

A. Ziólkowski

Three-dimensional phenomenological thermodynamic model of pseudoelasticity of shape memory alloys at finite strains

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Abstract The familiar small strain thermodynamic 3D theory of isotropic pseudoelasticity proposed by Raniecki and Lexcellent is generalized to account for geometrical effects. The Mandel concept of mobile isoclinic, natural reference configurations is used in order to accomplish multiplicative decomposition of total deformation gradient into elastic and phase transformation (p.t.) parts, and resulting from it the additive decomposition of Eulerian strain rate tensor. The hypoelastic rate relations of elasticity involving elastic strain rate $\underline{\mathbf{d}}^e$ are derived consistent with hyperelastic relations resulting from free energy potential. It is shown that use of Jaumann corotational rate of stress tensor in rate constitutive equations formulation proves to be convenient. The formal equation for p.t. strain rate $\underline{\mathbf{d}}^{\text{in}}$, describing p.t. deformation effects is proposed, based on experimental evidence. Phase transformation kinetics relations are presented in objective form. The field, coupled problem of thermomechanics is specified in rate weak form (rate principle of virtual work, and rate principle of heat transport). It is shown how information on the material behavior and motion inseparably enters the rate virtual work principle through the familiar bridging equation involving Eulerian rate of nominal stress tensor.

Keywords Shape memory alloys · NiTi · Pseudoelasticity · Thermoelastic martensitic transformation · Thermodynamic SMA constitutive model · Finite deformations · Hyperelastic–hypoelastic equivalence · Bridging equation · Coupled thermomechanics

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Abbreviations

p.t. phase transition
SMA shape memory alloys
i.n.s. instantaneous natural state

Notations

$$\underline{\mathbf{A}}\underline{\mathbf{B}} = A_{ijkl}B_{kl}\underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j, \quad \underline{\mathbf{A}}\underline{\mathbf{B}} = A_{ij}B_{jk}\underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_k, \quad \underline{\mathbf{1}} = \delta_{ij}\underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j, \\ \underline{\mathbf{I}}^{4s} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \otimes \underline{\mathbf{e}}_k \otimes \underline{\mathbf{e}}_l, \quad \text{tr}(\underline{\mathbf{A}}) = A_{ii}, \quad \underline{\mathbf{A}} \cdot \underline{\mathbf{B}} = \text{tr}(\underline{\mathbf{A}}\underline{\mathbf{B}}^T) = A_{ij}B_{ij}$$

1 Introduction

Special properties of so-called shape memory alloys (SMA) have resulted in a constantly growing number of structures and devices exploiting them; see Otsuka and Kakeshita [15] for a recent survey of application

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A. Ziólkowski
Institute of Fundamental Technological Research, Polish Academy of Sciences, Swietokrzyska 21, 00-049 Warsaw, Poland
E-mail: aziolk@ippt.gov.pl

areas. Devices containing elements made of SMA typically undergo moderate deformations not exceeding several percent during nominal operation; also typically they can undergo large rotations. These engineering conditions call for development of the SMA constitutive model, taking into account geometrical effects.

Extensive literature on constitutive modeling of SMA exists at present. The constitutive models of SMA available in the literature evolved from the prevailing one-dimensional models of the early 1990s to the three-dimensional thermodynamic models dominating at the turn of the century. The majority of the current 3D macroscopic constitutive models of SMA embrace the pseudoelastic range of SMA alloy behaviors and are usually written in small deformations formalism. A schematic map of the range of parameters in which various shape memory effects dominate is drawn in Fig. 1.

The interested reader can obtain information on different macroscopic models of polycrystalline SMA materials and their approaches, as well as advantages and drawbacks, from a very recent, broad, review paper by Lagoudas et al. [8]. Here in the context of taking into account geometrical effects, we shall mention the model of Auricchio and Taylor [1], as apparently it is the first macroscopic constitutive model of SMA written consistently in large deformations formalism. Closer analysis of mathematical expressions of the Auricchio and Taylor's model indicates that in the limit of small strains theory and disregarding the influence of the first stress invariant (pressure) on pseudoelastic flow criterion, the model constitutes a purely thermo-mechanical, special case of Raniecki and Lexcelent [20] in their model formulation from 1994. Taking into account pressure effects seems not to be of primary importance in view of experimental information available in literature that dilatational effects resulting from thermoelastic martensitic transformation responsible for shape memory effects are usually limited to 0.2%, see, e.g., Otsuka and Ren [16]. Besides formal mathematical identity of Auricchio, Taylor and the special case of Raniecki, Lexcelent models, the former one possesses essential deficiencies when aimed at modeling SMA materials behavior, resulting from generic origins of the concepts used in this model—namely generalized plasticity theory. The generalized plasticity theory aims at describing macroscopically physical mechanism of plastic slip—which involves microscopic scale of observation discontinuous displacement field. In contrast, the shape memory effects exhibited by SMA materials rely on the underlying physical mechanism of twinning, which involves a continuous microscopic displacement field. One of the consequences of this difference is that on the macroscopic scale of observation, microscopic coherency of the displacement field requires, in general, the presence of some energy term in macroscopic free energy potential—the so-called coherency energy. Without having some idea on how to explicitly describe coherency energy, it is impossible to evaluate reasonably in modeling terms thermal effects connected with martensitic transformation, for example to separate latent heat of martensitic transformation from dissipation of work. Auricchio and Taylor in their model from 1997 do not deliver any information on thermal effects, and in the present author opinion generalized plasticity concepts cannot help in view of the argumentation presented above. Concepts of non-equilibrium thermodynamics of phase transitions are necessary. Apparently the first complete, 3D phenomenological, thermodynamic, macroscopic theory of pseudoelasticity—model R_L was developed by Raniecki et al. [19]. Complete in the sense that it contained all elements enabling description of the most important effects connected with the phenomenon of pseudoelasticity, i.e., explicit form of free energy function, criteria determining when active forward or reverse phase transformation can take place, equations of phase transformation (p.t.) kinetics embracing description of internal hysteresis loops formation, evolution relations of p.t. strains enabling description of strain effects resulting from formation and reorienta-

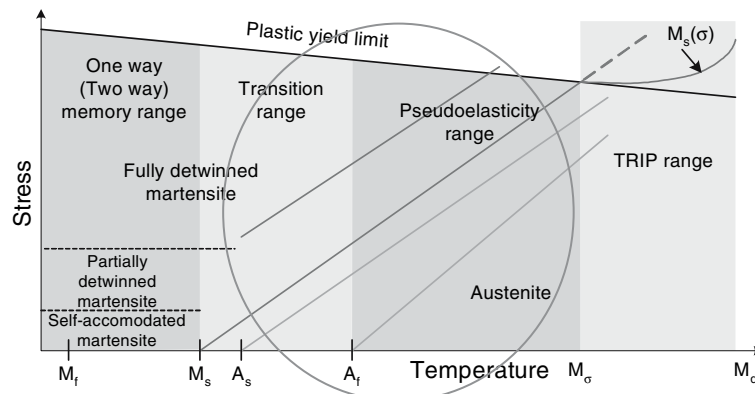


Fig. 1 Schematic map of range of parameters in which various shape memory effects dominate

tion of martensitic phase. The model was subsequently extended in the years 1994 [20] (to cover the case when austenitic and martensitic phase have different thermoelastic properties) and in 1998 [21] (to enable description of strength differential effect (SD) exhibited by SMA materials) i.e., the phenomenon of critical pseudoelastic flow stress dependence on the direction of stress tensor. Müller and Bruhns undertook very recently an effort to extend the 1992 version of the model R_L to take into account geometrical effects, cf. paper [12] from 2006. For that purpose they postulate additive decomposition of the Eulerian strain rate tensor into elastic and phase transformation part, but not multiplicative decomposition of deformation gradient, clearly trying to avoid explicit specification of evolution rule for inelastic spin. As a result these authors finally reach a very special rate constitutive equation of elasticity involving elastic stretching rate and corotational logarithmic derivative of Kirchoff stress— $\overset{\circ}{\boldsymbol{\tau}} = \underline{\mathbf{C}}_0 [\underline{\mathbf{d}}^e - \underline{\boldsymbol{\alpha}}_0 \dot{T}]$, cf. (88) in [12]. The rate relation effectively leads implicitly to a very special dependence of instantaneous elastic properties of SMA material on inelastic deformation state, connected with phase transition. This conclusion can be reached when one observes that logarithmic spin depends on the state of inelastic deformation—total principal stretches λ_i embrace p.t. principal stretches λ_i^{in} , cf. (A1), (A3). The above is inconsistent with the non-rate constitutive relation of elasticity (57), postulated in [12] (identical with relation (24) of the present paper upon substitution $\underline{\mathbf{L}} = \underline{\mathbf{C}}_0 = \text{const}$), where elastic properties do not depend on inelastic deformation state.

In the present work enhanced by Raniecki and Lexcelent, a version of model R_L [20,21] is extended into the large deformations regime, allowing one to model the SD effect in a large deformation regime. For that purpose the concept of multiplicative decomposition of the total deformation gradient is used together with the concept of a family of virtual, isoclinic, unloaded elastically configurations serving as reference configurations for description of elastic deformation—Mandel formalism¹ [10]. The Lagrangian logarithmic elastic strain tensor, temperature and mass fraction of martensitic phase $\{\underline{\mathbf{E}}^e, T, z\}$ are used as a set of state parameters entering macroscopic free energy function describing two-phase states of SMA macroelement in mobile Lagrangian description. The set $\{\underline{\mathbf{e}}^e, T, z\}$ of state parameters in Eulerian description corresponds to the set $\{\underline{\mathbf{E}}^e, T, z\}$, where $\underline{\mathbf{e}}^e$ denotes spatial logarithmic (Hencky) elastic strain. The state equations of thermoelasticity are obtained by formal differentiation of free energy potential in accordance with the formalism of thermodynamics. In order to describe deformation effects connected with martensitic phase transition or/and martensitic phase reorientation, the equation of pseudoelastic flow law for Eulerian inelastic strain rate $\underline{\mathbf{d}}^{\text{in}}$ is proposed. The formal equations of p.t. kinetics and criteria for active forward and reverse transformation are specified in the objective form, i.e., invariant with respect to rigid body rotations when expressed on actual configuration. Rate constitutive relations of elasticity are formulated in Eulerian description using Zaremba–Jaumann elastic corotational rate of Kirchoff stress in view of favorable properties of this particular rate. Selection of family of unloaded elastically reference isoclinic configurations by accepting assumption that inelastic Eulerian spin $\underline{\boldsymbol{\omega}}^{\text{in}}$ is identically equal to zero leads to considerable simplification of mathematical formulation of the proposed SMA materials model. It is shown how information on the material behavior and motion inseparably enters a global weak form of rate mechanical balance equation through a familiar bridging equation involving the Eulerian rate of the nominal stress tensor.

The proposed 3D phenomenological macroscopic model of SMA allows in a comprehensive way for quantitative description of their pseudoelastic behavior, taking into account geometrical effects resulting from finite deformations. As the model is developed within non-equilibrium thermodynamics formalism in a natural manner, it allows for prediction of coupled mechanical-thermal and phase transformation progress effects. The presently developed model upon its implementation into finite element code is very well suited for performing engineering design computations of structures containing elements made of SMA in analyzing situations when large rotations of structural elements appear during nominal operating conditions, or in analyzing emergency situations when also large strains may appear.

2 Kinematics relations at finite deformations

Consider a polycrystalline body B made of shape memory alloy occupying at a certain time instant t_0 configuration 0B , see Fig. 2.

The body B undergoes motion $\underline{\mathbf{x}}(\underline{\mathbf{X}}, t)$ due to applied thermo-mechanical loads, and it takes at the generic time instant t of a process actual, deformed configuration tB . For the purposes of building macroscopic

¹ The term Mandel formalism (description) is used interchangeably with the term mobile Lagrangian description, and they are synonymous here.

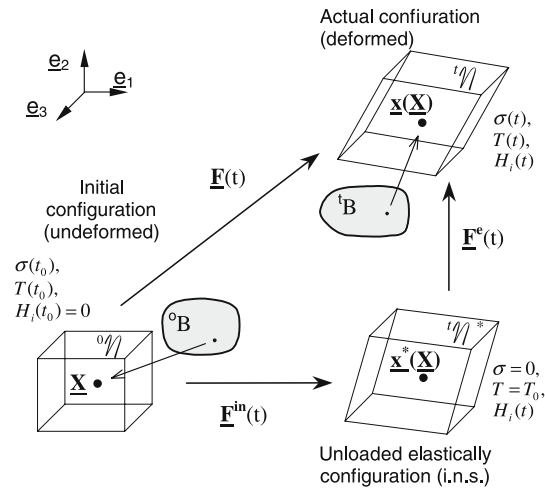


Fig. 2 Schematic illustration of configurations involved in the concept of multiplicative decomposition of total deformation gradient

constitutive model of SMA, it is assumed that in the neighborhood of an arbitrary material point remaining at initial position $\underline{\mathbf{X}}$ in initial configuration 0B there can be distinguished a macroelement, so-called representative volume element (RVE). The RVE must be large enough to grasp essential microstructural features of the investigated material and small enough in comparison to the characteristic dimension of the engineering structure for description of which the present model is to be employed, that fields in RVE volume could be treated as homogeneous. The macroelement at location $\underline{\mathbf{X}}$ in initially undeformed configuration is symbolically represented with hexahedron in Fig. 2. The macroelement undergoes deformation as a result of applied external loadings and at instant t takes the location $\underline{\mathbf{x}}(\underline{\mathbf{X}}, t)$. In the sequel, the deformation gradient $\underline{\mathbf{F}} = \partial \underline{\mathbf{x}} / \partial \underline{\mathbf{X}}$ is taken as homogeneous within the volume of RVE at all time instants of deformation process. More precise definition and discussion of the RVE concept can be found in the book by Nemat-Naser and Hori [13]. It is known that shape memory alloys, when loaded thermomechanically, can undergo forward or reverse martensitic p.t., which results in two-phase SMA macroelement microstructure. The inelastic deformation effects are connected with martensitic phase transition and with macroelement microstructure evolution, e.g., reorientation of martensitic variants. In the macroscopic model of SMA developed in the present work inelastic, “phase” deformation effects are described with the aid of two macroscopic parameters z —volume fraction of martensitic phase, and $\underline{\boldsymbol{\kappa}}$ —isotropic tensor function of a certain number of scalar internal parameters H_i characterizing microstructure of the macroelement. Parameter z characterizes advancement of phase transition, while parameter $\underline{\boldsymbol{\kappa}}$ called macroscopic tensor of phase eigenstrains characterizes phase transition deformation effects. Similarly like in the case of model R_L it is adopted conjecture that SMA macroelement always tends to reach thermodynamic microstructural equilibrium, i.e., its microstructure “exhibits tendency to adapt to changing external loading”. In the case of small deformations Raniecki and Lexcellent [20, 21] formally showed that in states of thermodynamic microstructural equilibrium $H_i = H_i^{\text{eq}}$, the free energy reaches minimum with respect to internal state parameters H_i . As a consequence requirement of “optimal adaptation of microstructure” led these authors to the conclusion that tensor $\underline{\boldsymbol{\kappa}}(H_i)$ in states of microstructural equilibrium ($H_i = H_i^{\text{eq}}$) must be certain function of macroscopic state parameters— $\underline{\boldsymbol{\kappa}}(H_i^{\text{eq}}) = \underline{\boldsymbol{\kappa}}^{\text{eq}}(H_i^{\text{eq}}(\underline{\boldsymbol{\sigma}}, T)) = \underline{\boldsymbol{\kappa}}^{\text{eq}}(\underline{\boldsymbol{\sigma}}, T)$. In the present work, accepting similar argumentation as in small deformations theory, without formal proof, it is adopted that tensor $\underline{\boldsymbol{\kappa}}$ is a function of external state parameters ($\underline{\boldsymbol{\sigma}}, T$) through equilibrium values of internal state parameters $H_i = H_i^{\text{eq}}$. Hence, it is assumed that also in the case of finite deformations microstructure of SMA macroelement optimally adapts to the external thermo-mechanical loading. It is also assumed, like in small deformations theory, that there exists inelastic potential $g^{\text{ph}}(\underline{\boldsymbol{\sigma}}, T)$, which generates tensor $\underline{\boldsymbol{\kappa}}$.

