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TRANSFORMATION INDUCED PLASTICITY REVISED AN UPDATED FORMULATION†

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Abstract—An externally stressed specimen in the process of a phase transformation may show a significant nonlinear behavior which is known as transformation-induced plasticity (TRIP). The TRIP-strain can be irreversible as in the case of steels, or reversible with a certain hysteresis as in the case of shape memory alloys. The basic mechanisms contributing to this nonlinear phenomena are the accommodation process of the transformation strain and the orientation process of the transforming microregions. TRIP strain formulations carried out so far do not meet both effects. A thermodynamical concept is presented in this paper to find a TRIP strain rate which takes into account the coupling of phase transformation and microplasticity. The start and progress of the transformation condition, during which the plastic behavior governs the transformation/plastic processes, are derived by solving a conditional extremum problem, composed of the dissipation inequality and the constraint conditions: the transformation condition and the yield condition. The thermomechanical and calorimetric constitutive equations are derived in rate form when the transformation and the plastic processes are fully coupled. Some illustrative examples are discussed by assuming a concrete form of the Gibbs free energy and the transformation/yield conditions. The cross-coupling effect of the transformation and plasticity is well understood in the TRIP strain rate and the transformation kinetics. © 1998 Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

In the only existing monography entirely devoted to transformation-induced plasticity (TRIP), Mitter (1987) describes TRIP as "significantly increased plasticity during a phase change. Even under an externally applied load stress with the corresponding equivalent stress being small in relation to the 'normal' yield stress of the material, plastic deformation occurs".

During a transformation, a part of a material (let us say, a microregion) may change its volume and occasionally its shape, too. As explained in more detail in the next chapter, the geometrical change of a microregion is described by a transformation tensor ε^*. To achieve compatibility between the neighboring material and the transformating microregion under consideration, the misfit must be compensated (or accommodated) by an eigenstress state which may vary within a grain of a polycrystalline material, but at least from grain to grain. In many cases (e.g. in the case of "classical" transformations of steel during quenching) the misfit leads to at least a plastification of the neighboring material of the microregion, sometimes even to a plastification of the microregions themselves. It can be easily imagined that the development of this local eigenstress state is influenced by an externally applied global stress state on a certain given specimen. The superposition of these two stressing or straining "mechanisms" may initiate or even promote plastification. Therefore,

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† Dedicated to Prof. Haupt on the occasion of his 60th birthday.

a macroscopic plastic deformation of the specimen can be observed. This mechanical effect, associated with a phase transformation, was originally considered as TRIP. Several continuum mechanics treatments have appeared in the past [see Johnson and Greenwood (1962); Greenwood and Johnson (1965); Leblond *et al.* (1986)]. The latter authors, however, were among the first reporting a rigorous concept. Their starting point is that the plastic strain $\mathbf{E}^p$ in a transforming material must be considered as the average of the local plastic strain, ε^p, of both phases:

$$\mathbf{E}^p = \langle \varepsilon^p \rangle = \xi \langle \varepsilon^p \rangle_n + (1-\xi) \langle \varepsilon^p \rangle_o \tag{1}$$

where ξ is the transformed volume fraction. $\langle . \rangle$ means the mesodomain average of an entity and can be split into

$$\langle . \rangle = \xi \langle . \rangle_n + (1-\xi) \langle . \rangle_o .$$

$\langle\,\rangle$ is defined by (see e.g. Kreher, 1990)

$$\langle f \rangle = \frac{1}{8\pi^2} \int f(\omega) g(\omega)\,\mathrm{d}\omega = \frac{1}{8\pi^2} \int_0^{\pi} \int_0^{2\pi} \int_0^{2\pi} f(\omega) g(\omega)\,\mathrm{d}\psi\,\mathrm{d}\phi\,\mathrm{d}\theta$$

where $\omega^T = (\theta, \psi, \phi)$ are the Euler angles between the local coordinate system attached to the microregion and the global coordinate system attached to the sample specimen, and $g(\omega)$ is a normalized distribution function.

The labels "n" and "o", refer to the new (product) and old (parent) phase, respectively, and its rate

$$\dot{\mathbf{E}}^p = \xi \langle \dot\varepsilon^p \rangle_n + (1-\xi) \langle \dot\varepsilon^p \rangle_o + \dot\xi \langle \Delta\varepsilon^p \rangle_{\tilde{S}} . \tag{2}$$

$\langle \Delta\varepsilon^p \rangle_{\tilde{S}}$ must be considered as the surface average of the plastic strain difference along the transformation front $\tilde{\mathbf{S}} \cdot \dot\varepsilon^p$ resp. $\dot\varepsilon^p$, in turn depends on the local stress $\boldsymbol{\Sigma}^{\mathrm{loc}}$ and the temperature T as

$$\dot\varepsilon^p = (\ldots) : \dot{\boldsymbol{\Sigma}}^{\mathrm{loc}} + (\ldots)\dot T \tag{3}$$

and $\boldsymbol{\Sigma}^{\mathrm{loc}}$ is assumed to depend on $\boldsymbol{\Sigma}$, the load stress, T and ξ as in

$$\dot{\boldsymbol{\Sigma}}^{\mathrm{loc}} = (\ldots) : \dot{\boldsymbol{\Sigma}} + (\ldots)\dot T + (\ldots)\dot\xi . \tag{4}$$

The insertion of eqn (4) into eqn (3) allows us to write $\dot\varepsilon^p$ as

$$\dot\varepsilon^p = (\ldots) : \dot{\boldsymbol{\Sigma}} + (\ldots)\dot T + (\ldots)\dot\xi \tag{5}$$

which finally leads to a splitting of the plastic rate $\dot{\mathbf{E}}^p$ into two parts

$$\dot{\mathbf{E}}^p = \dot{\mathbf{E}}^p_c + \dot{\mathbf{E}}^p_T \tag{6a}$$

$$\dot{\mathbf{E}}^p_c = [\ldots\ldots]_1 : \dot{\boldsymbol{\Sigma}} + [\ldots\ldots]_2 \dot T \tag{6b}$$

$$\dot{\mathbf{E}}^p_T = [\ldots\ldots]_3 \dot\xi + \langle \Delta\varepsilon^p \rangle_{\tilde{S}} \dot\xi . \tag{6c}$$

$\dot{\mathbf{E}}^p_c$ is considered the "classical" plastic strain rate which appears also for $\dot\xi$ and $\dot{\mathbf{E}}^p_T$ as the "TRIP" strain rate for $\dot\xi \neq 0$. Leblond *et al.* (1989) gave explicit expressions for the terms $[\ldots\ldots]_1$, $[\ldots\ldots]_2$ and $[\ldots\ldots]_3$ and neglected $\langle \Delta\varepsilon^p \rangle_{\tilde{S}}$. The terms $[\ldots\ldots]_1$ (here in slightly modified form) and $[\ldots\ldots]_3$ yield

$$[\ldots\ldots]_1 = \frac{9}{4}\frac{(1-\xi)}{\xi E}\frac{1}{\Sigma_{yo}\Sigma_{eq}}\mathbf{S}\otimes\mathbf{S}, \mathbf{S}\otimes\mathbf{S} \rightarrow S_{ij}S_{kl} \tag{7a}$$

$$[\ldots\ldots]_3 = \frac{\varepsilon_0}{\Sigma_{yo}}(\ln\xi)\mathbf{S} \tag{7b}$$

where Σ_{yo} is the yield stress of the parent phase, E the Young's modulus, S the deviator of Σ, $\Sigma_{eq} = (\frac{3}{2}\mathbf{S}:\mathbf{S})^{1/2}$, ε_0 the transformation volume strain.

The merits of Leblond's work are without any doubt based on a systematic treatment of a "tridimensional" formulation of the plastic behavior of a transforming metal despite some "obvious" and "hidden" shortcomings that have come to light in the last few years. First of all, one can learn from eqn (7b) that only the volume change ε_0 enters the TRIP strain rate. Since in the case of a displacive (martensitic) transformation also a significant transformation shear γ occurs in a microregion, γ must be accommodated by the neighboring material, too. Fischer gave a proposal for taking into account γ in a (7b)-type equation, see Fischer (1990) for an isotropic and Fischer and Schlögl (1995) for an anisotropic material.

It should be mentioned that the splitting of the plastic strain rate $\dot{\mathbf{E}}_p$ into three parts due to $\dot{\mathbf{\Sigma}}$, $\dot{T}$, $\dot{\xi}$ can be directly performed by introducing a yield function $f(\mathbf{\Sigma}, T, \kappa, \xi)$, $\kappa = (\frac{2}{3}\mathbf{E}^p:\mathbf{E}^p)^{1/2}$, and a flow rule $\dot{\mathbf{E}}_p = \dot{\lambda}(\partial f/\partial\mathbf{\Sigma})$, following the standard procedure in plasticity [see e.g. Tanaka and Nagaki (1982); Inoue and Wang (1985)].

From experiments, one knows that the transformation kinetics represented by $\dot{\xi}$ depends explicitly on $\dot{\mathbf{\Sigma}}$ and $\dot{T}$. Since this paper concentrates mainly on martensitic transformations, we are referring to the "classical" martensite kinetics formulation by Koistinen and Marburger (1959) with respect to T, and to a micromechanically based extended version with respect to T and Σ by Oberaigner *et al.* (1993)

$$\dot{\xi} = k_1(\mathbf{\Sigma}, T;\ldots):\dot{\mathbf{\Sigma}} + k_2(\mathbf{\Sigma}, T;\ldots)\dot{T}. \tag{8}$$

The consequence is that a splitting of $\dot{\mathbf{E}}^p$ into $\dot{\mathbf{E}}^p_c$ and $\dot{\mathbf{E}}^p_T$ as outlined in eqn (6) cannot physically by justified, in general, since e.g. $\dot{\mathbf{\Sigma}}$ may drive both the transformation process and the plastification.

