kappa) = f(\boldsymbol{\sigma} - \boldsymbol{\alpha}) - \kappa(\bar{\epsilon}, \theta, \xi) = 0, \quad \dot{\bar{\epsilon}}^2 = \tfrac{2}{3}\boldsymbol{D}_{PD} : \boldsymbol{D}_{PD}, \tag{9}$$

where $F(\boldsymbol{\sigma}, \boldsymbol{\alpha}, \kappa) = 0$ is a yield function, $\bar{\epsilon} = \int \dot{\bar{\epsilon}} dt$ an equivalent or effective plastic strain, $\kappa(\bar{\epsilon}, \theta, \xi)$ strain hardening and temperature softening parameter depending on the amount of the product phase ξ, $\boldsymbol{\alpha}$ is orientational microstress which results in controlling the kinematic hardening according to the standard definition of a back stress. It is represented by a linear combination of deformation rates due to dislocation plasticity and transformation induced plasticity with the corresponding constants–weights which control the influence of each particular term:

$$\overset{\nabla}{\boldsymbol{\alpha}} = \dot{\boldsymbol{\alpha}} + \boldsymbol{\Omega}^{\alpha} : \boldsymbol{L} = \alpha_1 \boldsymbol{D}_{PD} + \alpha_2 \boldsymbol{D}_{PT}. \tag{10}$$

The function $f(\boldsymbol{\sigma} - \boldsymbol{\alpha})$ in (9) represents a hypersurface in the space of stresses $\boldsymbol{\sigma}$ and microstresses $\boldsymbol{\alpha}$. In the most general case, for $f(\boldsymbol{\sigma} - \boldsymbol{\alpha})$ to represent a scalar invariant under the orthogonal isotropy group, we have the dependence

$$f(\boldsymbol{\sigma} - \boldsymbol{\alpha}) = f(\mathscr{I}_{1\sigma}, \mathscr{I}_{2\sigma}, \mathscr{I}_{3\sigma}, \mathscr{I}_{1\alpha}, \mathscr{I}_{2\alpha}, \mathscr{I}_{3\alpha}, \mathscr{I}_{\sigma\alpha}, \mathscr{I}_{\sigma\sigma\alpha}, \mathscr{I}_{\sigma\alpha\alpha}),$$

where the invariants are defined by

$$\begin{aligned} &\mathscr{I}_{1\sigma} = \mathrm{Tr}\boldsymbol{\sigma}, && \mathscr{I}_{1\alpha} = \mathrm{Tr}\boldsymbol{\alpha}, && \mathscr{I}_{2\sigma} = \mathrm{Tr}(\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}), \\ &\mathscr{I}_{2\alpha} = \mathrm{Tr}(\boldsymbol{\alpha} \cdot \boldsymbol{\alpha}), && \mathscr{I}_{3\sigma} = \mathrm{Tr}(\boldsymbol{\sigma} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{\sigma}), && \mathscr{I}_{3\alpha} = \mathrm{Tr}(\boldsymbol{\alpha} \cdot \boldsymbol{\alpha} \cdot \boldsymbol{\alpha}), \\ &\mathscr{I}_{\sigma\alpha} = \mathrm{Tr}(\boldsymbol{\sigma} \cdot \boldsymbol{\alpha}), && \mathscr{I}_{\sigma\sigma\alpha} = \mathrm{Tr}(\boldsymbol{\sigma} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{\alpha}), && \mathscr{I}_{\sigma\alpha\alpha} = \mathrm{Tr}(\boldsymbol{\sigma} \cdot \boldsymbol{\alpha} \cdot \boldsymbol{\alpha}). \end{aligned}$$

For example, one among possible choices for the function f belongs to the J_2 class of yield surfaces

$$f(\boldsymbol{\sigma} - \boldsymbol{\alpha}) = \tfrac{1}{2}\mathrm{Dev}(\boldsymbol{\sigma} - \boldsymbol{\alpha}) : \mathrm{Dev}(\boldsymbol{\sigma} - \boldsymbol{\alpha}) = \tfrac{1}{2}\mathscr{I}_{2\sigma} - \mathscr{I}_{\sigma\alpha} + \tfrac{1}{2}\mathscr{I}_{2\alpha} - \tfrac{1}{6}(\mathscr{I}_{1\sigma} - \mathscr{I}_{1\alpha})^2. \tag{11}$$