In order to properly describe inelastic deformation effects connected with phase transition, it is convenient to introduce known concept of virtual, unloaded elastically, instantaneous, “natural” reference configurations. The instantaneous, natural configuration is the kind of configuration that would be attained by SMA macroelement (a material point neighborhood) at particular time instant t , had the surface tractions $\underline{\mathbf{t}}_n$ been momentarily reduced to zero ($\underline{\boldsymbol{\sigma}} = \mathbf{0}$) and temperature had been brought to temperature $T = T_0$, where T_0 denotes certain fixed reference temperature—while keeping the internal microstructure of the macroelement fixed, “frozen”, i.e., va-

lues of set of internal parameters characterizing microstructure would be kept constant during elastic unloading process $z = \text{const}$, ($H_i = \text{const}$) \Leftrightarrow ($\kappa = \text{const}$). The natural configuration at time t is symbolically marked ${}^t\mathbf{N}^*$ in Fig. 2. State of macroelement (RVE) remaining in described above virtual, unloaded elastically configuration would be called instantaneous, natural state, where ($\boldsymbol{\sigma} = \mathbf{0}$, $T = T_0$, $z = \text{const}$, $H_i = \text{const}$). The concept of natural states is useful when building a macroscopic model of shape memory alloys valid at finite strains. It allows one to conveniently uncouple effects of elastic deformation from inelastic one—here connected with martensitic p.t. or possible evolution of two-phase, martensitic microstructure. The modeling approach is that instead of investigating the real deformation process of SMA macroelement when simultaneously elastic and inelastic deformations take place, there is investigated virtual pure inelastic deformation process from initial configuration to instantaneous natural configuration ${}^0\mathbf{N} \rightarrow {}^t\mathbf{N}^*$ —described by deformation gradient $\underline{\mathbf{F}}^{\text{in}}$, and next virtual pure elastic deformation from natural configuration to actual configuration ${}^t\mathbf{N}^* \rightarrow {}^t\mathbf{N}$ —described with deformation gradient $\underline{\mathbf{F}}^{\text{e}}$. Effectively in this way deformation is obtained from initial configuration to actual one ${}^0\mathbf{N} \rightarrow {}^t\mathbf{N}$ —described by actual deformation gradient $\underline{\mathbf{F}}$. This construction leads to the known concept of multiplicative decomposition of total deformation gradient

$$\underline{\mathbf{F}} = \underline{\mathbf{F}}^{\text{e}} \underline{\mathbf{F}}^{\text{in}}. \quad (1)$$

Variables in time configurations ${}^t\mathbf{N}^*$ constitute convenient reference configurations for operational definition of elastic deformation. Even when configuration ${}^t\mathbf{N}^*$ is already fixed still, there remains freedom in selection of particular measure of elastic deformation. Knowledge of elastic deformation gradient allows for determination of the value of elastic strain tensor—the state parameter appearing in free energy thermodynamic potential—and hence providing a convenient description of elastic branch of material behavior. In accordance with its definition, any natural configuration ${}^t\mathbf{N}^*$ defining tensor $\underline{\mathbf{F}}^{\text{e}}$ must be a stress-free configuration which imposes constraints on its selection but still orientation of the configuration ${}^t\mathbf{N}^*$ with respect to the fixed laboratory coordinates frame can be selected at free will. Freedom in selection of orientation of natural configurations ${}^t\mathbf{N}^*$ finds its reflection in non-uniqueness of multiplicative decomposition of deformation gradient into elastic and inelastic part. Premises of the physical nature may predetermine selection of specific orientation of natural configuration with respect to laboratory coordinates frame, like it is in the case of crystallographic theory of plasticity. Then such orientation is an element of constitutive model. Alternatively, if premises of physical nature for selection of natural configuration orientation are non-existent, as in the case of a macroscopic isotropic model of material behavior, then specific selection of orientation is dictated by the strive to obtain mathematical simplicity in material behavior description. The constraint equation determining uniquely family of natural configurations for developed here model of SMA materials is delivered in Sect. 4.2. The multiplicative decomposition of total deformation gradient (1) leads to the following known kinematical relations:

$$\underline{\mathbf{L}} = \partial \underline{\mathbf{v}} / \partial \underline{\mathbf{x}} = \dot{\underline{\mathbf{F}}} \underline{\mathbf{F}}^{-1} = \underline{\mathbf{L}}^{\text{e}} + \underline{\mathbf{L}}^{\text{in}}, \quad \underline{\mathbf{L}}^{\text{e}} = \dot{\underline{\mathbf{F}}}^{\text{e}} \underline{\mathbf{F}}^{\text{e}-1}, \quad \underline{\mathbf{L}}^{\text{in}} = \underline{\mathbf{F}}^{\text{e}} \underline{\mathbf{L}}^* \underline{\mathbf{F}}^{\text{e}-1}, \quad \underline{\mathbf{L}}^* = \dot{\underline{\mathbf{F}}}^{\text{in}} \underline{\mathbf{F}}^{\text{in}-1}, \quad (2)$$

$$\underline{\mathbf{d}} = \frac{1}{2} \left[\underline{\mathbf{L}} + \underline{\mathbf{L}}^T \right] = \underline{\mathbf{d}}^{\text{e}} + \underline{\mathbf{d}}^{\text{in}}, \quad \underline{\mathbf{d}}^{\text{e}} = \frac{1}{2} \left[\underline{\mathbf{L}}^{\text{e}} + \underline{\mathbf{L}}^{\text{e}T} \right], \quad \underline{\mathbf{d}}^{\text{in}} = \frac{1}{2} \left[\underline{\mathbf{L}}^{\text{in}} + \underline{\mathbf{L}}^{\text{in}T} \right], \quad \underline{\mathbf{D}}^* = \frac{1}{2} \left[\underline{\mathbf{L}}^* + \underline{\mathbf{L}}^{*T} \right], \quad (3)$$

$$\underline{\boldsymbol{\omega}} = \frac{1}{2} \left[\underline{\mathbf{L}} - \underline{\mathbf{L}}^T \right] = \underline{\boldsymbol{\omega}}^{\text{e}} + \underline{\boldsymbol{\omega}}^{\text{in}}, \quad \underline{\boldsymbol{\omega}}^{\text{e}} = \frac{1}{2} \left[\underline{\mathbf{L}}^{\text{e}} - \underline{\mathbf{L}}^{\text{e}T} \right], \quad \underline{\boldsymbol{\omega}}^{\text{in}} = \frac{1}{2} \left[\underline{\mathbf{L}}^{\text{in}} - \underline{\mathbf{L}}^{\text{in}T} \right], \quad \underline{\boldsymbol{\Omega}}^* = \frac{1}{2} \left[\underline{\mathbf{L}}^* - \underline{\mathbf{L}}^{*T} \right], \quad (4)$$

where $\underline{\mathbf{L}}$ denotes velocity gradient tensor, $\underline{\mathbf{d}}$ is Eulerian strain rate tensor and $\underline{\boldsymbol{\omega}}$ is material spin (vorticity) tensor. Superscripts denote objects connected with respective type of deformation—“e” purely elastic, “in” elastic–inelastic, “*” purely inelastic (here phase transformation/martensitic phase reorientation).

3 Elastically isotropic SMA alloys

3.1 State variables

It is assumed here that two-phase macroelement (RVE) of shape memory alloy is a thermodynamic system remaining in constrained thermodynamic equilibrium at any two-phase stage of deformation process similarly

like in the case of small deformations theory, cf. [21]. The experimental evidence shows that polycrystalline shape memory alloys with good accuracy can be treated as elastically isotropic, i.e., their elastic properties do not depend on orientation in space—cf., e.g., Chap. 5 in [27]. As a consequence it is adopted here that free energy potential ϕ for these materials is a scalar function isotropic with respect to its canonic arguments—parameters of state. The elastic logarithmic strain $\underline{\mathbf{E}}^e$, temperature T and volume fraction of martensitic phase z are adopted as variables characterizing thermodynamic state of SMA macroelement— $\{\underline{\mathbf{E}}^e, T, z\}$. In mobile Lagrangian description elastic logarithmic strain is expressible with tensor $\underline{\mathbf{U}}^e$, while in Eulerian description, it is expressible with tensor $\underline{\mathbf{V}}^e$, as follows:

$$\begin{aligned} \underline{\mathbf{E}}^e &= \ln(\underline{\mathbf{U}}^e) = \sum E_i^e \underline{\mathbf{N}}_i^e \otimes \underline{\mathbf{N}}_i^e, \quad \underline{\mathbf{e}}^e = \ln(\underline{\mathbf{V}}^e) = \sum e_i^e \underline{\mathbf{n}}_i^e \otimes \underline{\mathbf{n}}_i^e, \quad e_i^e = \ln(\lambda_i^e) = E_i^e, \\ \underline{\mathbf{e}}^e &= \underline{\mathbf{R}}^e \underline{\mathbf{E}}^e (\underline{\mathbf{R}}^e)^T, \\ \underline{\mathbf{E}}^e &= \sum \bar{E}_i^e \underline{\mathbf{N}}_i^e \otimes \underline{\mathbf{N}}_i^e = \underline{\mathbf{E}}^e - \frac{1}{3} \text{tr}(\underline{\mathbf{E}}^e) \underline{\mathbf{I}}, \quad \text{tr}(\underline{\mathbf{E}}^e) = \ln(J^e), \quad J^e \equiv \det(\underline{\mathbf{F}}^e) = \rho^*/\rho = \lambda_1^e \lambda_2^e \lambda_3^e, \end{aligned} \quad (5)$$

where the positive definite, symmetric tensors $\underline{\mathbf{U}}^e, \underline{\mathbf{V}}^e$ are right and left elastic stretch tensors, respectively ($\underline{\mathbf{F}}^e = \underline{\mathbf{R}}^e \underline{\mathbf{U}}^e = \underline{\mathbf{V}}^e \underline{\mathbf{R}}^e$). The scalars λ_i^e are common for them principal elastic stretches, $\underline{\mathbf{N}}_i^e$ and $\underline{\mathbf{n}}_i^e$ are Lagrangian (material) and Eulerian (spatial) principal directions of elastic stretch tensors $\underline{\mathbf{U}}^e$ and $\underline{\mathbf{V}}^e$. The symbol $\underline{\mathbf{E}}^e$ denotes a deviator of logarithmic elastic strain ($\bar{E}_1^e + \bar{E}_2^e + \bar{E}_3^e = 0$), ρ denotes density in the actual configuration and ρ^* density in stress free, natural configuration. Principal directions vectors $\underline{\mathbf{N}}_i^e$ can be rotated to principal directions $\underline{\mathbf{n}}_i^e$ with the aid of the rotation tensor $\underline{\mathbf{R}}^e$ ($\underline{\mathbf{n}}_i^e = \underline{\mathbf{R}}^e \underline{\mathbf{N}}_i^e, \underline{\mathbf{R}}^e = \underline{\mathbf{n}}_i^e \otimes \underline{\mathbf{N}}_i^e$). The logarithmic elastic strain measure $\underline{\mathbf{E}}^e$ was selected as a state variable in view of its known, valuable property (among others) that of having a spherical part that describes the purely dilatational deformation of a material element, while its deviatoric part describes the purely non-dilatational deformation at large deformations.

In the course of elastic deformation of macroelement the power of elastic work per unit of mass of the deforming material \dot{w}_e can be expressed as follows (regardless of any symmetry of a material constitutive rule)

$$\rho^0 \dot{w}_e = \text{tr}(\underline{\boldsymbol{\tau}} \underline{\mathbf{d}}^e), \quad \underline{\boldsymbol{\tau}} \equiv J \underline{\boldsymbol{\sigma}}, \quad \underline{\boldsymbol{\tau}} = \Sigma \tau_{ij} \underline{\mathbf{n}}_i^e \otimes \underline{\mathbf{n}}_j^e, \quad \underline{\mathbf{d}}^e = \Sigma d_{ij}^e \underline{\mathbf{n}}_i^e \otimes \underline{\mathbf{n}}_j^e, \quad J \equiv \det(\underline{\mathbf{F}}) = \rho^0/\rho, \quad (6)$$

where $\underline{\boldsymbol{\tau}}$ denotes classical Kirchoff stress, $\underline{\boldsymbol{\sigma}}$ is Cauchy stress, $\underline{\mathbf{d}}^e$ is elastic part of stretching—cf. (3)₂, ρ^0 denotes density in initial configuration. It is straightforward to show that the following relation is valid

$$\rho^0 \dot{w}_e = \text{tr}(\underline{\boldsymbol{\tau}} \underline{\mathbf{d}}^e) = \text{tr} \left(\begin{matrix} T \\ \underline{\mathbf{R}}^e \underline{\boldsymbol{\tau}} \underline{\mathbf{R}}^e \end{matrix} \begin{matrix} T \\ \underline{\mathbf{R}}^e \underline{\mathbf{d}}^e \underline{\mathbf{R}}^e \end{matrix} \right) = \text{tr}(\underline{\mathbf{T}}^{\text{Re}} \underline{\mathbf{D}}^e), \quad (7)$$

$$\underline{\mathbf{T}}^{\text{Re}} \equiv \begin{matrix} T \\ \underline{\mathbf{R}}^e \underline{\boldsymbol{\tau}} \underline{\mathbf{R}}^e \end{matrix}, \quad \underline{\mathbf{T}}^{\text{Re}} = T_{ij}^{\text{Re}} \underline{\mathbf{N}}_i^e \otimes \underline{\mathbf{N}}_j^e, \quad \underline{\mathbf{D}}^e \equiv \begin{matrix} T \\ \underline{\mathbf{R}}^e \underline{\mathbf{d}}^e \underline{\mathbf{R}}^e \end{matrix}, \quad \underline{\mathbf{D}}^e = \Sigma D_{ij}^e \underline{\mathbf{N}}_i^e \otimes \underline{\mathbf{N}}_j^e,$$

where $\underline{\mathbf{T}}^{\text{Re}}$ denotes “rotated” elastically Kirchoff stress tensor, and $\underline{\mathbf{D}}^e$ is rotated elastically Eulerian elastic strain rate.