A further point is that materials like shape memory alloys and some ceramics do not show any local plastification. However, a significant TRIP effect appears during martensitic transformation driven by a stress state $\mathbf{\Sigma}$ and additionally by the temperature T. Here, we are referring to pioneering contributions by Berveiller and cooperators [see e.g. Patoor *et al.* (1988)], who introduced, for such materials, a quasi-yield surface and a quasi-flow rule as

$$\dot{\mathbf{E}}^p_T = [\ldots\ldots]_4:\dot{\mathbf{\Sigma}} + [\ldots\ldots]_5\dot{T} \tag{6d}$$

where $[\ldots\ldots]_4$ and $[\ldots\ldots]_5$ include corresponding terms for the interaction energy of different martensitic variants. Since in the case of various shape memory alloys (nearly) no volume change exists, i.e. $\varepsilon_0 = 0$, relations (6c) and (7b) would not deliver any TRIP effect either. Here, the orientation effect comes into play. Martensitic variants, being the smallest transformed microregions, arrange themselves so that the thermodynamical "driving force" of the transforming microregions will be maximized (see also section 4). The transformation shear (which is significant in martensitic transformation) then contributes to a length change of a material element with respect to the principal stress directions [for details see Marketz and Fischer (1995)]. It is interesting to note that the orientation effect can be observed in case of steels too. Gautier *et al.* (1989) found in their experiments that the martensitic microregions orient themselves initially with respect to the load stress and, with the progress of transformation, more and more with respect to the local stress state.

Considering the deformation behavior of loaded specimens during a martensitic phase transformation it is obviously necessary to take into account both the accommodation process of the transformation strain and the orientation of the transformed microregions.

This makes it necessary to introduce, additionally to the plasticity concept, transformation thermodynamics by applying a transformation condition which must be formulated at the specimen level to allow any practical application. In the light of these aspects the TRIP effect is revised. Based on a thermodynamics concept, a new and generally applicable TRIP–strain rate term is formulated for an elastoplastic material.

The transformation strain tensor in the mesodomain $\mathbf{E}^*$ can be defined in an analogous way as for the plastic strain.

$$\mathbf{E}^* = \langle \varepsilon^* \rangle = \xi \langle \varepsilon^* \rangle_{\mathrm{n}}. \tag{9a}$$

It should be noted that $\mathbf{E}^*$ starts increasing just after the onset of transformation at some microregions in the mesodomain.

The microregions additionally experience an elastic deformation ε^{e} when they are mechanically loaded. They may also exhibit a plastic deformation ε^{p}, before or during or after the transformation. By averaging microscopic strains over the mesodomain one can identify on the level of the mesodomain the elastic strain $\mathbf{E}^{\mathrm{e}}$ and the plastic strain $\mathbf{E}^{\mathrm{p}}$

$$\mathbf{E}^{\mathrm{e}} = \langle \varepsilon^{\mathrm{e}} \rangle \quad \mathbf{E}^{\mathrm{p}} = \langle \varepsilon^{\mathrm{p}} \rangle. \tag{9b,c}$$

To demonstrate the TRIP–strain, reference is made to the "classical" TRIP-test where a longitudinal specimen is subjected to a constant load stress and the martensitic transformation is driven by cooling only, see e.g. the experiments by Gautier and Simon (1988) for a Fe-31% Ni–steel. The TRIP–strain $\mathbf{E}^{\mathrm{TP}}$ is defined as the deviator of the nonelastic part of the total strain tensor $\mathbf{E}$:

$$\mathbf{E}^{\mathrm{TP}} = (\mathbf{E} - \mathbf{E}^{\mathrm{e}})^{\mathrm{D}} \neq \mathbf{E}^{\mathrm{T}}_{\mathrm{P}}. \tag{10}$$

The label "D" refers to the deviator. It should be mentioned that $\mathbf{E}^{\mathrm{TP}} \neq \mathbf{E}^{\mathrm{T}}_{\mathrm{P}}$ is due to the influence of $\dot{\xi}$. Going back to the work of Greenwood and Johnson (1985) the TRIP–strain rate $\mathbf{E}^{\mathrm{T}}$ is assumed as

$$\dot{\mathbf{E}}^{\mathrm{TP}} = \tilde{K} f(\xi) \mathbf{S} \dot{\xi}. \tag{11}$$

$\tilde{K}$ and $f(\xi)$ are taken from experimental data. Various proposals are discussed in an overview paper by Fischer *et al.* (1994). Recently Gautier *et al.* (1995) reviewed the stress effect on the mechanical behavior and the morphology of martensite in steels. They presented a micromechanical interpretation of the TRIP-test too. Figure 1 demonstrates TRIP–strain

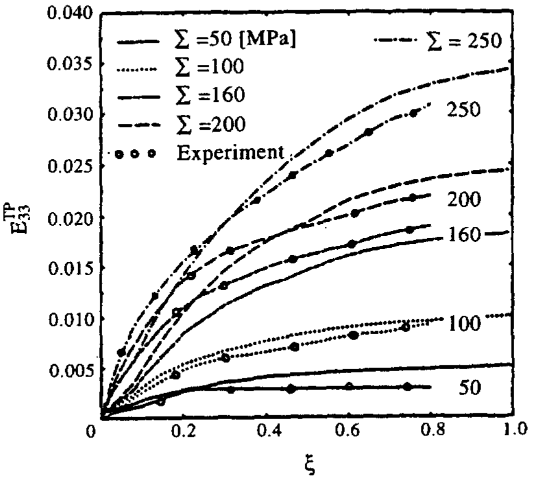

Fig. 1. TRIP–strain E^{TP}_{33} in dependence on martensite volume fraction ξ for different levels of uniaxial load tensile stress Σ. The open circles represent the experimental data by Gautier *et al.* (1988).

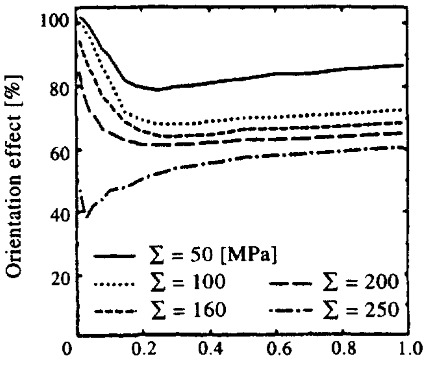

Fig. 2. Orientation effect contributing to the TRIP–strain in dependence on martensite volume fraction ξ for different levels of uniaxial load tensile stress Σ.

curves depending on the transformed volume fraction ξ. Experimental data and the curves from the simulation by Marketz and Fischer (1994) are being compared. This micromechanical simulation allows also to distinguish between $\mathbf{E}^*$ and $\mathbf{E}^p$, so the orientation effect on the total TRIP–strain can be quantified (see Fig. 2). One can learn from this experimental and simulation work that both plastification, E^p, and orientation, $\mathbf{E}^*$, contributed to the TRIP–strain in the same order.

2. EXTERNAL AND INTERNAL VARIABLES FOR TRIP

Obviously, the temperature T and/or the loadstress Σ control the transformation process in a specimen. If we assume locally constant T and a homogeneous loadstress Σ, the specimen level coincides with the mesoscopic level. From here on, we concentrate on the mesoscopic level, and consider Σ and T to be the external state variables in a material point. The material itself possesses a microstructure consisting of transformed and untransformed microregions. We take this microstructure into account and describe it by a set of observables, the internal state variables, which are, however, not controllable. ξ represents the transformed volume fraction and $\mathbf{E}^*$ the average of the transformation tensors ε^*. ξ can be detected, e.g. by magnetic permeability measurement. If we start with the first law of thermodynamics, we have to switch to the total strain $\mathbf{E}$ and to the entropy density η as external state variables.

In order to describe the situation exactly, let us assume that the Green strain tensor defined by:

$$\mathbf{E} = (\mathbf{F}^T \cdot \mathbf{F} - \mathbf{I})/2 \tag{12a}$$

with the deformation gradient $\mathbf{F}$ and the unit tensor $\mathbf{I}$ can be additively decomposed in the rate form

$$\dot{\mathbf{E}} = \dot{\mathbf{E}}^e + \dot{\mathbf{E}}^p + \dot{\mathbf{E}}^* \tag{12b}$$

where $\dot{\mathbf{E}}^e$ and $\dot{\mathbf{E}}^p$ stand for the elastic and plastic components, respectively.

The decomposition of the rate of the entropy density η [see Tanaka and Nagaki (1982)], is also assumed here by

$$\dot{\eta} = \dot{\eta}^e + \dot{\eta}^p + \dot{\eta}^*. \tag{13}$$

The thermomechanical process is then understood to be fully specified by a set of state variables $j = (\mathbf{E}^e, \eta^e; \xi, \mathbf{E}^*, \eta^*; \kappa, \mathbf{E}^p, \eta^p)$.

κ specifies the workhardening of the materials, e.g. in the sense of an equivalent plastic strain. The last six variables are the internal state variables. It should be mentioned that the use of $\mathbf{E}^e$ (which is, however, not directly controllable), instead of $\mathbf{E}$ as external state variable brings along a computational advantage, which will be outlined later.

3. MESOSCOPIC DESCRIPTION OF TRANSFORMATION/DEFORMATION PROCESSES

The thermomechanical transformation process on the mesoscopic level of the material can be described by the energy balance and the Clausius–Duhem inequality [see Tanaka *et al.* (1986)]:

$$\rho \dot{u} - \boldsymbol{\sigma} : \mathbf{L} + \operatorname{div} \mathbf{q} - \rho r = 0 \tag{14}$$

$$\rho \dot{\eta} - \rho \frac{r}{T} + \operatorname{div}\left(\frac{\mathbf{q}}{T}\right) \geqslant 0 \tag{15}$$

where, as in all following formulae the following physical entities are employed:

ρ, ρ_0 are the densities in the current and reference configurations, respectively
u is the internal energy density,
$\boldsymbol{\sigma}$ is the Cauchy stress tensor,
$\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1}$ is the velocity gradient,
$\mathbf{q}$ is the heat flux,
r is the heat production term,
η is the entropy density,
T is the temperature.

Throughout this study the notation "div" stands for the divergence with respect to the Eulerian coordinate system, while "Grad" means the gradient with respect to the Lagrangian coordinate system.

The internal energy density u contains the strain energy due to external load and due to interaction of grains, which leads to internal eigenstresses. The strain energy due to internal stress has to be expressed with mesoscopic variables. See Kreher (1990) concerning averaging of microscopic variables in order to get mesoscopic variables.