By employing a consistency condition $\dot{F} = 0$ and solving for $\dot{\lambda}$ we obtain

$$\begin{aligned} \dot{\lambda} = \Lambda^{-1}\Big[\Big(&\boldsymbol{p} - \alpha_2 \boldsymbol{p} : \mathcal{S}_2 - \frac{\partial \kappa}{\partial \xi}\boldsymbol{X}_{\boldsymbol{\sigma}}\Big) : \dot{\boldsymbol{\sigma}} - \dot{\theta}\Big(\alpha_2 \boldsymbol{p} : \boldsymbol{H}_2 + \frac{\partial \kappa}{\partial \theta} + \frac{\partial \kappa}{\partial \xi} X_\theta\Big) + \\ &+ \boldsymbol{p} : \boldsymbol{\Omega}^{\alpha} : \boldsymbol{L}\Big], \quad \text{where} \quad \Lambda = \alpha_1 \boldsymbol{p} : \boldsymbol{p} + \frac{\partial \kappa}{\partial \bar{\epsilon}}\left(\tfrac{2}{3}\boldsymbol{p} : \boldsymbol{p}\right)^{1/2}, \quad \text{and} \quad \boldsymbol{p} = \frac{\partial f}{\partial \boldsymbol{\sigma}} = -\frac{\partial f}{\partial \boldsymbol{\alpha}}. \end{aligned} \tag{12}$$

Consequently, on a macroscale the rate of deformation tensor due to dislocation plasticity can be written as

$$\begin{aligned} \boldsymbol{D}_{PD} &= \boldsymbol{H}_3\,\dot{\theta} + \mathcal{S}_3\!:\dot{\boldsymbol{\sigma}} + \Lambda^{-1}\boldsymbol{p}\otimes\boldsymbol{p}\!:\boldsymbol{\Omega}^{\alpha}\!:\boldsymbol{L} = \\ &= (H_{3ij}\,\dot{\theta} + \mathcal{S}_{3ijkl}\,\dot{\sigma}_{kl} + \Lambda^{-1}p_{ij}\,p_{rs}\,\Omega^{\alpha}_{rskl}\,L_{kl})\mathbf{e}_i\mathbf{e}_j, \end{aligned} \tag{13}$$

where the constitutive tensors $\boldsymbol{H}_3$ and $\mathcal{S}_3$ are defined as

$$\begin{aligned} \boldsymbol{H}_3 &= -\Lambda^{-1}\Big\{\alpha_2 X_\theta\big[\chi_0(\boldsymbol{p}\!:\boldsymbol{I}) + \chi_1(\boldsymbol{p}\!:\mathrm{Dev}\boldsymbol{\sigma})\big] + \partial\kappa/\partial\theta + X_\theta\partial\kappa/\partial\xi\Big\}\boldsymbol{p} = \\ &= -\Lambda^{-1}\Big\{\alpha_2 X_\theta\big[\chi_0(p_{mn}\delta_{mn}) + \chi_1(p_{mn}\mathrm{Dev}\sigma_{mn})\big] + \partial\kappa/\partial\theta + X_\theta\partial\kappa/\partial\xi\Big\}p_{ij}\mathbf{e}_i\mathbf{e}_j, \\ \mathcal{S}_3 &= \Lambda^{-1}\Big\{\boldsymbol{p}\otimes\boldsymbol{p} - \big[\alpha_2\big(\chi_0(\boldsymbol{p}\!:\boldsymbol{I}) + \chi_1(\boldsymbol{p}\!:\mathrm{Dev}\boldsymbol{\sigma})\big) + \partial\kappa/\partial\xi\big]\boldsymbol{p}\otimes\boldsymbol{X}_{\boldsymbol{\sigma}}\Big\} = \\ &= \Lambda^{-1}\Big\{p_{ij}p_{kl} - \big[\alpha_2\big(\chi_0(p_{mn}\delta_{mn}) + \chi_1(p_{mn}\mathrm{Dev}\sigma_{mn})\big) + \partial\kappa/\partial\xi\big]p_{ij}X^{\sigma}_{kl}\Big\}\mathbf{e}_i\mathbf{e}_j\mathbf{e}_k\mathbf{e}_l. \end{aligned} \tag{14}$$