Hill [6], using total Lagrangian description, introduced the concept of stress measures $\underline{\mathbf{T}}(n)$ work conjugate to a class of Lagrangian total strain measures $\underline{\mathbf{E}}(n)$ —defined on total stretch tensor $\underline{\mathbf{U}}(\underline{\mathbf{F}} = \underline{\mathbf{R}}\underline{\mathbf{U}})$. In this he relied on the presumption that the power of total work in the deformation process cannot depend on the way of its description—remains invariant under change of the strain measure. Adopting the presumption that also the power of elastic work in the deformation process cannot depend on the way of its description, it is used here the concept of stress measure $\underline{\mathbf{T}}^e$ elastic work conjugate to Lagrangian logarithmic elastic strain $\underline{\mathbf{E}}^e$, according to the definition

$$\rho^0 \dot{w}_e = \text{tr}(\underline{\mathbf{T}}^e \dot{\underline{\mathbf{E}}}^e), \quad \underline{\mathbf{T}}^e = T_{ij}^e \underline{\mathbf{N}}_i^e \otimes \underline{\mathbf{N}}_j^e, \quad (8)$$

here $\dot{\underline{\mathbf{E}}}^e$ denotes the usual material derivative of Lagrangian logarithmic elastic strain—cf. (5)₁, and $\underline{\mathbf{T}}^e$ is the stress measure elastic work conjugate to $\underline{\mathbf{E}}^e$.

When material is isotropic elastically, i.e., its elastic properties do not depend on orientation in space, then constitutive relation in Lagrangian description linking tensors $\underline{\mathbf{T}}^e$ and $\underline{\mathbf{E}}^e$, and corresponding relation in Eulerian description linking tensors $\underline{\boldsymbol{\tau}}$ and $\underline{\mathbf{e}}^e$ must be isotropic tensor functions.² Hence, then tensor $\underline{\mathbf{T}}^e$ must

² Isotropic tensor function $\chi(\underline{\mathbf{T}})$ of tensorial argument $\underline{\mathbf{T}}$ by definition fulfills the relation $\chi(\underline{\mathbf{Q}}\underline{\mathbf{T}}\underline{\mathbf{Q}}^T) = \underline{\mathbf{Q}}\chi(\underline{\mathbf{T}})\underline{\mathbf{Q}}^T$ for all proper orthogonal tensors $\underline{\mathbf{Q}}$.

have principal directions $\underline{\mathbf{N}}_i^e$ and it commutes with tensor $\underline{\mathbf{U}}^e$, while the Kirchoff stress $\underline{\boldsymbol{\tau}}$ (Cauchy stress $\underline{\boldsymbol{\sigma}}$) must have principal directions $\underline{\mathbf{n}}_i^e$, and it commutes with tensor $\underline{\mathbf{V}}^e$

$$\begin{aligned} \underline{\mathbf{T}}^e &= \Sigma T_i^e \underline{\mathbf{N}}_i^e \otimes \underline{\mathbf{N}}_i^e, \quad \underline{\mathbf{T}}^e \underline{\mathbf{U}}^e = \underline{\mathbf{U}}^e \underline{\mathbf{T}}^e, \quad \underline{\mathbf{T}}^e \underline{\mathbf{E}}^e = \underline{\mathbf{E}}^e \underline{\mathbf{T}}^e, \\ \underline{\boldsymbol{\tau}} &= \Sigma \tau_i \underline{\mathbf{n}}_i^e \otimes \underline{\mathbf{n}}_i^e, \quad \underline{\boldsymbol{\tau}} \underline{\mathbf{V}}^e = \underline{\mathbf{V}}^e \underline{\boldsymbol{\tau}}, \quad \underline{\boldsymbol{\tau}} \underline{\mathbf{e}}^e = \underline{\mathbf{e}}^e \underline{\boldsymbol{\tau}}. \end{aligned} \tag{9}$$

Formal proof of these statements can be found in many manuals, see, e.g., monograph by Ogden [14]. It was shown by Raniecki and Nguyen [18] that for isotropic elastically materials, the stress tensor $\underline{\mathbf{T}}^e$ elastic work conjugate to the elastic logarithmic strain $\underline{\mathbf{E}}^e$ is simply equal to “rotated” elastically Kirchoff stress tensor $\underline{\mathbf{T}}^{Re}$

$$\underline{\mathbf{T}}^e = \underline{\mathbf{T}}^{Re}, \quad \underline{\mathbf{T}}^{Re} = T_i^{Re} \underline{\mathbf{N}}_i^e \otimes \underline{\mathbf{N}}_i^e, \quad T_i^{Re} = \tau_i, \quad \underline{\mathbf{T}}^{Re} \underline{\mathbf{U}}^e = \underline{\mathbf{U}}^e \underline{\mathbf{T}}^{Re}. \tag{10}$$

3.2 Equations of state

Let us assume that free energy potential of isotropic elastically SMA alloy is known—not specifying it explicitly at present. Then ϕ must be isotropic scalar function with respect to each of its canonic arguments, i.e., state parameters $\{\underline{\mathbf{E}}^e, T, z\}$ in mobile Lagrangian description or equivalently $\{\underline{\mathbf{e}}^e, T, z\}$ in Eulerian description. The Gibbs fundamental equation of state—delivering operational definition of entropy, expressing total differential of free energy potential $\phi(\underline{\mathbf{E}}^e, T, z)$ takes the following form:

$$\begin{aligned} \dot{\phi} &= -s \dot{T} + \dot{w}_0, \\ \dot{w}_0 &= \text{tr}(\underline{\mathbf{T}}^{Re} \dot{\underline{\mathbf{E}}^e}) / \rho^0 - \pi_1 \dot{z}, \quad \dot{w}_0 = \text{tr}(\underline{\boldsymbol{\tau}} \dot{\underline{\mathbf{e}}^e}) / \rho^0 - \pi_1 \dot{z}, \quad \dot{w}_0 = \text{tr}(\underline{\boldsymbol{\tau}} \dot{\underline{\mathbf{d}}^e}) / \rho^0 - \pi_1 \dot{z} \text{ [J/kg]}, \end{aligned} \tag{11}$$

where s denotes specific entropy per unit of mass, π_1 is the thermodynamic driving force of martensitic p.t. at a stress-free state, \dot{w}_0 is specific power of work per unit of mass, which would have to be performed over macroelement in thermodynamically reversible process equivalent to the real one. Formula (11)₂ expresses power of reversible work \dot{w}_0 in Mandel description (mobile, natural, reference configuration), while formula (11)₃ expresses \dot{w}_0 in Eulerian description (actual configuration), the (11)₄ results from (11)₂ and (7), (8).

The following equations of state for a macroelement made of isotropic elastically SMA material are obtained in states of constrained thermodynamic equilibrium in mobile Lagrangian description

$$\begin{aligned} \underline{\mathbf{T}}^{Re} &= \rho^0 \frac{\partial \phi(\underline{\mathbf{E}}^e, T, z)}{\partial \underline{\mathbf{E}}^e}, \quad s = -\frac{\partial \phi(\underline{\mathbf{E}}^e, T, z)}{\partial T}, \quad \pi_1 = -\frac{\partial \phi(\underline{\mathbf{E}}^e, T, z)}{\partial z}, \\ \dot{\phi} &= (\partial \phi / \partial \underline{\mathbf{E}}^e) \dot{\underline{\mathbf{E}}^e} + (\partial \phi / \partial T) \dot{T} + (\partial \phi / \partial z) \dot{z}. \end{aligned} \tag{12}$$

The function ϕ is isotropic by assumption; hence its mathematical form does not change after expressing it in variables $\{\underline{\mathbf{e}}^e, T, z\}$, as tensors $\underline{\mathbf{E}}^e$ and $\underline{\mathbf{e}}^e$ differ only by rotation—cf. (5)₄. Due to this property counterpart of (12) in the Eulerian description for SMA alloy isotropic, with respect to elastic properties, can be immediately obtained

$$\underline{\boldsymbol{\tau}} \equiv \rho^0 \frac{\partial \phi(\underline{\mathbf{e}}^e, T, z)}{\partial \underline{\mathbf{e}}^e}, \quad s \equiv -\frac{\partial \phi(\underline{\mathbf{e}}^e, T, z)}{\partial T}, \quad \pi_1 \equiv -\frac{\partial \phi(\underline{\mathbf{e}}^e, T, z)}{\partial z}. \tag{13}$$

The collinearity of respective pairs of tensors $\underline{\boldsymbol{\tau}}, \underline{\mathbf{e}}^e$ and $\underline{\mathbf{T}}^{Re}, \underline{\mathbf{E}}^e$ —cf. (9), (10), lead to the conclusion that functional relations $\underline{\boldsymbol{\tau}} = \underline{\boldsymbol{\tau}}(\underline{\mathbf{e}}^e)$, $\underline{\mathbf{T}}^{Re} = \underline{\mathbf{T}}^{Re}(\underline{\mathbf{E}}^e)$ must be isotropic tensor valued functions of tensorial argument. The known property³ of such functions leads to the following formulae if conditions of their differentiability are fulfilled

$$\begin{aligned} (\partial \underline{\boldsymbol{\tau}} / \partial \underline{\mathbf{e}}^e) [\underline{\mathbf{e}}^e \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\mathbf{e}}^e] &= [\underline{\boldsymbol{\tau}} \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\boldsymbol{\tau}}], \\ (\partial \underline{\mathbf{T}}^{Re} / \partial \underline{\mathbf{E}}^e) [\underline{\mathbf{E}}^e \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\mathbf{E}}^e] &= [\underline{\mathbf{T}}^{Re} \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\mathbf{T}}^{Re}] \end{aligned} \tag{14}$$

for any spin tensor $\underline{\boldsymbol{\omega}}^Q$.

³ For any isotropic tensor function of tensorial argument it is $\underline{\mathbf{Q}} \underline{\boldsymbol{\chi}}(\underline{\mathbf{T}}) \underline{\mathbf{Q}}^T = \underline{\boldsymbol{\chi}}(\underline{\mathbf{Q}} \underline{\mathbf{T}} \underline{\mathbf{Q}}^T)$. Hence $\underline{\mathbf{Q}}[\dot{\underline{\boldsymbol{\chi}}} + \underline{\boldsymbol{\chi}} \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\boldsymbol{\chi}}] \underline{\mathbf{Q}}^T = \underline{\mathbf{Q}}(\partial \underline{\boldsymbol{\chi}} / \partial \underline{\mathbf{T}}) \underline{\mathbf{Q}}^T \underline{\mathbf{Q}}[\dot{\underline{\mathbf{T}}} + \underline{\mathbf{T}} \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\mathbf{T}}] \underline{\mathbf{Q}}^T$. This relation is valid for any spin $\underline{\boldsymbol{\omega}}^Q = \underline{\dot{\mathbf{Q}}} \underline{\mathbf{Q}}^T$, where $\underline{\mathbf{Q}}$ is proper orthogonal tensor ($\underline{\mathbf{Q}} \cdot \underline{\mathbf{Q}}^T = \underline{\mathbf{I}}, \det(\underline{\mathbf{Q}}) = 1$) and for any rate $\dot{\underline{\mathbf{T}}}$. Substituting $\dot{\underline{\mathbf{T}}} = \underline{\mathbf{0}}$, the properties (14) can be obtained.

3.3 Rate equations of state

Rate equations of state of SMA macroelement in Eulerian description can be obtained by calculating any corotational⁴ derivative of (13). However, due to reasons elucidated in this section below we use for this purpose elastic Zaremba–Jaumann corotational derivative. Then, rate constitutive relations in Eulerian description take the form

$$\begin{aligned}\overset{\circ}{\boldsymbol{\tau}}^{\text{Je}} &= J\mathbf{L}\overset{\circ}{\mathbf{e}}^{\text{Je}} - J\mathbf{B}\dot{T} - \rho^0(\partial\pi_1/\partial\mathbf{e}^e)\dot{z}, \\ T\dot{s} &= T(\mathbf{B}/\rho)\overset{\circ}{\mathbf{e}}^{\text{Je}} + c_\varepsilon\dot{T} + T(\partial\pi_1/\partial T)\dot{z}, \\ \dot{\pi}_1 &= \frac{\partial\pi_1}{\partial\mathbf{e}^e}\overset{\circ}{\mathbf{e}}^{\text{Je}} + \frac{\partial s}{\partial z}\dot{T} + \frac{\partial\pi_1}{\partial z}\dot{z},\end{aligned}\quad (15)$$

where \mathbf{L} is isotropic tensor of elastic stiffness moduli, $\mathbf{B} = \mathbf{L}\boldsymbol{\alpha}_0$ is tensor of elastic thermal stresses, $\boldsymbol{\alpha}_0 = \alpha_0\mathbf{I}$ is isotropic tensor of thermal expansion ($(\alpha_0)_{ij} = \alpha_0\delta_{ij}$), $c_\varepsilon \equiv T(\partial s/\partial T)$ denotes specific heat capacity per unit of mass at constant strain. In order to obtain relations (15), the property (14)₁ was used upon substitution of elastic spin $\boldsymbol{\omega}^e = \dot{\mathbf{R}}^e\mathbf{R}^e$ and using definition of \mathbf{L} —(16)₁. Knowledge of the explicit form of free energy potential ϕ allows for determination of instantaneous values of \mathbf{L} , \mathbf{B} and $\partial\pi_1/\partial\mathbf{e}^e$ with the aid of the following formula:

$$\begin{aligned}J\mathbf{L} &\equiv \rho^0 \frac{\partial^2\phi}{\partial\mathbf{e}^e\partial\mathbf{e}^e} = \frac{\partial\boldsymbol{\tau}}{\partial\mathbf{e}^e}, & J\mathbf{B} &\equiv -\rho^0 \frac{\partial^2\phi}{\partial T\partial\mathbf{e}^e} = \frac{\partial\boldsymbol{\tau}}{\partial T}, \\ \rho^0 \frac{\partial\pi_1}{\partial\mathbf{e}^e} &\equiv -\rho^0 \frac{\partial^2\phi}{\partial z\partial\mathbf{e}^e} = -\frac{\partial\boldsymbol{\tau}}{\partial z}.\end{aligned}\quad (16)$$