Introducing the Gibbs free energy density Ψ (using mesoscopic variables)

$$\Psi' = \Psi(\boldsymbol{\Sigma}, T; \xi, \mathbf{E}^*, \eta^*, \kappa, \mathbf{E}^{\mathrm{p}}, \eta^{\mathrm{p}}) = u - \eta^{\mathrm{e}} T - \frac{1}{\rho_0} \boldsymbol{\Sigma} : \mathbf{E}^{\mathrm{e}} \tag{16}$$

with the second Piola–Kirchhoff stress tensor $\boldsymbol{\Sigma}$ and the material heat flux $\mathbf{Q}$

$$\boldsymbol{\Sigma} = \frac{\rho_0}{\rho} \mathbf{F}^{-1} \cdot \boldsymbol{\sigma} \cdot (\mathbf{F}^{-1})^{\mathrm{T}} \quad \mathbf{Q} = \frac{\rho_0}{\rho} \mathbf{F}^{-1} \cdot \mathbf{q} \tag{17a,b}$$

the Clausius–Duhem inequality (15) is reduced to

$$-\left(\rho_0 \frac{\partial \Psi}{\partial \boldsymbol{\Sigma}} + \mathbf{E}^{\mathrm{e}}\right) : \dot{\boldsymbol{\Sigma}} - \rho_0 \left(\frac{\partial \Psi}{\partial T} + \eta^{\mathrm{e}}\right) \dot{T} + K_1 \dot{\xi} + \mathbf{K}_2 : \dot{\mathbf{E}}^* + K_3 \dot{\eta}^* + K_4 \dot{\kappa} + \mathbf{K}_5 : \dot{E}^{\mathrm{p}} + K_6 \dot{\eta}^{\mathrm{p}} - \frac{1}{T} \mathbf{Q} \cdot \operatorname{Grad} T \geqslant 0 \tag{18}$$

where the thermodynamic forces

$$K_1 = -\rho_0 \frac{\partial \Psi}{\partial \xi}, \quad \mathbf{K}_2 = \mathbf{\Sigma} - \rho_0 \frac{\partial \Psi}{\partial \mathbf{E}^*}, \quad K_3 = \rho_0 \left(T - \frac{\partial \Psi}{\partial \eta^*} \right) \tag{19a–c}$$

$$\mathbf{K}_4 = -\rho_0 \frac{\partial \Psi}{\partial \kappa}, \quad \mathbf{K}_5 = \mathbf{\Sigma} - \rho_0 \frac{\partial \Psi}{\partial \mathbf{E}^{\mathrm{p}}}, \quad K_6 = \rho_0 \left(T - \frac{\partial \Psi}{\partial \eta^{\mathrm{p}}} \right) \tag{19d–f}$$

are introduced. The thermodynamic force $\mathbf{K}_1$ is called the driving force of transformation in metallurgy [see e.g. Wayman (1983); Kaufman and Hillert (1992)].

For the sake of a clear presentation of the theory, the following generalized vectors are introduced. The generalized thermodynamic force $\mathbf{K}_{\mathrm{t}}$ relating to the transformation, and $\mathbf{K}_{\mathrm{p}}$ relating to the plastic deformation

$$\mathbf{K}_{\mathrm{t}} = (K_1, \mathbf{K}_2, K_3), \quad \mathbf{K}_{\mathrm{p}} = (K_4, \mathbf{K}_5, K_6) \tag{20a,b}$$

the corresponding generalized internal variables

$$\kappa_{\mathrm{t}} = (\xi, \mathbf{E}^*, \eta^*), \quad \kappa_{\mathrm{p}} = (\kappa, \mathbf{E}^{\mathrm{p}}, \eta^{\mathrm{p}}) \tag{21a,b}$$

and their material derivatives

$$\dot{\kappa}_{\mathrm{t}} = (\dot{\xi}, \dot{\mathbf{E}}^*, \dot{\eta}^*), \quad \dot{\kappa}_{\mathrm{p}} = (\dot{\kappa}, \dot{\mathbf{E}}^{\mathrm{p}}, \dot{\eta}^{\mathrm{p}}).$$

A generalized state variable composed of $\mathbf{\Sigma}$ and T,

$$\mathbf{\Omega} = (\mathbf{\Sigma}, T) \tag{22}$$

is also introduced for later use.

It is worth noting here that the Gibbs free energy (16) can be simply written as

$$\Psi = \Psi(\mathbf{\Omega}; \kappa_{\mathrm{t}}; \kappa_{\mathrm{p}}) \tag{23}$$

and, therefore, the same is true for the generalized thermodynamic forces

$$\mathbf{K}_{\mathrm{t}} = \mathbf{K}_{\mathrm{t}}(\mathbf{\Omega}; \kappa_{\mathrm{t}}; \kappa_{\mathrm{p}}), \quad \mathbf{K}_{\mathrm{p}} = \mathbf{K}_{\mathrm{p}}(\mathbf{\Omega}; \kappa_{\mathrm{t}}; \kappa_{\mathrm{p}}). \tag{24a,b}$$

The usual discussion in continuum thermodynamics leads from eqn (18) to the relations

$$\mathbf{E}^{\mathrm{e}} = -\rho_0 \frac{\partial \Psi}{\partial \mathbf{\Sigma}}, \quad \eta^{\mathrm{e}} = -\frac{\partial \Psi}{\partial T} \tag{25a,b}$$

$$D = \mathbf{K}_{\mathrm{t}} * \dot{\kappa}_{\mathrm{t}} + \mathbf{K}_{\mathrm{p}} * \dot{\kappa}_{\mathrm{p}} - \frac{1}{T}\mathbf{Q} \cdot \mathrm{Grad}\, T \geqslant 0. \tag{25c}$$

The inner product $*$ is explained in Appendix A.

Equation (25a,b) governs the reversible thermomechanical processes of the material, from which one can derive the thermomechanical and calorimetric constitutive equations in rate form if the elastic process is reasonably assumed not to be influenced by the irreversible processes [see Tanaka *et al.* (1986)]:

$$\dot{\mathbf{E}}^{\mathrm{e}} = \mathbf{D}^{-1} : \dot{\mathbf{\Sigma}} + \mathbf{\Theta} \dot{T}, \quad \dot{\eta}^{\mathrm{e}} = \frac{\boldsymbol{\theta}}{\rho_0} : \dot{\mathbf{\Sigma}} - c\dot{T} \tag{26a,b}$$

$$\mathbf{D}^{-1} = -\rho_0 \frac{\partial^2 \Psi}{\partial \mathbf{\Sigma}\, \partial \mathbf{\Sigma}}, \quad \mathbf{\Theta} = -\rho_0 \frac{\partial^2 \Psi}{\partial \mathbf{\Sigma}\, \partial T}, \quad c = -\rho_0 \frac{\partial^2 \Psi}{\partial T^2}. \tag{26c–e}$$

The material parameter tensors $\mathbf{D}$ and $\mathbf{\Theta}$, and the constant c, correspond to the elastic moduli tensor, the thermoelastic tensor and the specific heat, respectively. The dissipation inequality (25c) plays an important role in predicting the irreversible material behavior, which is elaborated in the next section.

4. CONSTITUTIVE EQUATIONS IN IRREVERSIBLE PROCESSES

Let us start from the dissipation inequality (25c). The conventional plasticity theory [see Lemaitre and Chaboche (1990)], requires that the plastic process must be restricted by a yield condition, which may generally be given in the present context as

$$f = f(\mathbf{\Omega}\,;\mathbf{K}_t,\mathbf{K}_p\,;\kappa_t,\kappa_p) = 0 \quad \text{and} \quad \dot{f} = 0. \tag{27a,b}$$

The second condition is referred to as the consistency condition.

Since the transformation condition must be fulfilled locally in each microregion, a global transformation condition can also be formulated at the mesoscopic level, which can be written in the most general ways as

$$g = g(\mathbf{\Omega}\,;\mathbf{K}_t,\mathbf{K}_p\,;\kappa_t,\kappa_p) = 0 \quad \text{and} \quad \dot{g} = 0. \tag{28a,b}$$

The time t is included in eqn (28) as an implicit parameter through the state variables, which reflects the fact that the martensitic transformation is of a diffusionless character [see Nishiyama (1978)]. The requirement of the second law of thermodynamics is now fulfilled by following the concept of maximum dissipation rate (25c) with the thermomechanical restrictions (27) and (28). This concept goes back to Onsager in the thirties and was outlined, e.g. by Edelen (1971), Eringen (1975), Peric (1993) and recently by Nguyen (1994) for a multiple plastic potential (a set of convex functions $f_1, \ldots, f_m = 0$). The problem can, therefore, be interpreted as an extremum problem of

$$\begin{aligned}\bar{D} &= D - \dot{\lambda} f - \dot{\mu} g \\ &= \mathbf{K}_t * \dot{\kappa}_t + \mathbf{K}_p * \dot{\kappa}_p - \frac{1}{T}\mathbf{Q}\cdot \operatorname{Grad} T - \dot{\lambda} f - \dot{\mu} g\end{aligned} \tag{29}$$

with the Lagrange multipliers $\dot{\lambda}$ and $\dot{\mu}$.

The usual mathematical procedure yields

$$\frac{\partial \bar{D}}{\partial \mathbf{K}_t} = 0 \quad \frac{\partial \bar{D}}{\partial \mathbf{K}_p} = 0 \quad \frac{\partial \bar{D}}{\partial \dot{\mu}} = 0 \quad \frac{\partial \bar{D}}{\partial \dot{\lambda}} = 0 \tag{30a–d}$$

which leads to the final formulae

$$\dot{\kappa}_t = \dot{\lambda}\frac{\partial f}{\partial \mathbf{K}_t} + \dot{\mu}\frac{\partial g}{\partial \mathbf{K}_t} \quad \dot{\kappa}_p = \dot{\lambda}\frac{\partial f}{\partial \mathbf{K}_p} + \dot{\mu}\frac{\partial g}{\partial \mathbf{K}_p} \tag{31a,b}$$

$$g = 0 \quad f = 0. \tag{32a,b}$$

Equations (31a, b) represent the evolution equations, or properly speaking, the constitutive equations for the generalized internal variables κ_t and κ_p.