3. THE STRUCTURE OF CONSTITUTIVE EQUATION

By substituting expressions (4),(7) and (13) representing different parts of rate of deformation tensor into Eq. (2), after multiplying by $\mathcal{C}$ and carrying out necessary algebraic manipulations we obtain the relation

$$\dot{\boldsymbol{\sigma}} = \mathcal{L}\!:\boldsymbol{L} - \Xi\,\dot{\theta} = (\mathcal{L}_{ijkl}\,L_{kl} - \Xi_{ij}\,\dot{\theta})\mathbf{e}_i\mathbf{e}_j, \tag{15}$$

where the constitutive tensor $\mathcal{L}$ is of the form

$$\begin{aligned} \mathcal{L} &= (\mathcal{I} - \mathcal{C}\!:\sum_{A=2}^{3}\mathcal{S}_A)^{-1}\!:(\mathcal{C} - \boldsymbol{\Omega}^{\sigma} - \mathcal{X}) = \mathcal{L}_{ijkl}\mathbf{e}_i\mathbf{e}_j\mathbf{e}_k\mathbf{e}_l, \\ \mathcal{L}_{ijkl} &= (\mathcal{I}_{ijmn} - \mathcal{C}_{ijrs}\sum_{A=2}^{3}\mathcal{S}^{(A)}_{rsmn})^{-1}(\mathcal{C}_{mnkl} - \Omega^{\sigma}_{mnkl} - \mathcal{X}_{mnkl}). \end{aligned} \tag{16}$$

The tensor χ which originates from the corotational rate of the back stress is given by

$$\mathcal{X} = \Lambda^{-1}\mathcal{C}\!:\boldsymbol{p}\otimes\boldsymbol{p}\!:\boldsymbol{\Omega}^{\alpha} = (\Lambda^{-1}\mathcal{C}_{ijmn}\,p_{mn}\,p_{rs}\,\Omega^{\alpha}_{rskl})\mathbf{e}_i\mathbf{e}_j\mathbf{e}_k\mathbf{e}_l, \tag{17}$$

while the coupling between the stress rate and the temperature rate in the constitutive relation (15) is represented by the tensor Ξ

$$\begin{aligned} \Xi &= (\mathcal{I} - \mathcal{C}\!:\sum_{A=2}^{3}\mathcal{S}_A)^{-1}\!:(\mathcal{C}\!:\sum_{A=0}^{3}\boldsymbol{H}_A) = \Xi_{ij}\mathbf{e}_i\mathbf{e}_j, \\ \Xi_{ij} &= (\mathcal{I}_{ijmn} - \mathcal{C}_{ijrs}\sum_{A=2}^{3}\mathcal{S}^{(A)}_{rsmn})^{-1}(\mathcal{C}_{mnkl}\sum_{A=0}^{3}\boldsymbol{H}^{(A)}_{kl}). \end{aligned} \tag{18}$$

Equations displayed above represent a formal structure of a set of constitutive relations describing the behavior of shape memory alloys. The equations are based on an additive decomposition of the strain rate tensor. Such a decomposition will always lead to the above structure of equations providing that the evolution equations of each particular part in the decomposition (2) are of the similar form as chosen in this work. In the explicit form the part described by Eq. (16) that pertains to the velocity gradient reads