It seems that for the first time Raniecki and Nguyen [18] delivered the exact, explicit mathematical formula between elastic Zaremba–Jaumann derivative of elastic logarithmic strain $\overset{\circ}{\mathbf{e}}^{\text{Je}} \equiv \dot{\mathbf{e}}^e + \mathbf{e}^e\boldsymbol{\omega}^e - \boldsymbol{\omega}^e\mathbf{e}^e$ and Eulerian elastic strain rate \mathbf{d}^e . It is recalled here in more convenient form [24]:

$$\begin{aligned}\overset{\circ}{\mathbf{e}}^{\text{Je}} &= [\mathbf{I}^{(4)} + \mathbf{E}^{\text{de}}(\mathbf{V}^e)]\mathbf{d}^e, & \overset{\circ}{\mathbf{e}}^{\text{Je}} &= \Sigma e_{ij}^c \mathbf{n}_i^c \otimes \mathbf{n}_j^c, \\ \mathbf{E}_{ijkl}^{\text{de}} d_{kl}^e &= e_{ij}^{\text{Je}} - d_{ij}^e = \begin{cases} 0, & i = j \\ \left[\frac{(\lambda_i^e/\lambda_j^e)^2 + 1}{(\lambda_i^e/\lambda_j^e)^2 - 1} \ln(\lambda_i^e/\lambda_j^e) - 1 \right] d_{ij}^e, & i \neq j, \end{cases}\end{aligned}\quad (17)$$

where $\mathbf{I}^{(4)}$ denotes unit tensor of the fourth order. The components of the fourth-order tensor \mathbf{E}^{de} depend only on the state of elastic deformation of the material but not on the components of \mathbf{d}^e . The tensor \mathbf{E}^{de} has at most three independent components $\mathbf{E}_{1212}^{\text{de}}$, $\mathbf{E}_{1313}^{\text{de}}$, $\mathbf{E}_{2323}^{\text{de}}$ different from zero. It is easy to show that tensor \mathbf{E}^{de} possesses interesting properties in the case of materials exhibiting isotropy of elastic properties. In such a case it commutes with tensor of elastic moduli $\mathbf{L}(\mathbf{L}\mathbf{E}^{\text{de}} = \mathbf{E}^{\text{de}}\mathbf{L})$, and $\mathbf{E}^{\text{de}}\mathbf{s} = \mathbf{0}$ for any second-order tensor \mathbf{s} collinear with tensor \mathbf{V}^e ($\mathbf{s}\mathbf{V}^e = \mathbf{V}^e\mathbf{s}$), e.g., $\mathbf{E}^{\text{de}}\boldsymbol{\tau} = \mathbf{E}^{\text{de}}\boldsymbol{\sigma} = \mathbf{E}^{\text{de}}\mathbf{e}^e = \mathbf{0}$. Substituting relation (17)–(15), one obtains the following

$$\begin{aligned}\overset{\circ}{\boldsymbol{\tau}}^{\text{Je}} &= J\mathbf{L}^{\text{Je}}\mathbf{d}^e - J\mathbf{L}\boldsymbol{\alpha}_0\dot{T} - \rho^0 \frac{\partial\pi_1}{\partial\mathbf{e}^e}\dot{z}, & \mathbf{L}^{\text{Je}} &\equiv \mathbf{L}(\mathbf{I}^{(4)} + \mathbf{E}^{\text{de}}(\mathbf{V}^e)), \\ \dot{s} &= (\mathbf{L}^{\text{Je}}/\rho)\boldsymbol{\alpha}_0\mathbf{d}^e + (c_\varepsilon/T)\dot{T} + (\partial\pi_1/\partial T)\dot{z}, & \dot{s} &= \boldsymbol{\alpha}_0 \cdot \overset{\circ}{\boldsymbol{\tau}}^{\text{Je}} + (c_p/T)\dot{T} + (\partial\pi_1/\partial T)\dot{z}, \\ \dot{\pi}_1 &= \frac{\partial\pi_1}{\partial\mathbf{e}^e} [\mathbf{I}^{(4)} + \mathbf{E}^{\text{de}}(\mathbf{V}^e)]\mathbf{d}^e + \frac{\partial s}{\partial z}\dot{T} + \frac{\partial\pi_1}{\partial z}\dot{z},\end{aligned}\quad (18)$$

where $J\mathbf{L}^{\text{Je}}$ is the current (instantaneous) elastic Zaremba–Jaumann tangent.

⁴ Corotational derivative of any second-order tensor \mathbf{T} is defined as follows, $\overset{\circ}{\mathbf{T}} \equiv \mathbf{Q}^{\text{D}}_{\text{Dt}}(T\mathbf{Q}\mathbf{T}\mathbf{Q})^T\mathbf{Q} = \dot{\mathbf{T}} + \mathbf{T}\boldsymbol{\omega}^Q - \boldsymbol{\omega}^Q\mathbf{T}$ where $\boldsymbol{\omega}^Q$ is a spin generating particular corotational derivative. After substituting respective spins various corotational derivatives can be obtained, e.g., Zaremba–Jaumann— $\overset{\circ}{\boldsymbol{\tau}}^{\text{J}} = \dot{\boldsymbol{\tau}} + \boldsymbol{\tau}\boldsymbol{\omega} - \boldsymbol{\omega}\boldsymbol{\tau} = J[\dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\boldsymbol{\omega} - \boldsymbol{\omega}\boldsymbol{\sigma} + \boldsymbol{\sigma}\text{tr}(\mathbf{d})]$ —the last equality is obtained upon use of local mass balance, elastic Zaremba–Jaumann— $\overset{\circ}{\boldsymbol{\tau}}^{\text{Je}} = J[\dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\boldsymbol{\omega}^e - \boldsymbol{\omega}^e\boldsymbol{\sigma} + \boldsymbol{\sigma}\text{tr}(\mathbf{d})]$, Green–Naghdi, etc.

Relation (17) is of the utmost importance for modeling constitutive behavior of metallic materials at large deformations. Experimental investigations show that all metallic materials undergo only small elastic non-dilatational deformations at arbitrary multiaxial loadings, while at the same time they can undergo large dilatational elastic deformations, e.g., at impact loadings. This special physical property of metallic materials leads to the known estimation—cf. [18], that if elastic principal stretches fulfill condition $\frac{5}{6} \leq \lambda_i^e / \lambda_j^e \leq \frac{7}{6}$ ($\mathbf{e}^e \left(\frac{\lambda_i^e}{\lambda_j^e} = 0.85 \right) = -0.16$) then the component wise difference between components of elastic Zaremba–Jaumann derivative of logarithmic strain and components of elastic stretching tensor expressed on Eulerian principal axes fulfill the condition $|e_{ij}^{Je} - d_{ij}^e| \leq 1.1\%$. The stress corresponding to 16% elastic strain upon assumption of linear elastic behavior is $\sigma = 2\mu \cdot (-0.16) = -0.32\mu$, where μ denotes shear modulus. The symbol $| \cdot |$ denotes here differences between individual components of the tensors. In majority of cases of shape memory alloys elastic strains do not exceed 1%, as at larger strains the material starts to flow pseudoelastically due to the initiation and progress of p.t. At this level of elastic strain, the following inequality is valid:

$$\left(e_{eq}^e = 0.01 \right) \Rightarrow \left(|e_{ij}^{Je} - d_{ij}^e| \leq 3 \cdot 10^{-5} = 0.003\% \right). \quad (19)$$

The above estimate indicates that in engineering design computations involving SMA, it can be accepted with perfect accuracy that—cf. (17), (18)₂

$$\frac{\circ}{\mathbf{e}}^{Je} = \mathbf{d}^e, \quad \mathbf{L}^{Je} = \mathbf{L}. \quad (20)$$

The (20) points out elastic Zaremba–Jaumann derivative to be especially useful in the task of formulating rate constitutive relations of elasticity, as in majority of practical cases the same instantaneous tensor of moduli of elasticity which are present in non-rate equations of state, e.g., $\mathbf{L} = \text{const}$, can be immediately used in corresponding rate equations of state expressed with the use of elastic stretching \mathbf{d}^e . This allows for large computational savings.

It is worth noting that (18)₁ constitutes exact mathematical transition from mechanical equations of *hyperelasticity*—(13)₁, to fully equivalent equations of *hypoelasticity*—(18)₁. In particular, taking the special case of isothermal elasticity ($\dot{T} = 0, \dot{z} = 0$) the exact mathematical counterpart of possibly non-linear hyperelasticity law $\underline{\boldsymbol{\tau}} = \rho^0 \partial \phi / \partial \mathbf{e}^e$ is the hypoelastic law $\underline{\boldsymbol{\tau}}^{\circ Je} = J \mathbf{L}^{Je} \mathbf{d}^e$. The approximation (20) is used with success in computational mechanics of elastic–plastic materials for many years now basing on the estimates delivered by Hill and Rice [7]. Hill and Rice did not elucidate explicit, exact equivalence (13)₁ \leftrightarrow (18)₁.

3.4 Work dissipation

Specific power of total work \dot{w} per unit of mass, done over the SMA macroelement, can be expressed with the following formula in Eulerian description:

$$\dot{w} = \text{tr}(\underline{\boldsymbol{\tau}} \mathbf{d}) / \rho^0 [\text{J/kg}]. \quad (21)$$

According to the concepts of non-equilibrium thermodynamics, in homogeneous processes the specific power of work dissipation \dot{w}_{Disp} is a difference between specific power of total work \dot{w} and reversible work \dot{w}_0 —cf. (11)₄

$$\dot{w}_{\text{Disp}} \equiv \dot{w} - \dot{w}_0 = \text{tr}(\underline{\boldsymbol{\tau}} \mathbf{d}^{\text{in}}) / \rho^0 + \pi_1 \dot{z} \geq 0. \quad (22)$$

In accordance with the second law of thermodynamics, mechanical work dissipation in any thermodynamic process must be greater or equal to zero. The relations between respective thermodynamic forces and fluxes determine its magnitude $\underline{\boldsymbol{\tau}} \leftrightarrow \mathbf{d}^{\text{in}}, \pi_1 \leftrightarrow \dot{z}$. At the same time the same principle indicates that such relations must exist. It should be pointed out that second law of thermodynamics does not impose any limitations on inelastic spin $\underline{\boldsymbol{\omega}}^{\text{in}}$ —cf. (4)₃.

4 Special elastically linear model of pseudoelasticity of shape memory alloys

In the previous section, a very general thermodynamic framework was presented enabling formulation of phenomenological, macroscopic model of SMA alloys behavior taking into account, e.g., different elastic properties of austenitic and martensitic phase or material damaging effects. In the present section the specific, complete, 3D SMA materials constitutive model of pseudoelasticity is specified linear elastic in logarithmic strain measure. The following elements of the model are proposed in explicit form:

- Free energy potential— $\phi(\underline{\mathbf{e}}^e, T, z)$,
- Eulerian representation of inelastic spin— $\underline{\boldsymbol{\omega}}^{\text{in}}$
- Pseudoelastic flow equation— $\underline{\mathbf{d}}^{\text{in}}(\text{tr}(\underline{\mathbf{d}}^{\text{in}}) = 0)$
- Formal p.t. kinetics relations written in objective form proper in finite deformation formalism— \dot{z}

The model constitutes extension of model R_L proposed by Raniecki and Lexcellent in 1998 into finite deformations regime.

4.1 Free energy function

The specific free energy potential of a two-phase shape memory alloy macroelement (RVE) remaining in state of “constrained phase equilibrium” and undergoing finite deformations is conjectured in mobile Lagrangian description in the following form:

$$\begin{aligned}\phi(\underline{\mathbf{E}}^e, T, z) &= \phi^0(T) + \phi^{\text{tm}}(\underline{\mathbf{E}}^e, T) + \phi^{\text{int}}(T, z), \\ \phi^0(T) &= u_0^{*(1)} - T s_0^{*(1)} - z \pi_0^f(T) + c_\varepsilon [(T - T_0) - T \ln(T/T_0)], \\ \rho^0 \phi^{\text{tm}}(\underline{\mathbf{E}}^e, T) &= \underline{\mathbf{E}}^e \cdot (\underline{\mathbf{JL}}) \underline{\mathbf{E}}^e / 2 - (T - T_0) \underline{\boldsymbol{\alpha}}_0 \cdot (\underline{\mathbf{JL}}) \underline{\mathbf{E}}^e, \\ \phi^{\text{int}}(T, z) &= \phi_{it}(T)(1 - z)z, \\ \phi_{it}(T) &= \bar{u}_0 - T \bar{s}_0, \quad \pi_0^f(T) = \Delta u^* - T \Delta s^*, \quad \Delta u^* = u_0^{*(1)} - u_0^{*(2)}, \quad \Delta s^* = s_0^{*(1)} - s_0^{*(2)}.\end{aligned}\tag{23}$$

Terms $\phi^0(T)$ and $\phi^{\text{tm}}(\underline{\mathbf{E}}^e, T)$ denote the thermal and thermoelastic part of SMA macroelement free energy, while $\phi^{\text{int}}(T, z)$ denotes the so-called internal interactions energy, $u_0^{*(\alpha)}$, $s_0^{*(\alpha)}$ are specific internal energies and entropies of austenitic ($\alpha = 1$) and martensitic ($\alpha = 2$) phase formation at thermodynamic reference state, i.e., in stress free state ($\underline{\boldsymbol{\sigma}} = \underline{\mathbf{0}}$), and at thermodynamic reference temperature $T = T_0$, z is mass fraction of martensitic phase, the term $\pi_0^f(T)$ is so-called “chemical thermodynamic driving force of p.t.”, $c_\varepsilon = \text{const}$ is heat capacity at fixed strain, $\underline{\mathbf{JL}}$ is isotropic tensor of elastic moduli assumed to be constant ($\underline{\mathbf{JL}}_{ijkl} = [\mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \lambda\delta_{ij}\delta_{kl}] = \text{const}$, $\lambda = (K - 2\mu/3)$), \bar{u}_0 , \bar{s}_0 are material constants.

The above explicit form of free energy potential corresponds to the one postulated by Raniecki and Lexcellent for small deformations in 3D case [20,21] and Müller and Xu in 1D case [11]. The difference between specification of free energy potential given here and that given by Raniecki and Lexcellent is that here elastic strain is used directly as a state variable, while the previous authors expressed this potential with the aid of total and phase transition strains tensors. After using additive decomposition of total strain tensor into elastic and inelastic part, valid in small deformations theory, Raniecki and Lexcellent’s potential takes the formal mathematical form identical with that specified here by formulae (23). In order to obtain the free energy potential in Eulerian description, it is sufficient to replace Lagrangian logarithmic strain $\underline{\mathbf{E}}^e$ with Eulerian logarithmic strain $\underline{\mathbf{e}}^e$, in view of elastic isotropy. The inverted strain–stress constitutive relations corresponding to stress–strain relations originating from free-energy potential can be easily obtained by formal differentiation of Gibbs potential. The Gibbs potentials on actual configurations can be constructed in a classical way with the aid of Legendre transformation $g(\underline{\boldsymbol{\tau}}, T, z) \equiv \phi - (1/\rho^0)\underline{\boldsymbol{\tau}} \cdot \underline{\mathbf{e}}^e$ [J/kg].