Equation (31a), which is explicitly read as

$$\dot{\xi} = \dot{\lambda}\frac{\partial f}{\partial K_1} + \dot{\mu}\frac{\partial g}{\partial K_1} \quad \dot{\mathbf{E}}^* = \dot{\lambda}\frac{\partial f}{\partial \mathbf{K}_2} + \dot{\mu}\frac{\partial g}{\partial \mathbf{K}_2} \tag{33a,b}$$

$$\dot{\eta}^* = \dot{\lambda}\frac{\partial f}{\partial K_3} + \dot{\mu}\frac{\partial g}{\partial K_3} \tag{33c}$$

is discussed elsewhere [see Tanaka *et al.* (1994)], in the case of no plastic deformation. Equation (33a) is called the transformation kinetics in metallurgy (Raghavan, 1992), which governs the progress of transformation. The component equations in eqn (32b) are written as follows:

$$\dot{\kappa} = \dot{\lambda}\frac{\partial f}{\partial K_4} + \dot{\mu}\frac{\partial g}{\partial K_4} \quad \dot{\mathbf{E}}^{\mathrm{p}} = \dot{\lambda}\frac{\partial f}{\partial \mathbf{K}_5} + \dot{\mu}\frac{\partial g}{\partial \mathbf{K}_5} \tag{34a,b}$$

$$\dot{\eta}^{\mathrm{p}} = \dot{\lambda}\frac{\partial f}{\partial K_6} + \dot{\mu}\frac{\partial g}{\partial K_6}. \tag{34c}$$

Equation (34a) governs the work-hardening of the material while eqn (34b) is called the thermomechanical flow rule in plasticity and eqn (34c) the calorimetric flow rule (Tokuoka, 1982). The second terms on the right-hand side in eqns (34a–c) represents the contribution from the transformation.

The first term on the right-hand side of eqn (33a), $\dot{\lambda}(\partial f/\partial K_1)$, states that the plastic process can activate the transformation, resulting in an irreversible strain rate $\dot{\lambda}(\partial f/\partial \mathbf{K}_2)$ in eqn (33b) and an irreversible entropy density rate $\dot{\lambda}(\partial f/\partial K_3)$ in eqn (33c). This effect stems solely from the assumption that the yield condition $f = 0$ includes also the thermodynamic force $\mathbf{K}_{\mathrm{t}}$ as variable. On the other hand, the second term on the right-hand side of eqn (34a), $\dot{\mu}(\partial g/\partial K_4)$, expresses that the work-hardening process is influenced by the progress of transformation, too. As a result an irreversible strain rate $\dot{\mu}(\partial g/\partial \mathbf{K}_5)$ and an irreversible entropy density rate $\dot{\mu}(\partial g/\partial K_6)$ are observed.

A conventional TRIP formulation (see section 1) refers only to the term $\dot{\lambda}(\partial f/\partial \mathbf{K}_5)$ in eqn (34b). Such a formulation of the TRIP–strain rate proportional to S, see eqns (7b) and (11), does not envisage plastification after unloading. This contradicts recent experiments by Videau *et al.* (1996) where a TRIP–strain rate has been observed after total unloading. The conventional TRIP–strain rate formulation, however, neither takes into account $\dot{\mathbf{E}}^*$, consisting of two terms not the second term $\dot{\mu}(\partial g/\partial \mathbf{K}_5)$ in $\dot{\mathbf{E}}^{\mathrm{p}}$. The latter may stem from a redistribution of the dislocations due to the transformation processes.

However, shape memory alloys remain within the elastic range in almost all technical cases. The strain rate $\dot{\mu}(\partial f/\partial \mathbf{K}_2)$ plays a major role then [see Tanaka *et al.* (1994, 1996)]. The so-called transformation superplasticity [see e.g. Padmanabhan and Davies (1980); Tanaka *et al.* (1984)], is observed to take place solely due to the progress of the transformation without any motion of dislocations.

This phenomenon can also be explained by means of the terms $\dot{\mu}(\partial g/\partial \mathbf{K}_2)$ and $\dot{\mu}(\partial g/\partial \mathbf{K}_5)$. The Lagrange multipliers $\dot{\lambda}$ and $\dot{\mu}$ introduced in eqn (29) can be determined from the consistency conditions eqns (27b) and (28b),

$$\dot{f} = \frac{\partial f}{\partial \mathbf{\Omega}} \circ \dot{\mathbf{\Omega}} + \frac{\partial \mathbf{f}}{\partial \mathbf{K}_{\mathrm{t}}} * \left(\frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \mathbf{\Omega}} \circ \dot{\mathbf{\Omega}} + \frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \kappa_{\mathrm{t}}} * \dot{\kappa}_{\mathrm{t}} + \frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \kappa_{\mathrm{p}}} * \dot{\kappa}_{\mathrm{p}}\right) + \frac{\partial f}{\partial \mathbf{K}_{\mathrm{p}}} * \left(\frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \mathbf{\Omega}} \circ \dot{\mathbf{\Omega}} + \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \kappa_{\mathrm{t}}} * \dot{\kappa}_{\mathrm{t}} + \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \kappa_{\mathrm{p}}} * \dot{\kappa}_{\mathrm{p}}\right)$$

$$+ \frac{\partial f}{\partial \kappa_{\mathrm{t}}} * \dot{\kappa}_{\mathrm{t}} + \frac{\partial f}{\partial \kappa_{\mathrm{p}}} * \dot{\kappa}_{\mathrm{p}} = 0 \tag{35a}$$

$$\dot{g} = \frac{\partial g}{\partial \mathbf{\Omega}} \circ \dot{\mathbf{\Omega}} + \frac{\partial \mathbf{g}}{\partial \mathbf{K}_{\mathrm{t}}} * \left(\frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \mathbf{\Omega}} \circ \dot{\mathbf{\Omega}} + \frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \kappa_{\mathrm{t}}} * \dot{\kappa}_{\mathrm{t}} + \frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \kappa_{\mathrm{p}}} * \dot{\kappa}_{\mathrm{p}}\right) + \frac{\partial g}{\partial \mathbf{K}_{\mathrm{p}}} * \left(\frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \mathbf{\Omega}} \circ \dot{\mathbf{\Omega}} + \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \kappa_{\mathrm{t}}} * \dot{\kappa}_{\mathrm{t}} + \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \kappa_{\mathrm{p}}} * \dot{\kappa}_{\mathrm{p}}\right)$$

$$+ \frac{\partial g}{\partial \kappa_{\mathrm{t}}} * \dot{\kappa}_{\mathrm{t}} + \frac{\partial g}{\partial \kappa_{\mathrm{p}}} * \dot{\kappa}_{\mathrm{p}} = 0 \tag{35b}$$

where the inner product $\circ$ is defined in Appendix A.

The above relation holds only if the plastic deformation as well as the transformation progresses. By substituting the evolution eqns (31a, b) for κ_{t} and κ_{p} into eqn (35), one arrives, after straightforward calculation, at an explicit expression for $\dot{\lambda}$ and $\dot{\mu}$:

$$\dot{\lambda} = \mathbf{L} \circ \dot{\mathbf{\Omega}}, \quad \dot{\mu} = \mathbf{M} \circ \dot{\mathbf{\Omega}} \tag{36a,b}$$

where

$$\mathbf{L} = \Delta\left[\left(F_g \frac{\partial g}{\partial \mathbf{K}_t} - G_g \frac{\partial f}{\partial \mathbf{K}_t}\right) * \frac{\partial \mathbf{K}_t}{\partial \Omega} + \left(F_g \frac{\partial g}{\partial \mathbf{K}_p} - G_g \frac{\partial f}{\partial \mathbf{K}_p}\right) * \frac{\partial \mathbf{K}_p}{\partial \Omega} + \left(F_g \frac{\partial g}{\partial \Omega} - G_g \frac{\partial f}{\partial \Omega}\right)\right] \tag{37a}$$

$$\mathbf{M} = \Delta\left[\left(G_f \frac{\partial f}{\partial \mathbf{K}_t} - F_f \frac{\partial g}{\partial \mathbf{K}_t}\right) * \frac{\partial \mathbf{K}_t}{\partial \Omega} + \left(G_f \frac{\partial f}{\partial \mathbf{K}_p} - F_f \frac{\partial g}{\partial \mathbf{K}_p}\right) * \frac{\partial \mathbf{K}_p}{\partial \Omega} + \left(G_f \frac{\partial f}{\partial \Omega} - F_f \frac{\partial g}{\partial \Omega}\right)\right] \tag{37b}$$

$$F_f = f_{\kappa_t} * \frac{\partial f}{\partial \mathbf{K}_t} + f_{\kappa_p} * \frac{\partial f}{\partial \mathbf{K}_p}, \quad F_g = f_{\kappa_t} * \frac{\partial g}{\partial \mathbf{K}_t} + f_{\kappa_p} * \frac{\partial g}{\partial \mathbf{K}_p} \tag{38a,b}$$

$$G_f = g_{\kappa_t} * \frac{\partial f}{\partial \mathbf{K}_t} + g_{\kappa_p} * \frac{\partial f}{\partial \mathbf{K}_p}, \quad G_g = g_{\kappa_t} * \frac{\partial g}{\partial \mathbf{K}_t} + g_{\kappa_p} * \frac{\partial g}{\partial \mathbf{K}_p} \tag{38c,d}$$

$$f_{\kappa_t} = \frac{\partial f}{\partial \mathbf{K}_t} * \frac{\partial \mathbf{K}_t}{\partial \kappa_t} + \frac{\partial f}{\partial \mathbf{K}_p} * \frac{\partial \mathbf{K}_p}{\partial \kappa_t} + \frac{\partial f}{\partial \kappa_t} \tag{39a}$$

$$f_{\kappa_p} = \frac{\partial f}{\partial \mathbf{K}_t} * \frac{\partial \mathbf{K}_t}{\partial \kappa_p} + \frac{\partial f}{\partial \mathbf{K}_p} * \frac{\partial \mathbf{K}_p}{\partial \kappa_p} + \frac{\partial f}{\partial \kappa_p} \tag{39b}$$

$$g_{\kappa_t} = \frac{\partial g}{\partial \mathbf{K}_t} * \frac{\partial \mathbf{K}_t}{\partial \kappa_t} + \frac{\partial g}{\partial \mathbf{K}_p} * \frac{\partial \mathbf{K}_p}{\partial \kappa_t} + \frac{\partial g}{\partial \kappa_t} \tag{39c}$$

$$g_{\kappa_p} = \frac{\partial g}{\partial \mathbf{K}_t} * \frac{\partial \mathbf{K}_t}{\partial \kappa_p} + \frac{\partial g}{\partial \mathbf{K}_p} * \frac{\partial \mathbf{K}_p}{\partial \kappa_p} + \frac{\partial g}{\partial \kappa_p} \tag{39d}$$

$$\Delta^{-1} = F_f G_g - F_g G_f. \tag{40}$$

The constitutive equations for the internal variables κ_t and κ_p in relation to the generalized state variable $\mathbf{\Omega}$ are now finally given by

$$\dot{\kappa}_t = \left(\frac{\partial f}{\partial \mathbf{K}_t} \otimes \mathbf{L} + \frac{\partial g}{\partial \mathbf{K}_t} \otimes \mathbf{M}\right) \circ \dot{\mathbf{\Omega}} \tag{41a}$$

$$\dot{\kappa}_p = \left(\frac{\partial f}{\partial \mathbf{K}_p} \otimes \mathbf{L} + \frac{\partial g}{\partial \mathbf{K}_p} \otimes \mathbf{M}\right) \circ \dot{\mathbf{\Omega}}. \tag{41b}$$

It should be mentioned that both the case of pure plasticity ($f = 0, g < 0$) and pure transformation ($f < 0, g = 0$), as in the case of shape memory alloys, cannot directly be deduced from eqn (41), since these equations stem from extremizing D with the two constraints $f = 0$ and $g = 0$.