$$\begin{aligned} \mathcal{L} = {} & \ell_0\mathcal{J} + \ell_1\mathcal{K} + \ell_2\mathrm{Dev}\boldsymbol{p}\otimes\mathrm{Dev}\boldsymbol{p} + \ell_3\boldsymbol{I}\otimes\mathrm{Dev}\boldsymbol{p} + \ell_4\mathrm{Dev}\boldsymbol{p}\otimes\boldsymbol{I} + \ell_5\mathrm{Dev}\boldsymbol{\sigma}\otimes\boldsymbol{I} + \\ & + \ell_6\mathrm{Dev}\boldsymbol{\sigma}\otimes\mathrm{Dev}\boldsymbol{p} + \ell_7\mathrm{Dev}\boldsymbol{\sigma}\otimes\mathrm{Dev}\boldsymbol{X}_{\boldsymbol{\sigma}} + \ell_8\boldsymbol{I}\otimes\mathrm{Dev}\boldsymbol{X}_{\boldsymbol{\sigma}} + \ell_9\mathrm{Dev}\boldsymbol{p}\otimes\mathrm{Dev}\boldsymbol{X}_{\boldsymbol{\sigma}} + \jmath_0\boldsymbol{\Omega}^{\sigma} + \\ & + \jmath_1\boldsymbol{I}\otimes(\mathrm{Dev}\boldsymbol{\sigma}\cdot\mathrm{Dev}\boldsymbol{p} - \mathrm{Dev}\boldsymbol{p}\cdot\mathrm{Dev}\boldsymbol{\sigma}) + \jmath_2\mathrm{Dev}\boldsymbol{\sigma}\otimes(\mathrm{Dev}\boldsymbol{\sigma}\cdot\mathrm{Dev}\boldsymbol{p} - \mathrm{Dev}\boldsymbol{p}\cdot\mathrm{Dev}\boldsymbol{\sigma}) + \\ & + \jmath_3\mathrm{Dev}\boldsymbol{p}\otimes(\mathrm{Dev}\boldsymbol{\sigma}\cdot\mathrm{Dev}\boldsymbol{p} - \mathrm{Dev}\boldsymbol{p}\cdot\mathrm{Dev}\boldsymbol{\sigma}) + \jmath_4\boldsymbol{I}\otimes(\mathrm{Dev}\boldsymbol{\sigma}\cdot\mathrm{Dev}\boldsymbol{X}_{\boldsymbol{\sigma}} - \mathrm{Dev}\boldsymbol{X}_{\boldsymbol{\sigma}}\cdot\mathrm{Dev}\boldsymbol{\sigma}) + \\ & + \jmath_5\mathrm{Dev}\boldsymbol{\sigma}\otimes(\mathrm{Dev}\boldsymbol{\sigma}\cdot\mathrm{Dev}\boldsymbol{p} - \mathrm{Dev}\boldsymbol{p}\cdot\mathrm{Dev}\boldsymbol{\sigma}) + \jmath_6\mathrm{Dev}\boldsymbol{p}\otimes(\mathrm{Dev}\boldsymbol{\sigma}\cdot\mathrm{Dev}\boldsymbol{p} - \mathrm{Dev}\boldsymbol{p}\cdot\mathrm{Dev}\boldsymbol{\sigma}) + \\ & + \jmath_7\boldsymbol{I}\otimes(\mathrm{Dev}\boldsymbol{\alpha}\cdot\mathrm{Dev}\boldsymbol{p} - \mathrm{Dev}\boldsymbol{p}\cdot\mathrm{Dev}\boldsymbol{\alpha}) + \jmath_8\mathrm{Dev}\boldsymbol{\sigma}\otimes(\mathrm{Dev}\boldsymbol{\alpha}\cdot\mathrm{Dev}\boldsymbol{p} - \mathrm{Dev}\boldsymbol{p}\cdot\mathrm{Dev}\boldsymbol{\alpha}) + \\ & + \jmath_9\mathrm{Dev}\boldsymbol{p}\otimes(\mathrm{Dev}\boldsymbol{\alpha}\cdot\mathrm{Dev}\boldsymbol{p} - \mathrm{Dev}\boldsymbol{p}\cdot\mathrm{Dev}\boldsymbol{\alpha}), \end{aligned} \tag{19}$$

while Eq. (18) associated with the temperature rate term has the following form

$$\Xi = \varsigma_0 \boldsymbol{I} + \varsigma_1 \mathrm{Dev}\boldsymbol{\sigma} + \varsigma_2 \mathrm{Dev}\boldsymbol{p}. \tag{20}$$