In accordance with the formalism of thermodynamics, the equations of state in Eulerian description resulting from potential ϕ defined with (23) take the following (they constitute explicit specification of relations (13)) form:

$$\begin{aligned}\underline{\boldsymbol{\sigma}} &= J^{-1} \underline{\boldsymbol{\tau}} = \underline{\mathbf{L}} [\underline{\mathbf{e}}^e - \underline{\boldsymbol{\alpha}}_0(T - T_0)], \\ s &= c_v \ln(T/T_0) + s_0^{*(1)} - z \Delta s^* + \bar{s}_0(1 - z)z + \underline{\boldsymbol{\alpha}}_0 \cdot \underline{\mathbf{L}} \underline{\mathbf{e}}^e / \rho, \\ \pi_1 &= \pi_0^f(T) - (1 - 2z)\phi_{it}(T).\end{aligned}\tag{24}$$

4.2 Inelastic spin tensor $\underline{\omega}^{\text{in}}$

The selection of the evolution rule for the Eulerian inelastic spin $\underline{\omega}^{\text{in}}$ leads effectively to the selection of specific family of isoclinic configurations and, at the same time, removes ambiguity in multiplicative decomposition of total deformation gradient into elastic and inelastic parts—cf. (1). The concept of isoclinic configurations, except for uncoupling elastic and inelastic behavior of the material, allows for the harmonious and efficient introduction the elements of description of microscopic behavior of the material, such as evolution of texture or effect of large inelastic deformation-induced anisotropy into a macroscopic model. Such elements can also be introduced to further enhance the developed-here model of shape memory alloys, when such a need arises, but first of all when credible experimental data regarding, e.g., influence of evolution of microstructure on material properties, are available. Analysis of such data must lead to formulation of physically supported evolution rule of $\underline{\omega}^{\text{in}}$.

In the current case of the developed isotropic elastically SMA alloys model, there is no premises indicating that selection of some specific family of isoclinic, natural, reference configurations would be more advantageous from the physical point of view. However, the selection of particular family of isoclinic configurations is important from a pragmatic point of view. Its “proper” selection leads to the simplicity of mathematical formulas and consequently to better numerical effectiveness of the model with the same quality of modeling predictions. It is accepted here that Eulerian inelastic spin $\underline{\omega}^{\text{in}}$ is identically equal to zero during any deformation process

$$\underline{\omega}^{\text{in}} = \mathbf{0}, \quad (25)$$

$$(\underline{\omega}^{\text{in}} = \mathbf{0}) \iff \left(\underline{\omega}^{\text{e}} = \underline{\omega}, \quad \underline{\tau} = \underline{\tau} \right).$$

Then elastic Zaremba–Jaumann derivative defined with spin $\underline{\omega}^{\text{e}}$ becomes identically equal to Zaremba–Jaumann derivative defined with spin $\underline{\omega}$ —cf. (4)₁. The condition (25) makes it unnecessary to continuously track the evolution of spin $\underline{\omega}^{\text{in}}$, in order to be able to determine elastic spin $\underline{\omega}^{\text{e}} = \underline{\omega} - \underline{\omega}^{\text{in}}$. It was shown in [27] that condition (25) determines isoclinic family of natural configurations—cf. Appendix 7.4.

4.3 Tensor of phase eigenstrain rate in Eulerian description $\underline{\mathbf{d}}^{\text{in}}$

Results of isothermal tests of polycrystalline NiTi alloy submitted to stress controlled multiaxial proportional loading paths presented and discussed in [27]—cf. also [22] show that with good approximation ratios of velocities of components of macroscopic p.t. strain tensor remained constant, in response to keeping constant ratios of velocities of components of inducing stress tensor—cf. Figures 5.4, 5.10 in [27]. Hence, it can be indirectly presumed that principal axes of macroscopic phase transformation strain tensor remained constant when principal axes of inducing phase transition stress tensor remained constant. Experimental works done on CuZnAl alloy by Rogueda [25], on CuAlBe alloy by Bouvet et al.—cf. Figure 17, 18, 19 in [3], see also Bouvet et al. [4], on NiTi alloy by Helm and Haupt—cf. Figure 7, 8 in [5], for non-proportional loading paths indicate that ratios of increments of components of macroscopic phase transformation strain tensor followed after ratios of increments of components of inducing stress tensor. The above-listed experimental evidence constitutes, partly quantitative, partly qualitative support for the theoretical concept put forward by Raniecki and Lexcellent of “optimal adaptation of the SMA alloy microstructure to changing external loadings”. They deliver also an important premise indicating that it is well acceptable to express macroscopic phase transformation strain tensor, describing inelastic deformation effects connected with phase transition with the aid of tensor function isotropic with respect to macroscopic stress tensor. The concept of “optimal adaptation of the SMA alloy microstructure” together with investigations regarding conditions for microstructural thermodynamic equilibrium led Raniecki and Lexcellent to the supposition that macroscopic phase eigenstrains tensor $\underline{\kappa}$ admits the existence of generating it potential $g^{\text{ph}}(\underline{\sigma}, T)$. Thermodynamic considerations show that it can be conveniently postulated as homogeneous function of the first order with respect to stress tensor—cf. formulae (11)–(13) in [21]. Further, yet unpublished theoretical analyses (B. Raniecki private communication, 2006) indicated that phase strain energy potential g^{ph} plays an essential role not only in modeling discussed here of the pseudoelastic behavior of shape memory alloys but also in the case of one-way memory effect, as it constitutes energetic measure of phases microstructural interactions.

Due to the recalled premises of experimental and theoretical nature, the concept of “optimal adaptation of the SMA alloy microstructure” together with all resulting from it consequences is accepted as valid when

building model of SMA behavior valid for finite deformations. In particular hereby, the conjecture is adopted that there exists phase strain potential g^{ph} being isotropic function with respect to Cauchy (Kirchoff) stress, homogeneous of the first order. Its explicit form proposed here is identical with that proposed in model R_L

$$\rho^0 g^{\text{ph}}(\underline{\boldsymbol{\tau}}) = \underline{\boldsymbol{\kappa}} \cdot \underline{\boldsymbol{\tau}} = \eta f(y) \tau', \quad \rho g^{\text{ph}}(\underline{\boldsymbol{\sigma}}) = \rho^0 g^{\text{ph}}(\underline{\boldsymbol{\tau}})|_{\tau'=\sigma'} = \underline{\boldsymbol{\kappa}} \cdot \underline{\boldsymbol{\sigma}} = \eta f(y) \sigma', \quad (26)$$

where $\sigma' = (\underline{\boldsymbol{\sigma}} \cdot \underline{\boldsymbol{\sigma}})^{1/2}$, $\tau' = (\underline{\boldsymbol{\tau}} \cdot \underline{\boldsymbol{\tau}})^{1/2}$, $\underline{\boldsymbol{\sigma}} = \text{dev}(\underline{\boldsymbol{\sigma}})$, $\underline{\boldsymbol{\tau}} = \text{dev}(\underline{\boldsymbol{\tau}})$, $\tau_{ef} = \sqrt{3/2} \tau'$.

The phase strain energy potential (26) generates phase eigenstrain tensor $\underline{\boldsymbol{\kappa}}$

$$\underline{\boldsymbol{\kappa}} \equiv \rho^0 \partial g^{\text{ph}}(\underline{\boldsymbol{\tau}}) / \partial \underline{\boldsymbol{\tau}} = \rho \partial g^{\text{ph}}(\underline{\boldsymbol{\sigma}}) / \partial \underline{\boldsymbol{\sigma}} = \underline{\boldsymbol{\bar{\kappa}}} + \underline{\boldsymbol{\bar{\bar{\kappa}}}}, \quad (27)$$

$$\underline{\boldsymbol{\bar{\kappa}}} = \eta f(y) \underline{\boldsymbol{n}}_{\sigma}, \quad \underline{\boldsymbol{\bar{\bar{\kappa}}}} = \eta \tau' \frac{df(y)}{dy} \frac{\partial y}{\partial \underline{\boldsymbol{\tau}}} = 3 \eta \frac{df(y)}{dy} \left[\sqrt{6} (\underline{\boldsymbol{n}}_{\sigma}^2 - (1/3) \mathbf{1}) - y \underline{\boldsymbol{n}}_{\sigma} \right],$$

where η denotes pseudoelastic flow amplitude treated as material constant, $\underline{\boldsymbol{n}}_{\sigma}$ denotes versor of “direction” of the Cauchy (Kirchoff) stress tensor

$$\underline{\boldsymbol{n}}_{\sigma} \equiv \underline{\boldsymbol{\sigma}} / \sigma' = \underline{\boldsymbol{\tau}} / \tau' = \underline{\boldsymbol{n}}_{\tau}, \quad \underline{\boldsymbol{n}}_{\sigma} \cdot \underline{\boldsymbol{n}}_{\sigma} = 1. \quad (28)$$

The postulate (26) leads to the relation $J^p = \rho^0 / \rho^* = 1 (J = \rho^0 / \rho = J^e J^p = J^e)$, i.e., assumption that thermoelastic martensitic transformation itself does not lead to volumetric changes. Function $f(y)$ defines shape of pseudoelastic flow surface in space of stress tensor deviators $\underline{\boldsymbol{\sigma}}$. It is called “shape” function and is defined operationally as follows:

$$f(y) \equiv \sigma^{AM}(0, T) / \sigma^{AM}(y, T), \quad f(y=0) = 1, \quad (29)$$

where $\sigma^{AM}(0, T)$ denotes the critical effective stress at which forward (A→M) martensitic transformation starts during pure shear, while $\sigma^{AM}(y, T)$ denotes the critical effective stress at which martensitic transformation starts when stress tensor has the “direction” y . Function $f(y)$ constitutes the input parameter of the model and must be identified for each shape memory alloy from the experimental data. The following three-parameter form of shape function was proposed in [23] for investigated NiTi alloy:

$$f(y) = a_1 - a_2 \cdot \exp[-a_3 \cdot (y + 1)]. \quad (30)$$

Parameter y , argument of shape function, determining direction of stress tensor in space of stress deviators is defined as follows:

$$y \equiv \sqrt{6} \text{tr}(\underline{\boldsymbol{n}}_{\sigma}^3), \quad -1 \leq y \leq 1, \quad y(\underline{\boldsymbol{\sigma}}) \equiv \frac{3\sqrt{6} J'_3}{(J'_2)^{3/2}}, \quad J'_3 = \text{tr}(\underline{\boldsymbol{\sigma}}^3)/3, \quad J'_2 \equiv \text{tr}(\underline{\boldsymbol{\sigma}}^2). \quad (31)$$

For example value $y = -1$ corresponds to compression, $y = 1$ corresponds to tension, $y = 0$ corresponds to torsion.

The property of isotropy of the potential $g^{\text{ph}}(\underline{\boldsymbol{\tau}})$ with respect to stress tensor leads to collinearity ($\underline{\boldsymbol{\kappa}} \underline{\boldsymbol{\tau}} = \underline{\boldsymbol{\tau}} \underline{\boldsymbol{\kappa}}$) of phase eigenstrain tensor $\underline{\boldsymbol{\kappa}}$ and Kirchoff stress $\underline{\boldsymbol{\tau}}$ —cf. (27). The following equations are satisfied identically for any spin tensor $\underline{\boldsymbol{\omega}}^Q$ in view of the above

$$\underline{\boldsymbol{\kappa}} \cdot [\underline{\boldsymbol{\tau}} \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\boldsymbol{\tau}}] = \mathbf{0}, \quad \underline{\boldsymbol{\tau}} \cdot [\underline{\boldsymbol{\kappa}} \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\boldsymbol{\kappa}}] = \mathbf{0}. \quad (32)$$

The relation $\underline{\boldsymbol{\kappa}} = \underline{\boldsymbol{\kappa}}(\underline{\boldsymbol{\tau}})$ is tensor function isotropic with respect to its tensorial argument. Hence for any spin $\underline{\boldsymbol{\omega}}^Q$ ($\underline{\boldsymbol{\omega}}^Q \underline{\boldsymbol{\tau}} = -\underline{\boldsymbol{\omega}}^Q$) the following relation is valid—cf. (14):

$$(\partial \underline{\boldsymbol{\kappa}} / \partial \underline{\boldsymbol{\tau}}) [\underline{\boldsymbol{\tau}} \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\boldsymbol{\tau}}] = [\underline{\boldsymbol{\kappa}} \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\boldsymbol{\kappa}}]. \quad (33)$$

It is convenient to introduce the following denotation of the derivative $\partial \underline{\boldsymbol{\kappa}} / \partial \underline{\boldsymbol{\tau}}$

$$\underline{\boldsymbol{P}} \equiv \rho^0 \frac{\partial^2 g^{\text{ph}}(\underline{\boldsymbol{\tau}})}{\partial \underline{\boldsymbol{\tau}} \partial \underline{\boldsymbol{\tau}}} = \frac{\partial \underline{\boldsymbol{\kappa}}}{\partial \underline{\boldsymbol{\tau}}}, \quad \rho \frac{\partial^2 g^{\text{ph}}(\underline{\boldsymbol{\sigma}})}{\partial \underline{\boldsymbol{\sigma}} \partial \underline{\boldsymbol{\sigma}}} = \frac{\partial \underline{\boldsymbol{\kappa}}}{\partial \underline{\boldsymbol{\sigma}}} = J \underline{\boldsymbol{P}}. \quad (34)$$

The explicit form of the fourth-order tensor $\underline{\mathbf{P}}$ in the case of phase strain potential $g^{\text{ph}}(\underline{\boldsymbol{\sigma}})$ is given below:

$$\begin{aligned} \underline{\mathbf{P}}(\underline{\boldsymbol{\tau}}) &= -2\eta \frac{df(y)}{dy} \frac{\partial y}{\partial \underline{\boldsymbol{\tau}}} \otimes \underline{\mathbf{n}}_{\boldsymbol{\tau}} + \left[\eta f(y) - 3\eta y \frac{df(y)}{dy} \right] \frac{\partial \underline{\mathbf{n}}_{\boldsymbol{\tau}}}{\partial \underline{\boldsymbol{\tau}}} \\ &+ \left[\eta \tau' \frac{d^2 f(y)}{dy^2} \right] \frac{\partial y}{\partial \underline{\boldsymbol{\tau}}} \otimes \frac{\partial y}{\partial \underline{\boldsymbol{\tau}}} + 6\sqrt{6}\eta \frac{df(y)}{dy} \underline{\mathbf{n}}_{\boldsymbol{\tau}} \frac{\partial \underline{\mathbf{n}}_{\boldsymbol{\tau}}}{\partial \underline{\boldsymbol{\tau}}}, \end{aligned} \quad (35)$$

$$\frac{\partial y}{\partial \underline{\boldsymbol{\tau}}} = \frac{3}{\tau'} \left[\sqrt{6}(\underline{\mathbf{n}}_{\boldsymbol{\tau}}^2 - \frac{1}{3}\underline{\mathbf{1}}) - y \underline{\mathbf{n}}_{\boldsymbol{\tau}} \right] = J^{-1} \frac{\partial y}{\partial \underline{\boldsymbol{\sigma}}}, \quad \frac{\partial \underline{\mathbf{n}}_{\boldsymbol{\tau}}}{\partial \underline{\boldsymbol{\tau}}} = \frac{1}{\tau'} \left[(\underline{\mathbf{1}}^{(4)} - \frac{1}{3}\underline{\mathbf{1}} \otimes \underline{\mathbf{1}}) - \frac{\bar{\boldsymbol{\tau}} \otimes \bar{\boldsymbol{\tau}}}{(\tau')^2} \right] = J^{-1} \frac{\partial \underline{\mathbf{n}}_{\boldsymbol{\sigma}}}{\partial \underline{\boldsymbol{\sigma}}}.$$

The postulated form of potential $g^{\text{ph}}(\underline{\boldsymbol{\tau}})$ is a function homogeneous of order one, with respect to $\underline{\boldsymbol{\tau}}(\underline{\boldsymbol{\sigma}})$. Hence the functional relation $\underline{\boldsymbol{\kappa}}(\underline{\boldsymbol{\tau}})$ —cf. (27), is an isotropic function, homogeneous of order zero with respect to $\underline{\boldsymbol{\tau}}(\underline{\boldsymbol{\sigma}})$. As a consequence tensor $\underline{\mathbf{P}}$ has the property

$$\underline{\mathbf{P}} \underline{\boldsymbol{\tau}} = \frac{\partial \underline{\boldsymbol{\kappa}}}{\partial \underline{\boldsymbol{\tau}}} \underline{\boldsymbol{\tau}} = \underline{\mathbf{0}}, \quad J \underline{\mathbf{P}} \underline{\boldsymbol{\sigma}} = \frac{\partial \underline{\boldsymbol{\kappa}}}{\partial \underline{\boldsymbol{\sigma}}} \underline{\boldsymbol{\sigma}} = \underline{\mathbf{0}} \quad (36)$$

which can be verified by direct calculation.