For the sake of completeness $\boldsymbol{\lambda}$ for plasticity without transformation ($\lambda|_{f=0,g<0}$) and $\dot{\mu}$ for transformation only in the elastic range ($\dot{\lambda}|_{g=0,f<0}$) are presented as

$$\dot{\lambda}|_{f=0,g<0} = -\left[\left(\frac{\partial f}{\partial \mathbf{K}_p} * \frac{\partial \mathbf{K}_p}{\partial \kappa_p} + \frac{\partial f}{\partial \kappa_p}\right) * \frac{\partial f}{\partial \mathbf{K}_p}\right]^{-1} \left[\left(\frac{\partial f}{\partial \mathbf{\Sigma}} + \frac{\partial f}{\partial \mathbf{K}_p} * \frac{\partial \mathbf{K}_p}{\partial \mathbf{\Sigma}}\right) : \dot{\mathbf{\Sigma}} + \left(\frac{\partial f}{\partial T} + \frac{\partial f}{\partial \mathbf{K}_p} * \frac{\partial \mathbf{K}_p}{\partial T}\right) \dot{T}\right] \tag{42a}$$

$$\dot{\mu}|_{g=0,f<0} = -\left[\left(\frac{\partial g}{\partial \mathbf{K}_t} * \frac{\partial \mathbf{K}_t}{\partial \kappa_t} + \frac{\partial g}{\partial \kappa_t}\right) * \frac{\partial g}{\partial \mathbf{K}_t}\right]^{-1} \left[\left(\frac{\partial g}{\partial \mathbf{\Sigma}} + \frac{\partial g}{\partial \mathbf{K}_t} * \frac{\partial \mathbf{K}_t}{\partial \mathbf{\Sigma}}\right) : \dot{\mathbf{\Sigma}} + \left(\frac{\partial g}{\partial T} + \frac{\partial g}{\partial \mathbf{K}_t} * \frac{\partial \mathbf{K}_t}{\partial T}\right)\dot{T}\right]. \tag{42b}$$

Substitution of eqns (31a, b) into the dissipation inequality (25c) leads to

$$D = \dot{\lambda}\left(\mathbf{K}_t * \frac{\partial f}{\partial \mathbf{K}_t} + \mathbf{K}_p * \frac{\partial f}{\partial \mathbf{K}_p}\right) + \dot{\mu}\left(\mathbf{K}_t * \frac{\partial g}{\partial \mathbf{K}_t} + \mathbf{K}_p * \frac{\partial g}{\partial \mathbf{K}_p}\right) - \frac{1}{T}\mathbf{Q}\cdot \mathrm{Grad}\, T \geqslant 0. \tag{43}$$

In the case of a homogeneous temperature T (Grad $T = 0$) eqn (43), together with the convexity conditions for f and g with respect to $\mathbf{K}_t$ and $\mathbf{K}_p$, which should be read in the present context as

$$\mathbf{K}_t * \frac{\partial f}{\partial \mathbf{K}_t} + \mathbf{K}_p * \frac{\partial f}{\partial \mathbf{K}_p} \geqslant 0, \quad \mathbf{K}_t * \frac{\partial g}{\partial \mathbf{K}_t} + \mathbf{K}_p * \frac{\partial g}{\partial \mathbf{K}_p} \geqslant 0 \tag{44a,b}$$

claims that the plastic deformation and the transformation process take place only if

$$\dot{\lambda} \geqslant 0 \quad \text{and} \quad \dot{\mu} \geqslant 0 \tag{45a,b}$$

are both satisfied.

Referring to the convexity conditions, f and g are assumed to have the structure

$$f = f_\Omega(\mathbf{\Omega}\,; \mathbf{K}_t, \mathbf{K}_p) - f_\kappa(\kappa_t, \kappa_p) = 0, \quad g = g_\Omega(\mathbf{\Omega}, \mathbf{K}_t, \mathbf{K}_p) - g_\kappa(\kappa_t, \kappa_p) = 0.$$

The homogeneous functions f_Ω and g_Ω of $\mathbf{K}_t$ and $\mathbf{K}_p$ of degree 1, ensure positive semidefiniteness in eqn (44).

5. ILLUSTRATIVE EXAMPLES

To show the capacity of the concept the evolution equations for $\dot{E}^p$, $\dot{\kappa}$, $\dot{E}^*$, $\dot{\xi}$ are derived on the basis of a broad function class of Ψ, f, g and are compared with existing concepts. Specifically the interaction of transformation and plasticity shall be demonstrated.

Let us assume a Gibbs free energy Ψ of the structure

$$\rho_0\Psi = -\tfrac{1}{2}\mathbf{\Sigma} : \mathbf{D}^{-1} : \mathbf{\Sigma} + h(\xi, \mathbf{E}^*, \mathbf{E}^p) + p(\xi, \kappa) + \rho_0(\phi_{\mathrm{ch,o}} - \xi\Delta\phi_{\mathrm{ch}}(T)]. \tag{46}$$

The effect of the interaction of the microregions and, therefore, of the internal stress state is reflected in h, the material hardening in p. The Gibbs free energy of the stress free specimen is the last part and depends on temperature only, see also eqn (53c). The (weak) thermomechanical coupling is neglected since the thermal strains are usually much smaller than $\mathbf{E}^*$ or E^p.

The yield condition f is defined as a function

$$f = f(K_4, \mathbf{K}_5, \xi, \mathbf{E}^*, \kappa, \mathbf{E}^p). \tag{47}$$

The transformation condition depends on K_1, $\mathbf{K}_2$ and ξ

$$g = g(K_1, \mathbf{K}_2, \xi). \tag{48}$$

This can be justified through consistency with the Koistinen–Marburger relation shown below.

Some algebraic computations, which are documented in Appendix B, yield

$$\dot{\lambda} = \frac{1}{F_\mathrm{f} - G_\mathrm{f}\dfrac{F_\mathrm{g}}{G_\mathrm{g}}}\left[\left(\frac{F_\mathrm{g}}{G_\mathrm{g}}\frac{\partial g}{\partial \mathbf{K}_2} - \frac{\partial f}{\partial \mathbf{K}_5}\right):\dot{\mathbf{\Sigma}} + \frac{F_\mathrm{g}}{G_\mathrm{g}}\frac{\partial g}{\partial \mathbf{K}_1}\rho_0\frac{\partial \Delta\phi_\mathrm{ch}}{\partial T}\dot{T}\right] \tag{49}$$

$$\dot{\mu} = \frac{1}{G_\mathrm{g} - F_\mathrm{g}\dfrac{G_\mathrm{f}}{F_\mathrm{f}}}\left[\left(-\frac{\partial g}{\partial \mathbf{K}_2} + \frac{G_\mathrm{f}}{F_\mathrm{f}}\frac{\partial f}{\partial \mathbf{K}_5}\right):\dot{\mathbf{\Sigma}} - \frac{\partial g}{\partial \mathbf{K}_1}\rho_0\frac{\partial \Delta\phi_\mathrm{ch}}{\partial T}\dot{T}\right]. \tag{50}$$

Equation (49) coincides with the case of pure plasticity for $F_\mathrm{g}/G_\mathrm{g} = 0$, and eqn (50) with the case of a pure transformation process for $G_\mathrm{f}/F_\mathrm{f} = 0$.

The evolution equations for the internal variables follow from eqns (33) and (34) as

$$\dot{\xi} = \dot{\mu}\frac{\partial g}{\partial \mathbf{K}_1} \quad \dot{\mathbf{E}}^* = \dot{\mu}\frac{\partial g}{\partial \mathbf{K}_2} \tag{51a,b}$$

$$\dot{\kappa} = \dot{\lambda}\frac{\partial f}{\partial \mathbf{K}_4} \quad \dot{\mathbf{E}}^\mathrm{p} = \dot{\lambda}\frac{\partial f}{\partial \mathbf{K}_5}. \tag{51c,d}$$

Special, but reasonable functions for f and g are assumed in order to simplify the structure of the evolution equations:

$$f = \tfrac{1}{2}\mathbf{K}_5^\mathrm{D} : \mathbf{K}_5^\mathrm{D} - f_0(K_4, \xi, \kappa) \tag{52}$$

$$g = K_1 + \mathbf{E}_\mathrm{f}^* : \mathbf{K}_2 - g_0(\xi). \tag{53a}$$

$\mathbf{K}_5^\mathrm{D}$ is the deviator of the tensor $\mathbf{K}_5$.

A simple example of a local transformation condition is (Fischer *et al.*, 1992, 1994; Levitas, 1995a, b)

$$\rho\Delta\phi_\mathrm{ch}(T) + (\mathbf{\Sigma} + \tau) : \varepsilon^* = F^* + F_\mathrm{m}. \tag{53b}$$

In general, the right side depends on

$$\Delta\phi_\mathrm{ch}(T) = \phi_\mathrm{ch,o}(T) - \phi_\mathrm{ch,n}(T). \tag{53c}$$

$\Delta\phi_\mathrm{ch}$ represents the chemical "driving force" being the difference in the free energy of the stress-free material. $(\mathbf{\Sigma} + \tau) : \varepsilon^*$ can be considered as the mechanical "driving force" where τ represents the internal stress state in addition to the load stress state. The driving forces must be in balance with the transformation barrier F^* and the mechanical barrier F_m.

Again one has to average in order to get a mesoscopic transformation condition. Since both, external temperature and external load stress, occur not only in the Gibbs free energy density, but also in the transformation condition, both quantities are essential for the transformation mechanism. Therefore, the model has no limitations in considering the transformation due to stress and/or temperature.

The microstructure is reflected in an average sense by the variable $\mathbf{K}_2$ which includes the internal variable $\mathbf{E}^*$ via the Gibbs free energy. It turns out in eqn (56b) that $\mathbf{E}_\mathrm{f}^*$ has the physical meaning of a maximum recoverable strain tensor during transformation if it is a constant tensor.