The coefficients ℓ_K, $\jmath_K$, and ς_L form an integrity basis for the representation of constitutive tensors $\mathcal{L}$ and Ξ. The representation can be considered irreducible. Beside other material constants the coefficients of the representation depend on the mixed invariants of the tensors $\boldsymbol{p}$, $\boldsymbol{\sigma}$, and $\boldsymbol{X}_{\boldsymbol{\sigma}}$

$$\begin{aligned} \ell_K &= \ell_K(\mathscr{J}_1, \mathscr{J}_2, \mathscr{J}_3, \mathscr{J}_4, \mathscr{J}_5), \quad K = 0, \ldots, 9 \\ \jmath_K &= \jmath_K(\mathscr{J}_1, \mathscr{J}_2, \mathscr{J}_3, \mathscr{J}_4, \mathscr{J}_5), \quad K = 0, \ldots, 9 \\ \varsigma_L &= \varsigma_L(\mathscr{J}_1, \mathscr{J}_2, \mathscr{J}_3, \mathscr{J}_4, \mathscr{J}_5), \quad L = 0, \ldots, 2 \end{aligned}$$

where the invariants $\mathscr{J}_M, M = 1, \ldots, 5$ are defined as

$$\begin{aligned} &\mathscr{J}_1 = \mathrm{Tr}(\boldsymbol{X}_{\boldsymbol{\sigma}}), \quad \mathscr{J}_2 = \mathrm{Tr}(\mathrm{Dev}\boldsymbol{p} \cdot \mathrm{Dev}\boldsymbol{p}), \quad \mathscr{J}_3 = \mathrm{Tr}(\mathrm{Dev}\boldsymbol{p} \cdot \mathrm{Dev}\boldsymbol{\sigma}), \\ &\mathscr{J}_4 = \mathrm{Tr}(\mathrm{Dev}\boldsymbol{p} \cdot \mathrm{Dev}\boldsymbol{X}_{\boldsymbol{\sigma}}), \quad \mathscr{J}_5 = \mathrm{Tr}(\mathrm{Dev}\boldsymbol{\sigma} \cdot \mathrm{Dev}\boldsymbol{X}_{\boldsymbol{\sigma}}). \end{aligned} \tag{21}$$

In the derivation of (16), (17) and (18) it has been assumed that the tensor $\boldsymbol{p}$ represents the normal to the yield surface $f(\boldsymbol{\sigma} - \boldsymbol{\alpha})$ which in turn depends on the difference between the macro stress and the orientational back stress only. Moreover, for the yield surface (11) we have $\boldsymbol{p} = \mathrm{Dev}(\boldsymbol{\sigma} - \boldsymbol{\alpha})$ and the structure of (19) and (20) remains unchanged except for the slight simplifications in the coefficients ℓ_K, $\jmath_K$, ς_L, and in the invariants $\mathscr{J}_M$. If we decide not to use the corotational rates in our formulation, but material rates only, then the coefficients $\jmath_K$ drop out ($\jmath_K = 0 \; \forall \; K \in [0, 9]$), and the expression (19) simplifies significantly. Furthermore, neglecting the effect of orientational back stress, i.e. $\boldsymbol{\alpha} = \boldsymbol{0}$ so that $\mathrm{Dev}\boldsymbol{p} = \mathrm{Dev}\boldsymbol{\sigma}$, additionally simplifies the constitutive equation.

4. CONCLUDING REMARKS

In this paper we have considered a derivation and a formal structure of constitutive equations that tend to describe the material behavior of shape memory alloys. The concept of presentation was based on the classical concepts of phenomenological theory and was mainly discussed in terms of macroscopic thermoplasticity. The model presented in the paper can accommodate a variety of special models described in the literature by making appropriate adjustments among the coefficients and tensor invariants forming the equations of the model. In terms of future research the very important aspect that should be addressed is a detailed calibration and experimental characterization of the behavior of shape memory alloy under the conditions of multi–axial loading. Once such data is known and readily available, the identification of appropriate constitutive functions can be straightforward, and the theoretical modeling can make a significant progress.

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