Taking advantage of the formula (33), one can express any corotational derivative of tensor $\underline{\boldsymbol{\kappa}}$ with the aid of corresponding to it corotational derivative of Kirchoff stress tensor as follows—using notation (34):

$$\overset{\circ}{\underline{\boldsymbol{\kappa}}} = \dot{\underline{\boldsymbol{\kappa}}} + \underline{\boldsymbol{\kappa}} \underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q \underline{\boldsymbol{\kappa}} = \underline{\mathbf{P}} \underline{\boldsymbol{\tau}}, \quad \overset{\circ}{\underline{\boldsymbol{\kappa}}} = (J \underline{\mathbf{P}}) \underline{\boldsymbol{\sigma}}. \quad (37)$$

In the case of proposed here the linear elastically model of SMA materials, thermodynamic force π_1 does not depend on $\underline{\mathbf{e}}^e$ —cf. (24)₃. Hence it is

$$\frac{\partial \pi_1}{\partial \underline{\mathbf{e}}^e} = -\frac{\partial \sigma}{\partial z} = \underline{\mathbf{0}}. \quad (38)$$

The rate mechanical equation of state (24)₁—cf. also (18)₁, simplifies to the form

$$\underline{\boldsymbol{\tau}} = J \underline{\mathbf{L}}^{\text{Je}} (\underline{\mathbf{d}} - \underline{\mathbf{d}}^{\text{in}}) - J \underline{\mathbf{L}} \underline{\boldsymbol{\alpha}}_0 \dot{T}, \quad (39)$$

where it was used property $\underline{\mathbf{L}}^{\text{Je}} \underline{\boldsymbol{\alpha}}_0 = \underline{\mathbf{L}} \underline{\boldsymbol{\alpha}}_0$ valid for material exhibiting isotropic thermal expansion $\underline{\boldsymbol{\alpha}}_0 = \alpha_0 \underline{\mathbf{1}}$. The above relation requires specification of tensor of inelastic strain rate $\underline{\mathbf{d}}^{\text{in}}$. The pseudoelastic flow rule defining tensor $\underline{\mathbf{d}}^{\text{in}}$ is hereby postulated in the following form:

$$\underline{\mathbf{d}}^{\text{in}} = z \underline{\boldsymbol{\kappa}} = \dot{z} \underline{\boldsymbol{\kappa}} + z \underline{\boldsymbol{\kappa}}. \quad (40)$$

The elastic Zaremba–Jaumann derivative of tensor $\underline{\boldsymbol{\kappa}}$ can be expressed with the aid of elastic Zaremba–Jaumann derivative of Kirchoff stress as follows—cf. (37):

$$\underline{\boldsymbol{\kappa}} = \underline{\mathbf{P}} \underline{\boldsymbol{\tau}}. \quad (41)$$

Substituting in (39) relations (40) and (41), one obtains

$$\underline{\boldsymbol{\tau}} = J \underline{\mathbf{L}}^{\text{Je}} [\underline{\mathbf{d}} - \dot{z} \underline{\boldsymbol{\kappa}} - \underline{\boldsymbol{\alpha}}_0 \dot{T}] - z J \underline{\mathbf{L}}^{\text{Je}} \underline{\mathbf{P}} \underline{\boldsymbol{\tau}}, \quad (42)$$

Grouping terms with corotational derivative of stress, one obtains the following:

$$\underline{\boldsymbol{\tau}} = J \underline{\mathbf{L}}^{\text{S-Je}} [\underline{\mathbf{d}} - \dot{z} \underline{\boldsymbol{\kappa}} - \underline{\boldsymbol{\alpha}}_0 \dot{T}], \quad (43)$$

where

$$\underline{\mathbf{L}}^{\text{S-Je}} \equiv [\underline{\mathbf{1}}^{(4)} + z J \underline{\mathbf{L}}^{\text{Je}} \underline{\mathbf{P}}]^{-1} \underline{\mathbf{L}}^{\text{Je}}, \quad \underline{\mathbf{L}}^{\text{S}} \equiv [\underline{\mathbf{1}}^{(4)} + z J \underline{\mathbf{L}} \underline{\mathbf{P}}]^{-1} \underline{\mathbf{L}}. \quad (44)$$

Taking advantage of the mathematical formula $[\underline{\mathbf{A}}^{-1}\underline{\mathbf{B}}]^{-1} = \underline{\mathbf{B}}^{-1}\underline{\mathbf{A}}$, one can see that

$$\begin{aligned}\underline{\mathbf{L}}^{S-Je} &= [\underline{\mathbf{M}}^{Je} + z J\underline{\mathbf{P}}]^{-1}, \quad \underline{\mathbf{L}}^S = [\underline{\mathbf{M}} + z J\underline{\mathbf{P}}]^{-1}, \\ \underline{\mathbf{M}}^{Je} &= [\underline{\mathbf{L}}^{Je}]^{-1}, \quad \underline{\mathbf{M}} = \underline{\mathbf{L}}^{-1}.\end{aligned}\quad (45)$$

Using property $\underline{\mathbf{L}}^{S-Je} \underline{\boldsymbol{\alpha}}_0 = \underline{\mathbf{L}}^S \underline{\boldsymbol{\alpha}}_0 = \underline{\mathbf{L}} \underline{\boldsymbol{\alpha}}_0$ and relation (25)₁ one obtains the required rate form of mechanical equations of state:

$$\underline{\boldsymbol{\tau}}^{\circ J} = \underline{\boldsymbol{\tau}}^{\circ Je} = J\underline{\mathbf{L}}^{S-Je} [\underline{\mathbf{d}} - \dot{z}\underline{\boldsymbol{\kappa}}] - J\underline{\mathbf{L}}\underline{\boldsymbol{\alpha}}_0\dot{T}.\quad (46)$$

The rate equation of entropy change takes, in the case of proposed hereby SMA model, the following form—cf. (18)₄

$$\dot{s} = (c_p/T)\dot{T} + [-\Delta s^* + \bar{s}_0(1 - 2z)]\dot{z} + \underline{\boldsymbol{\alpha}}_0 \cdot \underline{\dot{\boldsymbol{\tau}}}/\rho_0.\quad (47)$$

4.4 Thermal effects and mechanical work dissipation

The following relation is obtained upon contracting (40) with $\underline{\boldsymbol{\tau}}$ and using property (36):

$$\underline{\boldsymbol{\tau}} \cdot \underline{\mathbf{d}}^{\text{in}} = \dot{z} \underline{\boldsymbol{\tau}} \cdot \underline{\boldsymbol{\kappa}} + z \underline{\boldsymbol{\tau}} \cdot \underline{\boldsymbol{\kappa}}^{\circ Je} = \dot{z} \underline{\boldsymbol{\tau}} \cdot \underline{\boldsymbol{\kappa}} + \underbrace{\underline{\boldsymbol{\tau}} \cdot \underline{\mathbf{P}} \underline{\boldsymbol{\tau}}}_{=0}^{\circ Je} = \dot{z} \underline{\boldsymbol{\tau}} \cdot \underline{\boldsymbol{\kappa}}.\quad (48)$$

The expression for mechanical work dissipation, taking place during any deformation process of SMA macroelement, can be obtained upon substituting in (22) expression (48) and using (24)₃:

$$\dot{w}_{\text{Disp}} = \dot{w} - \dot{w}_0 = \pi^f \dot{z} \geq 0, \quad \pi^f = \pi_1 + \underline{\boldsymbol{\kappa}} \cdot \underline{\boldsymbol{\tau}}/\rho_0 = \pi_0^f(T) - (1 - 2z)\phi_{it}(T) + \underbrace{\underline{\boldsymbol{\tau}} \cdot \underline{\boldsymbol{\kappa}}/\rho_0}_{=g^{\text{ph}}(\underline{\boldsymbol{\tau}})}.\quad (49)$$

Eliminating \dot{u} from the relation resulting from the definition of free energy $\dot{\phi} = \dot{u} - s\dot{T} - \dot{s}T$ and the equation expressing the first law of thermodynamics written in the form $\dot{u} = \dot{w} - \dot{q}$, and next substituting the obtained expression for $\dot{\phi}$ into the fundamental Gibbs equation of state $\dot{\phi} = -s\dot{T} + \dot{w}_0$ —cf. (11), and using the expression for work dissipation (49)₁, one obtains the following relation:

$$\dot{q} = \pi^f \dot{z} - \dot{s}T.\quad (50)$$

After substituting (49)₂ and (47) in the above formula, one obtains

$$\dot{q} = -c_p\dot{T} + [\Delta u^* - (1 - 2z)\bar{u}_0 + g^{\text{ph}}(\underline{\boldsymbol{\tau}})]\dot{z} - T\underline{\boldsymbol{\alpha}}_0 \cdot \underline{\dot{\boldsymbol{\tau}}}/\rho_0.\quad (51)$$

Let us denote by \dot{q}_{tr} specific power of heat sources (positive when removed to environment) connected with all thermal effects taking place in the SMA macroelement except for heat capacity, cf. (26)₁

$$\dot{q}_{\text{tr}} \equiv c_p\dot{T} + \dot{q} = [\Delta u^* - (1 - 2z)\bar{u}_0 + \eta f(y)\boldsymbol{\tau}'/\rho_0]\dot{z} - T\underline{\boldsymbol{\alpha}}_0 \cdot \underline{\dot{\boldsymbol{\tau}}}/\rho_0.\quad (52)$$

The first term on the right above in the combined way describes effects connected with the latent heat of p.t. and the mechanical work dissipation; the second term describes piezocaloric effect. Please note that in the case of isotropic thermal expansion, it is $\underline{\boldsymbol{\alpha}}_0 \cdot \underline{\dot{\boldsymbol{\tau}}} = 3 \dot{\boldsymbol{\tau}}_m \alpha_0/\rho_0$.

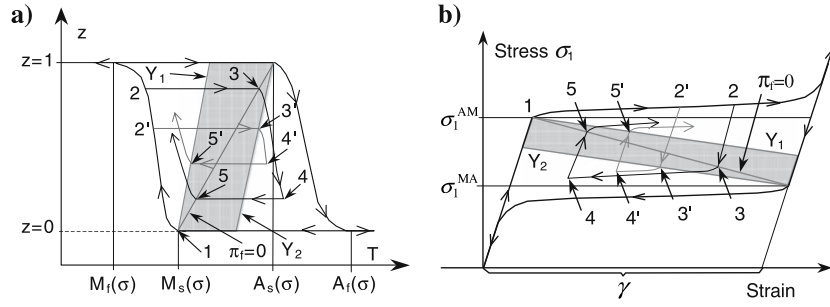


Fig. 3 Schematic illustration of external and internal hysteresis loops formation at partial and complete phase transformations, in accordance with phase transformation kinetics rules proposed by Raniecki and Lexcelent—RL kinetics [20]

4.5 Formal equation of martensitic phase transformation kinetics

The general formal thermoelastic martensitic p.t. kinetics relation fulfilling requirements imposed by the second law of thermodynamics proposed in very comprehensive form by Raniecki and Lexcelent [20]—the so-called RL kinetics relations, are adapted here for the purposes of finite deformations theory. The operation of RL kinetics relations in the case of full and partial, forward and reverse phase transitions, upon inducing them by temperature variation is illustrated schematically in Fig. 3a, while upon inducing them by stress variation in Fig. 3b. With dropping temperatures, forward p.t. (austenite \rightarrow martensite) starts after crossing the line $\pi^f = 0$, point 1. When temperature reduction is stopped in point 2 then p.t. also stops. With increasing temperature reverse p.t. (martensite \rightarrow austenite) starts after crossing line $\pi^f = 0$, point 3. When temperature increase is stopped in point 4, then reverse p.t. also stops (partial p.t.). When subsequently temperature again is lowered then partial forward p.t. starts in point 5, after crossing line $\pi^f = 0$. Such a scenario is realized in the case of those SMA, which do not exhibit appearance of threshold values for phase transitions, i.e., those for which there can be accepted with good approximation that threshold functions $Y_\alpha(\underline{\sigma}, T, z) \equiv 0$ ($\alpha = 1, 2$) identically equal to zero. SMA on the basis of iron instead of path 1-2-3-4-5 rather exhibit behavior consistent with path 1-2'-3'-4'-5'—marked light gray in Fig. 3. Respective forward phase transitions start in the case of such alloys after crossing line Y_1 (hence the name threshold function), while respective reverse transitions start after crossing line Y_2 .

