About modelling the shape memory alloy behaviour based on the phase transformation surface identification under proportional loading and anisothermal conditions

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Abstract

Based on the experimental identification of the phase transformation surface, a modelling of shape memory alloys anisothermal behaviour is proposed. Within the framework of the thermodynamics of irreversible processes, two internal variables are chosen: the stress-induced martensite volume fraction and the self-accommodating martensite volume fraction. A special attention is paid to take into account the asymmetry between tension and compression behaviours.
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1. Introduction

As in the classical plasticity theory, the determination of the forward phase transformation surface (austenite (A) → martensite (M)) or reverse $(M \rightarrow A)$ under evidently proportional loading, at least, for some different external conditions, constitutes a modelling key point.

The determination of these yield surfaces needs multiaxial experiments as tension (compression)–torsion or tension (compression)–internal pressure on tubular specimens and bi or tri-compression on cubes.

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Nowadays, some recent experimental determinations in 2D situations appear in the literature (Lim and Mac Dowell, 1999; Raniecki et al., 2001; Bouvet et al., 2002, 2003). One has to say that the yield loading point detection is more easy for the forward phase transformation $A \rightarrow M$ than for the reverse one $M \rightarrow A$ (see the usual shape of the shape memory alloys (SMA) stress–strain curve, particularly in the case of copper-based alloys).

The modelling of the phase transformation initiation surfaces can also be obtained by an homogenisation process of the basic crystallographic phase transformation between the mother phase A and the product phase M (cubic $\rightarrow$ tetragonal, orthorhombic, monoclinic, etc.). In this case, a particular attention must be paid to the Hadamard's conditions or interface compatibility between austenite and martensite variants which are twinned or untwinned (Lexcellent et al., 2002).

In the present paper, a classical phenomenological model with internal variables in the frame of the thermodynamics of irreversible processes is proposed. The shape of phase transformation initiation surfaces constitutes a serious ingredient of the model. This model is extended to describe the thermomechanical behaviour with the introduction of an additional internal variable linked to the thermal effects. In a first part, the main experimental characteristics of the SMA behaviour are described. In a second part, a model taking into account these characteristics is built.

2. Basic experimental features: Forward phase transformation initiation surface

For Ni–Ti alloys with different compositions, Raniecki et al. (2001) on one hand (Fig. 1) and Bouvet et al. (2003) on other hand (Fig. 2) realise tension (compression)–torsion tests on thin walled tubes. The two investigations lead to the prime observations:

(i) The asymmetry between tension and compression is obvious as it was observed on the same alloy for pure tension–compression tests made by Orgeas and Favier (1998). The critical stress for forward phase transformation in tension (initial limit of pseudoelastic flow) σ_T^{AM} is smaller than the absolute value of the corresponding critical stress $\sigma_C^{AM} < 0$ in compression, i.e. $\sigma_T^{AM} < -\sigma_C^{AM}$. Hence, an Huber–von Mises criterion cannot be suitable (Fig. 1).

(ii) The limit curve $(\sigma, \sqrt{3}\tau)$ in the stress space, does not depend on the sign of the shear stress τ (Fig. 2).

In this context, the limit surface can be described as

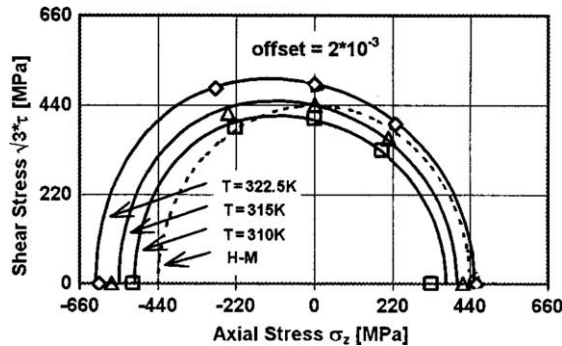$$\psi_F^\sigma(\underline{\sigma}, T) = \sigma_{\text{ef}} - \sigma_0^{AM}(T) = 0 \tag{1}$$

Fig. 1. Assymmetry of $A \rightarrow M$ pseudoelasticity limit surfaces for different temperatures. Dotted line: Huber–Von Mises modeling (Raniecki et al., 2001).
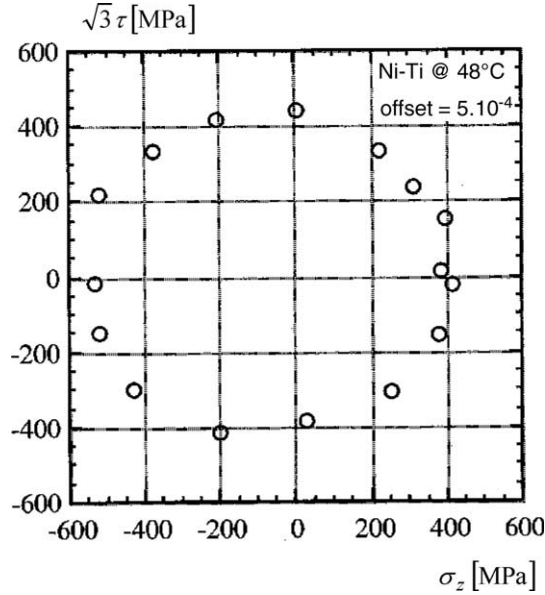
Fig. 2. Yield experimental points of phase transformation initiation for Ni–Ti polycrystal (Bouvet et al., 2003).