The physical justification for eqn (53a), more or less a simple formulation of g, lies in the fact that the famous Koistinen–Marburger kinetics relation (Koistinen *et al.*, 1959), with an additional stress term, can be derived in a straightforward manner as shown by Tanaka *et al.* (1994, 1996).

The Lagrange multipliers now follow as

$$\dot{\lambda} = \frac{1}{F_{\mathrm{f}} - G_{\mathrm{f}}\frac{F_{\mathrm{g}}}{G_{\mathrm{g}}}}\left[\left(\frac{F_{\mathrm{g}}}{G_{\mathrm{g}}}\mathbf{E}_{\mathrm{f}}^{*} - \mathbf{K}_5^{\mathrm{D}}\right):\dot{\mathbf{\Sigma}} + \frac{F_{\mathrm{g}}}{G_{\mathrm{g}}}\rho_0\frac{\partial\Delta\phi_{\mathrm{ch}}}{\partial T}\dot{T}\right] \tag{54a}$$

$$\dot{\mu} = \frac{1}{G_{\mathrm{g}} - F_{\mathrm{g}}\frac{G_{\mathrm{f}}}{F_{\mathrm{f}}}}\left[\left(-\mathbf{E}_{\mathrm{f}}^{*} + \frac{G_{\mathrm{f}}}{F_{\mathrm{f}}}\mathbf{K}_5^{\mathrm{D}}\right):\dot{\mathbf{\Sigma}} - \rho_0\frac{\partial\Delta\phi_{\mathrm{ch}}}{\partial T}\dot{T}\right] \tag{54b}$$

with

$$F_{\mathrm{f}} = \left(\frac{\partial f_0}{\partial K_4}\right)^2\frac{\partial^2 p}{\partial\kappa^2} + \frac{\partial f_0}{\partial\kappa}\frac{\partial f_0}{\partial K_4} - \mathbf{K}_5^{\mathrm{D}}:\frac{\partial^2 h}{\partial\mathbf{E}^{\mathrm{p}}\,\partial\mathbf{E}^{\mathrm{p}}}:\mathbf{K}_5^{\mathrm{D}} \tag{55a}$$

$$F_{\mathrm{g}} = \frac{\partial f_0}{\partial K_4}\frac{\partial^2 p}{\partial\xi\,\partial\kappa}\frac{\partial f_0}{\partial\xi} - \mathbf{K}_5^{\mathrm{D}}:\frac{\partial^2 h}{\partial\xi\,\partial\mathbf{E}^{\mathrm{p}}} - \mathbf{K}_5^{\mathrm{D}}:\frac{\partial^2 h}{\partial\mathbf{E}^{*}\,\partial\mathbf{E}^{\mathrm{p}}}:\mathbf{E}_{\mathrm{f}}^{*} \tag{55b}$$

$$G_{\mathrm{f}} = \frac{\partial f_0}{\partial K_4}\frac{\partial^2 p}{\partial\xi\,\partial\kappa} - \mathbf{K}_5^{\mathrm{D}}:\frac{\partial^2 h}{\partial\xi\,\partial\mathbf{E}^{\mathrm{p}}} \tag{55c}$$

$$G_{\mathrm{g}} = -\frac{\partial^2 h}{\partial\xi^2} - \frac{\partial^2 p}{\partial\xi^2} - \frac{\partial g_0}{\partial\xi} - 2\mathbf{E}_{\mathrm{f}}^{*}:\frac{\partial^2 h}{\partial\xi\,\partial\mathbf{E}^{*}} - \mathbf{E}_{\mathrm{f}}^{*}:\frac{\partial^2 h}{\partial\mathbf{E}^{*}\,\partial\mathbf{E}^{*}}:\mathbf{E}_{\mathrm{f}}^{*}. \tag{55d}$$

The above relations are derived in Appendix B.

The evolution equations (51) now read

$$\dot{\xi} = \dot{\mu}, \quad \dot{\mathbf{E}}^{*} = \mathbf{E}_{\mathrm{f}}^{*}\dot{\xi}, \quad \dot{\kappa} = -\frac{\partial f_0}{\partial K_4}\dot{\lambda}, \quad \dot{\mathbf{E}}^{\mathrm{p}} = \dot{\lambda}\mathbf{K}_5^{\mathrm{D}} \tag{56}$$

with $\mathbf{K}_5^{\mathrm{D}} = \mathbf{S} - (\partial h/\partial\mathbf{E}^{\mathrm{p}})^{\mathrm{D}}$. Again, the label "D" refers to the deviator.

5.1. *The TRIP–strain rate*

Referring to section 2 the TRIP–strain rate is defined as

$$\dot{\mathbf{E}}^{\mathrm{TP}} = \dot{\mathbf{E}}^{\mathrm{p}} + (\dot{\mathbf{E}}^{*})^{\mathrm{D}} \tag{57}$$

on the assumption of a constant external load stress, $\dot{\mathbf{\Sigma}} = 0$. Assuming that $\dot{\mathbf{\Sigma}} = 0$, relation $\dot{\xi} = \dot{\mu}$ and eqn (54a,b) allows us to write

$$\dot{\lambda} = -\frac{F_{\mathrm{g}}}{G_{\mathrm{f}}}\dot{\xi}, \quad \dot{\mathbf{E}}^{\mathrm{p}} = -\frac{F_{\mathrm{g}}}{G_{\mathrm{f}}}\left[\mathbf{S} - \left(\frac{\partial h}{\partial\mathbf{E}^{\mathrm{p}}}\right)^{\mathrm{D}}\right]\dot{\xi}. \tag{58a}$$

It follows for $\dot{\mathbf{E}}^{\mathrm{TP}}$ that

$$\dot{\mathbf{E}}^{\mathrm{TP}} = -\frac{F_{\mathrm{g}}}{G_{\mathrm{f}}}\left[\mathbf{S} - \left(\frac{\partial h}{\partial\mathbf{E}^{\mathrm{p}}}\right)^{\mathrm{D}}\right]\dot{\xi} + (\mathbf{E}_{\mathrm{f}}^{*})^{\mathrm{D}}\dot{\xi}. \tag{58b}$$

The following conclusions can be drawn from this newly derived TRIP–strain rate:

- If $\partial h/\partial\mathbf{E}^{\mathrm{p}}$ and $(\mathbf{E}_{\mathrm{f}}^{*})^{\mathrm{D}}$ are $\mathbf{0}$, the TRIP–strain rate corresponds to the conventional one (for comparison see eqns (10) and (11)).
- The TRIP–strain rate meets the orientation effect as explained in detail in section 2 by means of the term $(\mathbf{E}_{\mathrm{f}}^{*})^{\mathrm{D}}\dot{\xi}$.
- If unloading takes place, $\mathbf{S} = \mathbf{0}$, a TRIP–strain rate survives also in the case of $\mathbf{E}_{\mathrm{f}}^{*} = 0$. This agrees with the experimental results recently gained by Videau *et al.* (1996). This group proposed to introduce in eqn (11) a term $\mathbf{S} - \tilde{\mathbf{S}}$ [see Videau *et al.* (1994)] instead

of $\mathbf{S}.\tilde{\mathbf{S}}$ is interpreted as a backstress and acquires a physical meaning in the present derivation

$$\tilde{\mathbf{S}} = \left(\frac{\partial h}{\partial \mathbf{E}^{\mathrm{p}}}\right)^{\mathrm{D}}.$$

The backstress is derived with respect to $\mathbf{E}^{\mathrm{p}}$, but h contains also $\mathbf{E}^*$ and ξ. Therefore this backstress $\tilde{\mathbf{S}}$ comes from the transformation, too.

5.2. *Transformation kinetics*

Considering eqn (56a), eqn (54b) yields a kinetic relation. If we take the simplest case, i.e. that h does not depend on $\mathbf{E}^{\mathrm{p}}$ and $p(\xi, \kappa)$ can be decomposed into $p_1(\xi)+p_2(\kappa)$ leading to

$$\rho_0\Psi = -\tfrac{1}{2}\boldsymbol{\Sigma}:\mathbf{D}^{-1}:\boldsymbol{\Sigma}+h(\xi,\mathbf{E}^*)+p_1(\xi)+p_2(\kappa)+\rho_0(\phi_{\mathrm{ch,o}}-\xi\Delta\phi_{\mathrm{ch}}(T)) \tag{59}$$

relation (54b) yields after short calculation

$$\dot{\xi} = \frac{1}{G_{\mathrm{g}}}\left[-\mathbf{E}_{\mathrm{f}}^*:\dot{\boldsymbol{\Sigma}}-\rho_0\frac{\partial\Delta\phi_{\mathrm{ch}}}{\partial T}\dot{T}\right] \tag{60a}$$

$$G_{\mathrm{g}}(\xi) = -\left[\frac{\partial^2 h}{\partial\xi^2}+\frac{\partial^2 p_1}{\partial\xi^2}+2\mathbf{E}_{\mathrm{f}}^*:\frac{\partial^2 h}{\partial\xi\,\partial\mathbf{E}^*}+\mathbf{E}_{\mathrm{f}}^*:\frac{\partial^2 h}{\partial\mathbf{E}^*\,\partial\mathbf{E}^*}:\mathbf{E}_{\mathrm{f}}^*+\frac{\partial g_0}{\partial\xi}\right]. \tag{60b}$$

Now the famous Koistinen–Marburger kinetics (Koistinen and Marburger, 1959), as well as Magee's proposal for martensite kinetics (Magee, 1969) correspond directly to the case that eqn (60b) is of the form

$$G_{\mathrm{g}}(\xi) = -\frac{1}{k_0(1-\xi)}. \tag{61}$$

Then with the initial conditions $\boldsymbol{\Sigma} = \mathbf{0}$, $T = M_{\mathrm{S}}$, integration of eqn (60a) yields

$$\xi = 1-\exp\left[-k_0\mathbf{E}_{\mathrm{f}}^*:\boldsymbol{\Sigma}+k_0\rho_0\left|\frac{\partial\Delta\phi_{\mathrm{ch}}}{\partial T}\right|(T-M_{\mathrm{S}})\right]. \tag{62}$$

This is a generalized Koistinen–Marburger relation due to $\boldsymbol{\Sigma}$. The transformation start plane follows immediately from eqn (62) for $\xi = 0$ as

$$\mathbf{E}_{\mathrm{f}}^*:\boldsymbol{\Sigma}-\rho_0\left|\frac{\partial\Delta\phi_{\mathrm{ch}}}{\partial T}\right|(T-M_{\mathrm{S}}) = 0. \tag{63}$$

According to a discussion of transformations kinetics by Tanaka *et al.* (1985, 1986, 1990) on the shape memory effect, the condition $0 \leqslant \xi \leqslant 1$ restricts the argument of the exponential function in eqn (62) to

$$k_0\mathbf{E}_{\mathrm{f}}^*:\boldsymbol{\Sigma}-k_0\rho_0\left|\frac{\partial\Delta\phi_{\mathrm{chem}}}{\partial T}\right|(T-M_{\mathrm{S}}) \geqslant 0 \tag{64}$$

i.e. that region in the $\boldsymbol{\Sigma}-T$ space where the martensitic transformation progresses.