The actual “shape” of p.t. kinetics curves for various SMA alloys is described by so-called specific p.t. kinetics rules—functions λ_α^σ . These functions $0 \leq \lambda_\alpha^\sigma(\underline{\tau}, T, z; m_\alpha, p_\alpha, r_\alpha) < \infty$ ($\alpha = 1, 2$) depend on the state of the material and also on a set of parameters. Proper identification of $(m_\alpha, p_\alpha, r_\alpha)$ parameter values allow for a description of kinetics of various SMA alloys. The general RL kinetics relations written in objective form in Eulerian description are as follows:

$$\dot{z} = \lambda_1^\sigma \cdot \tilde{\pi}_\tau^f \text{ if } \left\{ \pi^f \geq Y_1 \text{ and } \tilde{\pi}_\tau^f > 0 \right\} \quad (\text{A} \rightarrow \text{M p.t.}), \quad (53)$$

$$\dot{z} = \lambda_2^\sigma \cdot \tilde{\pi}_\tau^f \text{ if } \left\{ \pi^f \leq Y_2 \text{ and } \tilde{\pi}_\tau^f < 0 \right\} \quad (\text{M} \rightarrow \text{A p.t.}), \quad \dot{z} = 0 \text{ in any other case,}$$

where π^f denotes thermodynamic driving force of phase transformation defined with the aid of formula (49)₂. The threshold value functions $Y_{(\alpha)}(\underline{\tau}, T, z) \geq 0$, $\alpha = 1, 2$, $Y_{(1)}|_{z=0} = Y_{(2)}|_{z=1} = 0$ denote thresholds upon reaching which, active forward (reverse) phase transition can be initiated. These functions impose additional restrictions to those imposed by the second law of thermodynamics. The physical reason for such restrictions in p.t. progress is not known at present, however they are observed experimentally for some SMA alloys. For example experimental data gathered by Pascal and Monasevich [17] for NiTi alloy indicate that it is reasonable to take $Y_{(1)} = \pi(\underline{0}, M_s^0, z)$ and $Y_{(2)} = \pi(\underline{0}, A_s^0, z)$, while the tests performed at the Institute of Fundamental Technological Research on NiTi alloy (unpublished) indicate that it is reasonable to take $Y_{(\alpha)} = 0$. Experimental data of Müller and Xu [11] for CuZnAl alloy also suggest that it is reasonable to take $Y_{(\alpha)} = 0$ for investigated by them alloy. The specific kinetics rules conjectured in [20] are defined with state functions of the form

$$\lambda_1^\sigma = \frac{(m_1/2)(1-z)D^{m_1-1}}{\bar{u}_0[p_1(1-z)+r_1]-m_1(1-z)\phi_{it}(T)D^{m_1-1}}, \quad \lambda_2^\sigma = \frac{(m_2/2)z(-D)^{m_2-1}}{\bar{u}_0[p_2z+r_2]-m_2z\phi_{it}(T)(-D)^{m_2-1}}, \quad (54)$$

where D denotes “normalized” dimensionless thermodynamic driving force of phase transition

$$D \equiv \pi^f / 2 \bar{u}_0 = D_T \cdot (M_s^0 - T) + D_\sigma \cdot f(y) \cdot \sigma_{ef} + D_z \cdot z, \quad (55)$$

$$D_z \equiv [1 - M_s^0 \bar{s}_0 / \bar{u}_0], \quad D_\sigma \equiv \gamma / (2 \bar{u}_0 \rho), \quad D_T \equiv [(\Delta s^* - \bar{s}_0(1 - 2z)) / 2 \bar{u}_0].$$

Identification of p.t. kinetics constants $m_1, r_1, p_1, m_2, r_2, p_2$ present in (54) can be most conveniently done using integrated form of (54) valid for piecewise continuous forward and reverse phase transition processes, respectively, which take the form

$$D^{m_1} + r_1 \ln(1 - z) - p_1 z = C_0^{(1)}(z^*) = \text{const}, \quad (56)$$

$$D^{m_2} + r_2 \ln(z) - p_2 (1 - z) = C_0^{(2)}(z^*) = \text{const}.$$

In the above z^* denotes starting value of mass fraction of martensite at the beginning of continuous p.t. process. Upon substituting of $C_0^{(1)}(z^* = 0) = 0$ in (56)₁ for forward p.t. curve and $C_0^{(2)}(z^* = 1) = 0$ in (56)₂ for reverse p.t. curve the “outer” hysteresis loop is obtained.

The power of the thermodynamic driving force inducing the process of active p.t. forward (A→M) or reverse (M→A) written in the objective form is

$$\tilde{\pi}_\tau^f \equiv \underline{\pi}_\tau^f \cdot \underline{\dot{\boldsymbol{\tau}}} + \pi_T^f \dot{T}, \quad (57)$$

$$\underline{\pi}_\tau^f \equiv \frac{\partial \pi^f}{\partial \underline{\boldsymbol{\tau}}} = \underline{\boldsymbol{\kappa}} / \rho^0, \quad \pi_T^f \equiv \frac{\partial \pi^f}{\partial T} = -[\Delta s^* - \bar{s}_0(1 - 2z)].$$

The above form is inconvenient in numerical computations as it is expressed through $\underline{\dot{\boldsymbol{\tau}}}$ ($\dot{\boldsymbol{\sigma}}$), i.e., quantity, which is one of the output data from the material behavior procedure. In a general case, such a situation requires application of some iteration scheme for checking whether criterion of active p.t. is fulfilled or not, which increases cost of numerical computations. Hence, it is advisable to search the functional form of (57)₁ that is expressed through input quantities to material behavior procedure, i.e., $\underline{\boldsymbol{d}}$ and \dot{T} . The searched relation was derived in Appendix and has the form

$$\tilde{\pi}_\tau^f \equiv \frac{(\underline{\boldsymbol{\kappa}} / \rho) \cdot \underline{\mathbf{L}}^S \underline{\boldsymbol{d}} + \pi_T^f \dot{T}}{[1 + \lambda_{(\omega)}^\sigma (\underline{\boldsymbol{\kappa}} / \rho) \cdot \underline{\mathbf{L}}^S \underline{\boldsymbol{\kappa}}]}. \quad (58)$$

The above result is extremely advantageous from a numerical efficiency point of view as it allows one to immediately find out whether in a particular time step active phase transition will or will not take place upon prescribed $\underline{\boldsymbol{d}}$, \dot{T} . The formal thermoelastic martensitic p.t. forward and reverse kinetic relations can conveniently be written in a compact form—cf. (53)–(55) and (58)

$$\dot{z} = \lambda_1^\sigma \cdot \bar{H}(\pi^f - Y_1) \cdot \left\langle \tilde{\pi}_\tau^f \right\rangle - \lambda_2^\sigma \cdot \bar{H}(-\pi^f - Y_2) \cdot \left\langle -\tilde{\pi}_\tau^f \right\rangle, \quad (59)$$

where an advantage is taken of the functions $\bar{H}(x)$ and $\langle x \rangle$ defined as follows: $\bar{H}(x) = \{1 \text{ if } x \geq 0; 0 \text{ if } x < 0\}$, $\langle x \rangle = \{x \text{ if } x \geq 0; 0 \text{ if } x < 0\}$.

The complete, specific, linear elastic in a logarithmic strain, macroscopic model of SMA alloys pseudoelastic behavior undergoing finite deformations consists of the set of rate relations (46), (40), (59), (52). The model input parameters are the velocity gradient $\underline{\mathbf{L}}$ and the material derivative of temperature \dot{T} . The model predicts quantitatively the extent of mechanical, thermal, progress of thermoelastic phase transition effects— $\underline{\dot{\boldsymbol{\sigma}}}$, $\underline{\dot{\boldsymbol{d}}}^m$, \dot{z} , \dot{q}_T . They are the output of the model. In the majority of the practical cases of problems involving behavior of shape memory alloys with perfect approximation—cf. (18), it can be adopted that $\underline{\mathbf{L}}^{S-Je} = \underline{\mathbf{L}}^S$ —cf. (44).

5 Field equations

The solution of any engineering design problem concerning a structure or device containing SMA materials requires finding fields of stress $\underline{\sigma}(\underline{\mathbf{x}}, t)$, strain $\underline{\epsilon}(\underline{\mathbf{x}}, t)$, temperature $T(\underline{\mathbf{x}}, t)$, volume fraction of martensitic phase $z(\underline{\mathbf{x}}, t)$ satisfying mechanical and heat transfer balance equations constituting relevant initial-boundary value problem. Due to the highly non-linear behavior of such materials, it is convenient to write balance equations in their rate form in terms of the velocity field $\underline{\mathbf{v}}$ and temperature rate \dot{T} to obtain coupled problem of thermomechanics. The current most common approach to solving such problems, i.e., the finite element method is written in the Lagrangian description variational formulation of mechanical equilibrium equations, also-called the “principle of virtual work” and variational formulation of heat transport equation, also-called the “principle of virtual heat transport”.

A concise formulation of the rate principle of virtual work valid for any fixed reference configuration, in which inertial effects are neglected, can be found in Hill [6]—cf. (3.21). The detailed derivation of the rate principle of virtual work, including inertial effects, and its final form written with respect to current configuration can be found in Lubarda [9]—cf. (3.11.8). Here the rate principle of virtual work is recalled in modified form to that cited by Hill

$$\int_{V^r} (J_r \underline{\mathbf{F}}_r^{-1} \underline{\boldsymbol{\Pi}}^P) \cdot (\underline{\nabla}^r \otimes \delta \underline{\mathbf{v}}^r) dV^r - \int_{\partial V^r} \underline{\mathbf{n}}^r (J_r \underline{\mathbf{F}}_r^{-1} \underline{\boldsymbol{\Pi}}^P) \cdot \delta \underline{\mathbf{v}}^r dS^r - \int_{V^r} \rho^r \underline{\dot{\mathbf{b}}}^r \cdot \delta \underline{\mathbf{v}}^r dV^r = 0. \quad (60)$$

The superscript “ r ” denotes that the relevant quantities are calculated with respect to some fixed reference configuration, $\underline{\nabla}^r = \frac{\partial}{\partial \xi_i} \mathbf{e}_i$ is the gradient operator with respect to coordinates ξ_i in some reference configuration, $\underline{\mathbf{n}}$ denotes the normal to the boundary of reference configuration, $\underline{\dot{\mathbf{b}}}$ is carried to the reference configuration rate of change of mass specific body forces, $\delta \underline{\mathbf{v}}$ denotes the virtual velocities field over the volume of reference configuration. It should be noted that the virtual velocities field $\delta \underline{\mathbf{v}}$ is not totally arbitrary but must fulfill the so-called essential boundary conditions, i.e., it must be null on those parts of the boundary on which the velocity boundary conditions are prescribed. The dV and dS denote elemental volume and elemental surface enclosing reference configuration. The $\underline{\boldsymbol{\Pi}}^P$ denotes the Eulerian rate of the nominal stress tensor. Elucidated by Hill and called by him the “bridging equation”, the following relation is valid —cf. [6]

$$\begin{aligned} \underline{\boldsymbol{\Pi}}^P &= \underline{\dot{\boldsymbol{\sigma}}} + \underline{\boldsymbol{\sigma}} \operatorname{tr}(\underline{\mathbf{d}}) - \underline{\mathbf{L}}\underline{\boldsymbol{\sigma}}, \\ \underline{\dot{\mathbf{P}}}_r &= J_r \underline{\mathbf{F}}_r^{-1} \underline{\boldsymbol{\Pi}}^P, \quad \underline{\mathbf{P}}_r = J_r \underline{\mathbf{F}}_r^{-1} \underline{\boldsymbol{\sigma}}, \end{aligned} \quad (61)$$

$\underline{\mathbf{P}}_r$ denotes the non-symmetric tensor of nominal stress calculated with respect to the fixed reference configuration ($\underline{\mathbf{P}}_r^T$ is corresponding first Piola–Kirchhoff stress).

The rate form of principle of virtual heat transport valid for any fixed reference configuration takes the form

$$\int_{V^r} \frac{1}{\rho^r} \lambda (\underline{\nabla}^r T)^T (\underline{\nabla}^r \delta T^r) dV^r - \int_{\partial V^r} q_s^r \delta T^r dS^r + \int_{V^r} (-\dot{q}_{\operatorname{tr}} + c_p \frac{\partial T}{\partial t}) \delta T^r dV^r = 0, \quad (62)$$

where λ denotes the isotropic heat conduction coefficient, δT denotes the virtual temperature field over the volume of reference configuration. The δT must fulfill so-called essential temperature boundary conditions, i.e., it must be null on those parts of the boundary on which temperature boundary conditions are prescribed. In the above Fourier law of heat conduction has been used $\underline{\mathbf{q}}^r = -\lambda \underline{\nabla}^r T$ ($\underline{\mathbf{n}}^r \underline{\mathbf{q}}^r = q_s^r$).

The classical total Lagrangian formulation can be recovered from (60) when reference configuration is identified with initial one (then $\underline{\nabla}^r \rightarrow \underline{\nabla}^0 = \frac{\partial}{\partial X_i} \mathbf{e}_i$, $\underline{\mathbf{F}}_r^{-1} \rightarrow \underline{\mathbf{F}}^{-1} J_r \rightarrow J$, $\underline{\mathbf{P}}_r \rightarrow \underline{\mathbf{P}}$, $\delta \underline{\mathbf{v}}^r \rightarrow \delta \underline{\mathbf{v}}^0$) and the updated Lagrangian formulation is recovered when reference configuration is identified with current one (then $\underline{\nabla}^r \rightarrow \underline{\nabla} = \frac{\partial}{\partial x_i} \mathbf{e}_i$, $\underline{\mathbf{F}}_r^{-1} \rightarrow \underline{\mathbf{I}} J_r \rightarrow 1$, $\underline{\mathbf{P}}_r \rightarrow \underline{\boldsymbol{\Pi}}^P$, $\delta \underline{\mathbf{v}}^r \rightarrow \delta \underline{\mathbf{v}}$). Beneath only the updated Lagrangian formulation of the coupled problem of pseudoelasticity is explicitly specified

$$\begin{aligned} \int_{V^t} \underline{\boldsymbol{\Pi}}^P \cdot (\underline{\nabla} \otimes \delta \underline{\mathbf{v}}) dV - \int_{\partial V^t} \underline{\dot{\mathbf{i}}}_s \cdot \delta \underline{\mathbf{v}} dS - \int_{V^t} \rho \underline{\dot{\mathbf{b}}} \cdot \delta \underline{\mathbf{v}} dV &= 0, \quad \underline{\mathbf{n}} \underline{\boldsymbol{\Pi}}^P = \underline{\dot{\mathbf{i}}}_s, \\ \int_{V^t} \frac{1}{\rho} \lambda (\underline{\nabla} T)^T \cdot (\underline{\nabla} \delta T) dV - \int_{\partial V^t} q_s \cdot \delta T dS + \int_{V^t} (-\dot{q}_{\operatorname{tr}} + c_p \partial T / \partial t) \cdot \delta T dV &= 0. \end{aligned} \quad (63)$$

In mathematical terms total Lagrangian and updated Lagrangian formulations are completely equivalent as can be inferred from (60) and lead to the same mathematical solution. Though, one or the other formulations may have merits in solving some specific problems. More extensive discussion on advantages and drawbacks of both techniques can be found in Bathe [2]—cf. Sect. 6.2.3. The formula (60) also indicates that all the necessary material behavior information is brought into global mechanical balance equation only through non-objective tensor $\underline{\Pi}^P$. This information in the case of investigated here SMA materials model can be delivered to it by elimination of $\underline{\dot{\boldsymbol{\sigma}}}$ between (61)₁ and (46) to obtain

$$\underline{\Pi}^P = \underline{\mathbf{L}}^{S\text{-Je}} [\underline{\mathbf{d}} - \dot{\underline{\boldsymbol{\kappa}}}] - \underline{\mathbf{L}} \alpha_0 \dot{T} - \underline{\mathbf{d}} \boldsymbol{\sigma} - \boldsymbol{\sigma} \boldsymbol{\omega}. \quad (64)$$

The coupled set of thermo-mechanical equations (63) is usually solved by staggered solution algorithm. Upon finding satisfying the equations, the fields of velocity $\underline{\mathbf{v}}(\underline{\mathbf{x}}, t)$ and temperature rate $\dot{T}(\underline{\mathbf{x}}, t)$ all the relevant state and kinematical variables can be updated by a time step dt .

6 Concluding remarks

In the present work, the very comprehensive general structure of the macroscopic thermodynamic theory of pseudoelasticity of shape memory alloys was presented taking into account geometrical effects, allowing for large rotations and large strains. Next a complete 3D macroscopic, phenomenological, thermodynamic model of shape memory alloys pseudoelastic behavior was formulated. The model is linearly elastic in terms of elastic logarithmic strain. Hypotheses on which the model is based are verified only partially at present, namely for isothermal proportional loadings. The presently developed model can be relatively easily extended to the range of impact loadings (high pressures), whenever there is known experimental characteristic pressure \leftrightarrow volumetric strain. As the model was developed in non-equilibrium thermodynamic formalism, its generalization to the case when elastic moduli depend on state of the material, e.g., different elastic moduli of austenitic and martensitic phases or to take into account some material damaging effects also does not present significant difficulties upon condition that relevant experimental data are available. Finally, it is worth mentioning that the model is very well suited for implementation into finite element code.

Appendix

Corotational elastic logarithmic derivative $\overset{\Omega_{e,\log}}{\underline{T}}$

Xiao et al. in their work [26] searching for corotational derivative of logarithmic total strain tensor, which would be equal to the tensor of total Eulerian strain rate $\underline{\mathbf{d}}$ introduced the concept of logarithmic spin $\underline{\boldsymbol{\omega}}^{\log}$, and next the concept of the corotational logarithmic derivative of any second-order tensor $\underline{\mathbf{T}}$ as specified below

$$\overset{\circ}{\underline{T}}^{\log} \equiv \dot{\underline{T}} + \underline{\mathbf{T}} \underline{\boldsymbol{\omega}}^{\log} - \underline{\boldsymbol{\omega}}^{\log} \underline{\mathbf{T}}. \quad (A1)$$

The spin $\underline{\boldsymbol{\omega}}^{\log}$ is such that the following relation is fulfilled identically

$$\overset{\circ}{\underline{\mathbf{e}}}^{\log} \equiv \dot{\underline{\mathbf{e}}} + \underline{\mathbf{e}} \underline{\boldsymbol{\omega}}^{\log} - \underline{\boldsymbol{\omega}}^{\log} \underline{\mathbf{e}} = \underline{\mathbf{d}}, \quad \underline{\mathbf{e}} = \ln(\underline{\mathbf{V}}). \quad (A2)$$

Xiao et al. delivered explicit expressions for $\underline{\boldsymbol{\omega}}^{\log}$

$$\underline{\boldsymbol{\omega}}^{\log} = \underline{\boldsymbol{\omega}} + \underline{\mathbf{N}}^{\log}, \quad \underline{\mathbf{N}}^{\log} = \sum N_{ij}^{\log} \underline{\mathbf{n}}_i \otimes \underline{\mathbf{n}}_j, \quad (A3)$$

$$N_{ij}^{\log} = 0 \quad i = j, \quad N_{ij}^{\log} = \left(\frac{2}{\ln(\chi_i/\chi_j)} + \frac{1 + (\chi_i/\chi_j)}{1 - (\lambda_i/\chi_j)} \right) d_{ij} \quad \chi_i \neq \chi_j \quad \text{and} \quad i \neq j,$$

where $\underline{\boldsymbol{\omega}}$ is body spin, $\underline{\mathbf{n}}_i$ denote principal directions of left total stretch tensor $\underline{\mathbf{V}}$, and χ_i denote principal values of $\underline{\mathbf{V}}^2$.

In full analogy it is introduced the concept of elastic logarithmic corotational derivative and elastic logarithmic spin as follows:

$$\overset{\circ}{\mathbf{T}}^{\text{e-log}} \equiv \dot{\mathbf{T}} + \mathbf{T}\underline{\boldsymbol{\omega}}^{\text{e-log}} - \underline{\boldsymbol{\omega}}^{\text{e-log}}\mathbf{T}, \quad (\text{A4})$$

where the spin $\underline{\boldsymbol{\omega}}^{\text{e-log}}$ by definition fulfills identically relation

$$\overset{\circ}{\mathbf{e}}^{\text{e-log}} \equiv \dot{\mathbf{e}}^{\text{e}} + \mathbf{e}^{\text{e}}\underline{\boldsymbol{\omega}}^{\text{e-log}} - \underline{\boldsymbol{\omega}}^{\text{e-log}}\mathbf{e}^{\text{e}} = \underline{\mathbf{d}}^{\text{e}}, \quad \mathbf{e}^{\text{e}} = \ln(\mathbf{V}^{\text{e}}). \quad (\text{A5})$$

Upon comparing (A5) with (17)

$$\overset{\circ}{\mathbf{e}}^{\text{e}} - \mathbf{E}^{\text{de}}(\mathbf{V}^{\text{e}})\underline{\mathbf{d}}^{\text{e}} \equiv \dot{\mathbf{e}}^{\text{e}} + \mathbf{e}^{\text{e}}(\underline{\boldsymbol{\omega}}^{\text{e}} + \underline{\mathbf{x}}^{\text{e}}) - (\underline{\boldsymbol{\omega}}^{\text{e}} + \underline{\mathbf{x}}^{\text{e}})\mathbf{e}^{\text{e}} = \underline{\mathbf{d}}^{\text{e}}. \quad (\text{A6})$$

It is straightforward to find out that

$$\underline{\boldsymbol{\omega}}^{\text{e-log}} = \underline{\boldsymbol{\omega}}^{\text{e}} + \underline{\mathbf{x}}^{\text{e}}, \quad \underline{\mathbf{x}}^{\text{e}} = -(\underline{\mathbf{x}}^{\text{e}})^T, \quad \underline{\mathbf{x}}^{\text{e}} = \Sigma x_{ij}^{\text{e}} \mathbf{n}_i^{\text{e}} \otimes \mathbf{n}_j^{\text{e}}, \quad (\text{A7})$$

$$x_{ij}^{\text{e}} = 0 \quad i = j, \quad x_{ij}^{\text{e}} = \left(\frac{1}{\ln(\lambda_i^{\text{e}}/\lambda_j^{\text{e}})} + \frac{1 + (\lambda_i^{\text{e}}/\lambda_j^{\text{e}})^2}{1 - (\lambda_i^{\text{e}}/\lambda_j^{\text{e}})^2} \right) d_{ij}^{\text{e}} \quad \lambda_i^{\text{e}} \neq \lambda_j^{\text{e}} \quad \text{and} \quad i \neq j,$$

where $\underline{\mathbf{x}}^{\text{e}}$ is a spin tensor, \mathbf{n}_i^{e} denote principal directions of left elastic stretch tensor \mathbf{V}^{e} , and λ_i^{e} denote principal values of \mathbf{V}^{e} . Whatever deformation in the form of dilatation does not change the value of tensor $\underline{\mathbf{x}}^{\text{e}}$, while for purely dilatational deformation $\lambda_1^{\text{e}} = \lambda_2^{\text{e}} = \lambda_3^{\text{e}}$ it is identically equal to zero $\underline{\mathbf{x}}^{\text{e}} \equiv 0$. Please note that

$\overset{\circ}{\mathbf{T}}^{\text{e-log}} \neq \overset{\circ}{\mathbf{T}}^{\text{log}}$ even when $\underline{\boldsymbol{\omega}}^{\text{in}} = \mathbf{0}$ ($\underline{\boldsymbol{\omega}}^{\text{e}} = \underline{\boldsymbol{\omega}}$).

In order to obtain (58) let us calculate corotational elastic logarithmic derivative (A4) of both sides of (24)₁, and use property (A5)₁. Substituting next (3)₁ and (40), one can express the rate constitutive relation of elasticity in the form

$$J^{-1} \overset{\circ}{\underline{\boldsymbol{\tau}}}^{\text{e-log}} = \underline{\mathbf{L}} \left[\underline{\mathbf{d}} - \dot{z}\underline{\boldsymbol{\kappa}} - z\overset{\circ}{\mathbf{J}}\mathbf{e} \right] - \underline{\mathbf{P}}\underline{\boldsymbol{\alpha}}_0\dot{T}. \quad (\text{A8})$$

In view of property (37), it is

$$J^{-1} \overset{\circ}{\underline{\boldsymbol{\tau}}}^{\text{e-log}} = \underline{\mathbf{L}} \left[\underline{\mathbf{d}} - \dot{z}\underline{\boldsymbol{\kappa}} - z\underline{\mathbf{P}}\overset{\circ}{\underline{\boldsymbol{\tau}}}^{\text{e-log}} - \underline{\boldsymbol{\alpha}}_0\dot{T} \right] - z\underline{\mathbf{L}} \left[\underline{\boldsymbol{\kappa}}(\underline{\boldsymbol{\omega}}^{\text{e}} - \underline{\boldsymbol{\omega}}^{\text{e-log}}) - (\underline{\boldsymbol{\omega}}^{\text{e}} - \underline{\boldsymbol{\omega}}^{\text{e-log}})\underline{\boldsymbol{\kappa}} \right], \quad (\text{A9})$$

$$J^{-1} \overset{\circ}{\underline{\boldsymbol{\tau}}}^{\text{e-log}} = \underline{\mathbf{L}}^S \left[\underline{\mathbf{d}} - \dot{z}\underline{\boldsymbol{\kappa}} - \underline{\boldsymbol{\alpha}}_0\dot{T} \right] - z\underline{\mathbf{L}}^S \left[\underline{\boldsymbol{\kappa}}(\underline{\boldsymbol{\omega}}^{\text{e}} - \underline{\boldsymbol{\omega}}^{\text{e-log}}) - (\underline{\boldsymbol{\omega}}^{\text{e}} - \underline{\boldsymbol{\omega}}^{\text{e-log}})\underline{\boldsymbol{\kappa}} \right],$$

$$\overset{\circ}{\underline{\boldsymbol{\tau}}}^{\text{e-log}} = J\underline{\mathbf{L}}^S \left[\underline{\mathbf{d}} - \dot{z}\underline{\boldsymbol{\kappa}} - \underline{\boldsymbol{\alpha}}_0\dot{T} \right] - z \left[\underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}}(\underline{\boldsymbol{\omega}}^{\text{e}} - \underline{\boldsymbol{\omega}}^{\text{e-log}}) - (\underline{\boldsymbol{\omega}}^{\text{e}} - \underline{\boldsymbol{\omega}}^{\text{e-log}})\underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}} \right].$$

In the above definition (44)₂ was used. In view of the isotropy of tensor $\underline{\mathbf{L}}^S$ —cf. (45) and (35), tensor $\underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}} \equiv J\underline{\mathbf{L}}^S\underline{\boldsymbol{\kappa}}$ is collinear with $\underline{\boldsymbol{\kappa}}(\underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}}\underline{\boldsymbol{\kappa}} = \underline{\boldsymbol{\kappa}}\underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}})$ and $\underline{\mathbf{L}}^S[\underline{\boldsymbol{\kappa}}\underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q\underline{\boldsymbol{\kappa}}] = \underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}}\underline{\boldsymbol{\omega}}^Q - \underline{\boldsymbol{\omega}}^Q\underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}}$ —cf. (33). Contracting both sides of (A9)₃ by $(\underline{\boldsymbol{\kappa}}/\rho^0)$ it is

$$(\underline{\boldsymbol{\kappa}}/\rho^0) \cdot \overset{\circ}{\underline{\boldsymbol{\tau}}}^{\text{e-log}} = (\underline{\boldsymbol{\kappa}}/\rho) \cdot \underline{\mathbf{L}}^S \underline{\mathbf{d}} - \dot{z}(\underline{\boldsymbol{\kappa}}/\rho) \cdot \underline{\mathbf{L}}^S \underline{\boldsymbol{\kappa}}, \quad (\text{A10})$$

as $\underline{\boldsymbol{\kappa}} \cdot [\underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}}(\underline{\boldsymbol{\omega}}^{\text{e}} - \underline{\boldsymbol{\omega}}^{\text{e-log}}) - (\underline{\boldsymbol{\omega}}^{\text{e}} - \underline{\boldsymbol{\omega}}^{\text{e-log}})\underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}}] = 0$ and $\underline{\boldsymbol{\kappa}} \cdot \underline{\mathbf{L}}^S \underline{\boldsymbol{\alpha}}_0\dot{T} = 0$.

In view of property (32)₁, it is

$$\underline{\boldsymbol{\kappa}} \cdot \underline{\boldsymbol{\tau}}^{\boldsymbol{\kappa}} = \underline{\boldsymbol{\kappa}} \cdot \overset{\circ}{\underline{\boldsymbol{\tau}}}^{\text{e-log}} = \underline{\boldsymbol{\kappa}} \cdot \dot{\underline{\boldsymbol{\tau}}}, \quad \overset{-\circ}{\pi}_{\underline{\boldsymbol{\tau}}}^{\text{Je}} = \overset{-\circ}{\pi}_{\underline{\boldsymbol{\tau}}}^{\text{e-log}} = \dot{\pi}_{\underline{\boldsymbol{\tau}}}^f. \quad (\text{A11})$$

Taking advantage of (A11)₁ and adding $\pi_T^f \dot{T}$ on both sides of (A10) one obtains

$$\left[(\underline{\boldsymbol{\kappa}}/\rho^0) \cdot \overset{\circ}{\underline{\boldsymbol{\tau}}}^{\text{e-log}} + \pi_T^f \dot{T} \right] + \dot{z}(\underline{\boldsymbol{\kappa}}/\rho) \cdot \underline{\mathbf{L}}^S \underline{\boldsymbol{\kappa}} = (\underline{\boldsymbol{\kappa}}/\rho) \cdot \underline{\mathbf{L}}^S \underline{\mathbf{d}} + \pi_T^f \dot{T}. \quad (\text{A12})$$

When criteria for active p.t. are fulfilled then $\dot{z} = \lambda_{(\alpha)}^{\sigma} \cdot \tilde{\pi}_{\tau}^f$ —cf. (53). Substituting this relation in the above equation, one obtains

$$\left[1 + \lambda_{(\alpha)}^{\sigma} (\underline{\kappa}/\rho) \cdot \underline{\mathbf{L}}^S \underline{\kappa} \right] \tilde{\pi}_{\tau}^f = (\underline{\kappa}/\rho) \cdot \underline{\mathbf{L}}^S \underline{\mathbf{d}} + \pi_T^f \dot{T}, \quad (\text{A13})$$

and finally

$$\tilde{\pi}_{\tau}^f = \frac{(\underline{\kappa}/\rho) \cdot \underline{\mathbf{L}}^S \underline{\mathbf{d}} + \pi_T^f \dot{T}}{\left[1 + \lambda_{(\alpha)}^{\sigma} (\underline{\kappa}/\rho) \cdot \underline{\mathbf{L}}^S \underline{\kappa} \right]} = f(\underline{\mathbf{d}}, \dot{T}). \quad (\text{A14})$$

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