6. CONCLUDING REMARKS

An updated formulation is presented, from the viewpoint of continuum mechanics, for transformation-induced plasticity (TRIP), which is often observed in certain types of steels under thermomechanical loading. TRIP, as an increased plastification of a specimen subjected to an applied stress during a solid state phase transformation, has its origin in the accommodation of the significant volume and shape change of the transforming microregions. In addition, the shape change may contribute to the global deformation due to a thermodynamically optimal orientation of the product phase particles.

In this paper the TRIP process is described on the mesoscopic structural level of the material by introducing the internal variables specifying both the processes of plasticity and transformation, which are assumed to start and progress following a yield condition and a transformation condition, respectively, along with their consistency condition. The evolution equations characterizing the two processes are derived by solving a conditional extremum problem governed by the dissipation inequality which is a consequence of standard thermodynamics starting from the energy balance and the Clausius–Duhem inequality, with the yield condition and the transformation condition as thermodynamic restrictions. One of the evolution equations presents the transformation kinetics which characterizes the progress of transformation. The constitutive equations for the strain rate and the entropy density rate are obtained in the case of full coupling between plasticity and transformation.

Contrary to the conventional TRIP–strain rate the inelastic strain rate formulated here shows a rational coupling between plasticity and transformation without any empirical assumption. Both the kinematic and the isotropic hardening are automatically included in the present theory depending on the expression of the Gibbs free energy and the yield condition. The back stress during TRIP, which was intensively discussed in recent experiments of TRIP steels, also originates from this theory. In other words, the experimental data can be used to identify the material parameters.

Employing a simple form of the yield condition and the transformation condition together with a quite general expression for the Gibbs free energy, exhibiting the effect of plasticity and transformation, allows to understand the cross coupling effect of both the process of plasticity and transformation in the derived flow rule for the plastic strain rate and the transformation kinetics. In the simplest case, the transformation kinetics is reduced to the Koistinen–Marburger and Magee-type kinetics, which, however, still exhibits the effect of a three-dimensional applied stress state.

The following additional points are worth noting:

- The theory is fully compatible with the second law of thermodynamics since the dissipation inequality is the starting point of the present discussion of the processes which exhibit both the plastic and transformation effects.
- The yield condition employed here is expressed as a function of the thermodynamic forces and the internal variables. However, the theory is shown to be equivalent to the conventional plasticity with a standard yield function expressed by the stress, the temperature and the internal state variables.
- The theory can also be reduced to the case of shape memory alloys without dislocation plasticity. In this case the TRIP strain rate due to the orientation effect as well as the transformation kinetics can be derived.

The task of the next study will be to identify the material parameters of some actual materials along with some numerical illustrations according to the theory developed here.

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APPENDIX A

Let us define a generalized vector $\mathbf{A} = (A_1, \mathbf{A}_2, A_3)$ with A_1, A_3 being scalars and $\mathbf{A}_2$ being a second-order tensor. We define a further vector $\mathbf{B} = (B_1, \mathbf{B}_2, B_3)$ in the same way. An inner product C with the operator "$*$" is introduced by

$$C = \mathbf{A} * \mathbf{B} = A_1 B_1 + \mathbf{A}_2 : \mathbf{B}_2 + A_3 B_3.$$

This inner product is extended to a case where A_1, A_3 are substituted by the second-order tensors and $\mathbf{A}_2$ by a fourth-order tensor. In this case the inner product produces the second order tensor $\mathbf{C}$.

We define another inner product $\tilde{C}$ with the operator "$\circ$" for the generalized vectors $\tilde{\mathbf{A}} = (\tilde{\mathbf{A}}_1, \tilde{A}_2)$. $\tilde{\mathbf{A}}_1$ is a second-order tensor, $\tilde{A}_2$ a scalar, and $\tilde{\mathbf{B}} = (\tilde{\mathbf{B}}_1, \tilde{B}_2)$ with the same structure as $\tilde{\mathbf{A}}$,

$$\tilde{C} = \tilde{\mathbf{A}} \circ \tilde{\mathbf{B}} = \tilde{\mathbf{A}}_1 : \tilde{\mathbf{B}}_1 + \tilde{A}_2 \tilde{B}_2.$$

This inner product is extended to a case where $\tilde{\mathbf{A}}_1$ is substituted by a fourth-order tensor and $\tilde{A}_2$ by a second-order tensor. In this case the result of the inner product becomes the second-order tensor $\tilde{\mathbf{C}}$.

APPENDIX B

This appendix presents the calculations leading to eqns (49) and (50). The starting points are the Gibbs free energy Ψ, the yield condition f and the transformation condition g.

$$\rho_0 \Psi = -\tfrac{1}{2}\boldsymbol{\Sigma} : \mathbf{D}^{-1} : \boldsymbol{\Sigma} + h(\xi, \mathbf{E}^*, E^{\mathrm{p}}) + p(\xi, \kappa) + \rho_0(\phi_{\mathrm{ch,o}} - \xi \Delta\phi_{\mathrm{ch}}(T)). \tag{B1}$$

The yield condition f is defined as a function

$$f = f(K_4, \mathbf{K}_5, \xi, \mathbf{E}^*, \kappa, \mathbf{E}^{\mathrm{p}}). \tag{B2}$$

The transformation condition depends on K_1, $\mathbf{K}_2$ and ξ

$$g = g(K_1, \mathbf{K}_2, \xi). \tag{B3}$$

Taking into account the definitions eqns (20) and (21) of $\mathbf{K}_{\mathrm{t}}$, $\mathbf{K}_{\mathrm{p}}$, κ_{t} and κ_{p} one gets

$$\frac{\partial f}{\partial \mathbf{K}_{\mathrm{t}}} = (0, \mathbf{0}, 0) \quad \frac{\partial f}{\partial \kappa_{\mathrm{t}}} = \left(\frac{\partial f}{\partial \xi}, \frac{\partial f}{\partial \mathbf{E}^*}, 0\right) \tag{B4}$$

$$\frac{\partial f}{\partial \mathbf{K}_{\mathrm{p}}} = \left(\frac{\partial f}{\partial K_4}, \frac{\partial f}{\partial \mathbf{K}_5}, 0\right) \quad \frac{\partial f}{\partial \kappa_{\mathrm{p}}} = \left(\frac{\partial f}{\partial \kappa}, \frac{\partial f}{\partial \mathbf{E}^{\mathrm{p}}}, 0\right) \tag{B5}$$

$$\frac{\partial g}{\partial \mathbf{K}_{\mathrm{t}}} = \left(\frac{\partial g}{\partial K_1}, \frac{\partial g}{\partial \mathbf{K}_2}, 0\right) \quad \frac{\partial g}{\partial \kappa_{\mathrm{t}}} = \left(\frac{\partial g}{\partial \xi}, \mathbf{0}, 0\right) \tag{B6}$$

$$\frac{\partial g}{\partial \mathbf{K}_{\mathrm{p}}} = (0, \mathbf{0}, 0) \quad \frac{\partial g}{\partial \kappa_{\mathrm{p}}} = (0, \mathbf{0}, 0). \tag{B7}$$

$\mathbf{K}_{\mathrm{t}}$ and $\mathbf{K}_{\mathrm{p}}$ are calculated with eqn (19)

$$\mathbf{K}_{\mathrm{t}} = \left(-\frac{\partial h}{\partial \xi} - \frac{\partial p}{\partial \xi} + \rho_0 \Delta\phi_{\mathrm{ch}}, \mathbf{\Sigma} - \frac{\partial h}{\partial \mathbf{E}^*}, \rho_0 T\right) \tag{B8}$$

$$\mathbf{K}_{\mathrm{p}} = \left(-\frac{\partial p}{\partial \kappa}, \mathbf{\Sigma} - \frac{\partial h}{\partial \mathbf{E}^{\mathrm{p}}}, \rho_0 T\right). \tag{B9}$$

The expressions

$$\frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \kappa_{\mathrm{t}}} \quad \frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \kappa_{\mathrm{p}}} \quad \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \kappa_{\mathrm{t}}} \quad \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \kappa_{\mathrm{p}}}$$

can be assembled in the following generalized matrices:

$$\frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \kappa_{\mathrm{t}}} = \begin{bmatrix} -\dfrac{\partial^2 h}{\partial \xi^2} - \dfrac{\partial^2 p}{\partial \xi^2} & -\dfrac{\partial^2 h}{\partial \xi\, \partial \mathbf{E}^*} & 0 \\ -\dfrac{\partial^2 h}{\partial \xi\, \partial \mathbf{E}^*} & -\dfrac{\partial^2 h}{\partial \mathbf{E}^*\, \partial \mathbf{E}^*} & \mathbf{0} \\ 0 & \mathbf{0} & 0 \end{bmatrix} \tag{B10}$$

$$\frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \kappa_{\mathrm{p}}} = \begin{bmatrix} -\dfrac{\partial^2 p}{\partial \xi\, \partial \kappa} & \mathbf{0} & 0 \\ -\dfrac{\partial^2 h}{\partial \xi\, \partial \mathbf{E}^{\mathrm{p}}} & -\dfrac{\partial^2 h}{\partial \mathbf{E}^*\, \partial \mathbf{E}^{\mathrm{p}}} & \mathbf{0} \\ 0 & \mathbf{0} & 0 \end{bmatrix} \tag{B11}$$

$$\frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \kappa_{\mathrm{t}}} = \begin{bmatrix} -\dfrac{\partial^2 p}{\partial \xi\, \partial \kappa} & -\dfrac{\partial^2 h}{\partial \xi\, \partial \mathbf{E}^{\mathrm{p}}} & \mathbf{0} \\ \mathbf{0} & -\dfrac{\partial^2 h}{\partial \mathbf{E}^*\, \partial \mathbf{E}^{\mathrm{p}}} & \mathbf{0} \\ 0 & \mathbf{0} & 0 \end{bmatrix} \tag{B12}$$

$$\frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \kappa_{\mathrm{p}}} = \begin{bmatrix} -\dfrac{\partial^2 p}{\partial \xi\, \partial \kappa} & \mathbf{0} & 0 \\ 0 & -\dfrac{\partial^2 h}{\partial \mathbf{E}^{\mathrm{p}}\, \partial \mathbf{E}^{\mathrm{p}}} & \mathbf{0} \\ 0 & \mathbf{0} & 0 \end{bmatrix}. \tag{B13}$$

Products like $\partial f/\partial \mathbf{K}_{\mathrm{t}} * \partial \mathbf{K}_{\mathrm{t}}/\partial \kappa_{\mathrm{t}}$ in eqn (39) can formally be built by multiplying the matrices (B10)–(B13) with the vectors (B4)–(B7). From eqn (39) it follows for $f_{\kappa_{\mathrm{t}}}, f_{\kappa_{\mathrm{p}}}, g_{\kappa_{\mathrm{t}}}, g_{\kappa_{\mathrm{p}}}$:

$$f_{\kappa_{\mathrm{t}}} := \left(\frac{\partial f}{\partial \mathbf{K}_4}\frac{\partial^2 p}{\partial \xi\, \partial \kappa} - \frac{\partial f}{\partial \mathbf{K}_5} : \frac{\partial^2 h}{\partial \xi\, \partial \mathbf{E}^{\mathrm{p}}}, -\frac{\partial f}{\partial \mathbf{K}_5} : \frac{\partial^2 h}{\partial \mathbf{E}^*\, \partial \mathbf{E}^{\mathrm{p}}}, 0\right)^{\mathrm{T}} + \left(\frac{\partial f}{\partial \xi}, \frac{\partial f}{\partial \mathbf{E}^*}, 0\right)^{\mathrm{T}} \tag{B14}$$

$$f_{\kappa_{\mathrm{p}}} = \left(\frac{\partial f}{\partial \mathbf{K}_4}\frac{\partial^2 p}{\partial \kappa^2}, -\frac{\partial f}{\partial \mathbf{K}_5} : \frac{\partial^2 h}{\partial \mathbf{E}^{\mathrm{p}}\, \partial \mathbf{E}^{\mathrm{p}}}, 0\right)^{\mathrm{T}} + \left(\frac{\partial f}{\partial \kappa}, \frac{\partial f}{\partial \mathbf{E}^{\mathrm{p}}}, 0\right)^{\mathrm{T}} \tag{B15}$$

$$g_{\kappa_{\mathrm{t}}} = \left(\frac{\partial g}{\partial \mathbf{K}_1}\left(-\frac{\partial^2 h}{\partial \xi^2} - \frac{\partial^2 p}{\partial \xi^2}\right) - \frac{\partial g}{\partial \mathbf{K}_2} : \frac{\partial^2 h}{\partial \xi\, \partial \mathbf{E}^*} - \frac{\partial g}{\partial \mathbf{K}_1}\frac{\partial^2 h}{\partial \xi\, \partial \mathbf{E}^*} - \frac{\partial g}{\partial \mathbf{K}_2} : \frac{\partial^2 h}{\partial \mathbf{E}^*\, \partial \mathbf{E}^*}, 0\right)^{\mathrm{T}} + \left(\frac{\partial g}{\partial \xi}, \mathbf{0}, 0\right)^{\mathrm{T}} \tag{B16}$$

$$g_{\kappa_{\mathrm{p}}} = \left(-\frac{\partial g_1}{\partial K_1}\frac{\partial^2 p}{\partial \xi\, \partial \kappa}, -\frac{\partial g}{\partial K_1}\frac{\partial^2 h}{\partial \xi\, \partial \mathbf{E}^{\mathrm{p}}} - \frac{\partial g}{\partial \mathbf{K}_2} : \frac{\partial^2 h}{\partial \mathbf{E}^*\, \partial \mathbf{E}^{\mathrm{p}}}, 0\right)^{\mathrm{T}}. \tag{B17}$$

A further formal vector multiplication gives us, due to eqn (38)

$$F_{\mathrm{f}} = -\left(\frac{\partial f}{\partial K_4}\right)^2 \frac{\partial^2 p}{\partial \kappa^2} - \frac{\partial f}{\partial \mathbf{K}_5} : \frac{\partial^2 h}{\partial \mathbf{E}^{\mathrm{p}}\,\partial \mathbf{E}^{\mathrm{p}}} : \frac{\partial f}{\partial \mathbf{K}_5} + \frac{\partial f}{\partial \kappa}\frac{\partial f}{\partial K_4} + \frac{\partial f}{\partial \mathbf{E}^{\mathrm{p}}} : \frac{\partial f}{\partial \mathbf{K}_5} \tag{B18}$$

$$F_{\mathrm{g}} = -\frac{\partial g}{\partial \mathbf{K}_1}\frac{\partial f}{\partial K_4}\frac{\partial^2 p}{\partial \xi\,\partial \kappa} - \frac{\partial g}{\partial K_1}\frac{\partial f}{\partial \mathbf{K}_5} : \frac{\partial^2 h}{\partial \xi\,\partial \mathbf{E}^{\mathrm{p}}} - \frac{\partial f}{\partial \mathbf{K}_5} : \frac{\partial^2 h}{\partial \mathbf{E}^*\,\partial \mathbf{E}^{\mathrm{p}}} : \frac{\partial g}{\partial \mathbf{K}_2} + \frac{\partial g}{\partial K_1}\frac{\partial f}{\partial \xi} + \frac{\partial f}{\partial \mathbf{E}^*} : \frac{\partial g}{\partial K_2} \tag{B19}$$

$$G_{\mathrm{f}} = -\frac{\partial f}{\partial K_4}\frac{\partial g}{\partial K_1}\frac{\partial^2 p}{\partial \xi\,\partial \kappa} - \frac{\partial g}{\partial K_1}\frac{\partial f}{\partial \mathbf{K}_5} : \frac{\partial^2 h}{\partial \xi\,\partial \mathbf{E}^{\mathrm{p}}} - \frac{\partial f}{\partial \mathbf{K}_5} : \frac{\partial^2 h}{\partial \mathbf{E}^*\,\partial \mathbf{E}^{\mathrm{p}}} : \frac{\partial g}{\partial \mathbf{K}_2} \tag{B20}$$

$$G_{\mathrm{g}} = -\left(\frac{\partial g}{\partial K_1}\right)^2 \left(\frac{\partial^2 h}{\partial \xi^2} + \frac{\partial^2 p}{\partial \xi^2}\right) + \frac{\partial g}{\partial K_1}\frac{\partial g}{\partial \xi} - 2\frac{\partial g}{\partial K_1}\frac{\partial g}{\partial \mathbf{K}_2} : \frac{\partial^2 h}{\partial \xi\,\partial \mathbf{E}^*} - \frac{\partial g}{\partial \mathbf{K}_2} : \frac{\partial^2 h}{\partial \mathbf{E}^*\,\partial \mathbf{E}^*} : \frac{\partial g}{\partial \mathbf{K}_2}. \tag{B21}$$

Now Δ can be evaluated from eqn (40). Relation (37) for the vectors **L** and **M** leading to $\dot{\lambda}$ and $\dot{\mu}$, together with eqn (36) yields the relations

$$\dot{\lambda} = \Delta\left[F_{\mathrm{g}}\frac{\partial g}{\partial \mathbf{K}_{\mathrm{t}}} * \frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \boldsymbol{\Omega}} - G_{\mathrm{g}}\frac{\partial f}{\partial \mathbf{K}_{\mathrm{p}}} * \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \boldsymbol{\Omega}}\right] \circ \dot{\boldsymbol{\Omega}} \tag{B22}$$

$$\dot{\mu} = \Delta\left[-F_{\mathrm{f}}\frac{\partial g}{\partial \mathbf{K}_{\mathrm{t}}} * \frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \boldsymbol{\Omega}} + G_{\mathrm{f}}\frac{\partial f}{\partial \mathbf{K}_{\mathrm{p}}} * \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \boldsymbol{\Omega}}\right] \circ \dot{\boldsymbol{\Omega}}. \tag{B23}$$

The explicit evaluation of eqns (B22) and (B23) can best be performed by introducing two further matrices

$$\frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \boldsymbol{\Omega}} = \begin{bmatrix} \mathbf{0} & \mathbf{II} & \mathbf{0} \\ \rho_0 \dfrac{\partial \Delta\phi_{\mathrm{ch}}}{\partial T} & 0 & \rho_0 \end{bmatrix}^{\mathrm{T}}, \quad \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \boldsymbol{\Omega}} = \begin{bmatrix} \mathbf{0} & \mathbf{II} & \mathbf{0} \\ 0 & 0 & \rho_0 \end{bmatrix}^{\mathrm{T}}. \tag{B24a,b}$$

II represents the fourth-order unit tensor.

The products $\partial g/\partial \mathbf{K}_{\mathrm{t}} * \partial \mathbf{K}_{\mathrm{t}}/\partial \boldsymbol{\Omega}$, $\partial f/\partial \mathbf{K}_{\mathrm{p}} * \partial \mathbf{K}_{\mathrm{p}}/\partial \boldsymbol{\Omega}$, respectively can be built by formal multiplication of the matrices $\partial \mathbf{K}_{\mathrm{t}}/\partial \boldsymbol{\Omega}$, $\partial \mathbf{K}_{\mathrm{p}}/\partial \boldsymbol{\Omega}$, respectively, with the vectors $\partial g/\partial \mathbf{K}_{\mathrm{t}}$, $\partial f/\partial \mathbf{K}_{\mathrm{p}}$,

$$\frac{\partial g}{\partial \mathbf{K}_{\mathrm{t}}} * \frac{\partial \mathbf{K}_{\mathrm{t}}}{\partial \boldsymbol{\Omega}} = \left(\frac{\partial g}{\partial \mathbf{K}_2}, \frac{\partial g}{\partial K_1}\rho_0\frac{\partial \Delta\phi_{\mathrm{ch}}}{\partial T}\right) \tag{B25a}$$

$$\frac{\partial f}{\partial \mathbf{K}_{\mathrm{p}}} * \frac{\partial \mathbf{K}_{\mathrm{p}}}{\partial \boldsymbol{\Omega}} = \left(\frac{\partial f}{\partial \mathbf{K}_5}, 0\right). \tag{B25b}$$