where $\underline{\sigma}$ being the Cauchy stresses tensor; $\sigma_0^{AM}(T)$ represents the scalar yield value of forward phase transformation. Hence under the external temperature T for pure tension $\sigma_0^{AM}(T) = \sigma_T^{AM}(T)$ and for pure compression $\sigma_0^{AM}(T) = -\sigma_C^{AM}(T)$

$$\sigma_{\text{ef}} = \bar{\sigma}f(y_\sigma), \quad \bar{\sigma} = \left(\frac{3}{2}\text{dev}\,\underline{\sigma} : \text{dev}\,\underline{\sigma}\right)^{1/2}, \quad y_\sigma = \frac{27}{2}\frac{\det(\text{dev}\,\underline{\sigma})}{\bar{\sigma}^3} \tag{2}$$

This choice of the effective stress σ_{ef} expression supposes that the phase transformation does not depend on the hydrostatic pressure. The explicit choice of the yield function ψ_F^σ is open but must guarantee its convexity in the stress space.

Referring to Fig. 1, the yield value $\sigma_0^{AM}(T)$ can be linearised as a function of the temperature T:

$$\sigma_0^{AM}(T) = b(T - M_s^0) \tag{3}$$

M_s^0 constitutes the classical martensite initiation temperature under stress free state.

This expression corresponds to the extension of the classical Clausius–Clapeyron diagram (σ, T) under multiaxial proportional loading.

Tension (compression)–internal pressure tests on tubes and bi-compression tests on cubes made of a Cu–Al–Be alloy (Bouvet et al., 2002) permit to gather important data making the choice of the function $f(y_\sigma)$ more easier. For instance, Bouvet et al. (2002) choose:

$$f(y_\sigma) = \cos\left[\frac{\cos^{-1}(1 - a(1 - y_\sigma))}{3}\right] \tag{4}$$

where a is a material parameter. This expression yields a convex forward phase transformation criterion for all values of a varying within the range $[0, 1]$ (Fig. 3). The value $a = 0.7$ has been experimentally identified by the authors. From tensile loading on the same Cu–Al–Be alloy it has been established that $b = 3$ MPa/°C.

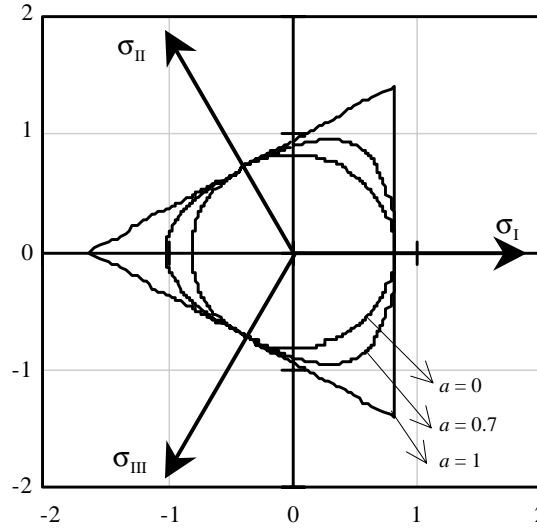Fig. 3. Pseudoelastic yield surface range in the deviatoric stress plane representation (σ_I, σ_{II}, σ_{III} eigen-stress).

Concerning the theoretical prediction of the yield surface (Fig. 1), Raniecki et al. (2001) postulate the following empirical formula for $f(y_\sigma)$, such as $f(y_\sigma = 0) = 1$, $y_\sigma = 0$ corresponding to pure shearing:

$$f(y_\sigma) = h - c \exp\left[-d(y_\sigma + 1)\right] \tag{5}$$

with $h = 1.17$, $c = 0.37$ and $d = 0.78$ for their Ni–Ti alloy.

Concerning the Cu–Al–Be alloy, the normality of the phase transformation strain rate to the yield surface has been clearly established (Fig. 4). In the particular case of a time-independent behaviour, the following flow rule can then be introduced for the forward transformation ($A \rightarrow M$):

$$\underline{\dot{\varepsilon}}^{\text{tr}} = \dot{\lambda}_F \frac{\partial \psi_F^\sigma}{\partial \underline{\sigma}} = \dot{\lambda}_F \frac{\partial \sigma_{\text{ef}}}{\partial \underline{\sigma}} \tag{6}$$

Following the classical plasticity theory, such a normal evolution law is established from the maximum dissipation principle associated with a constrained convex region $\Omega_\psi = \{\underline{\sigma}/\psi_F^\sigma(\underline{\sigma}) \leqslant 0\}$ defining the elastic domain. More generally, any convex region $\Omega_\kappa = \{\underline{\sigma}/\kappa(\underline{\sigma}) \leqslant 0\}$ with $\kappa(\underline{\sigma}) = 0$ when $\psi_F^\sigma(\underline{\sigma}) = 0$ and $\kappa(\underline{\sigma}) < 0$ when $\psi_F^\sigma(\underline{\sigma}) < 0$ can be used. This allows us to built normal evolution laws for the reverse phase transformation since in this case, the constraint elastic domain is not convex (see Eqs. (49) and (50)).

3. SMA behaviour modelling basic concepts

3.1. Thermodynamic potentials forms

Consider a representative volume element (RVE) of SMA in single solid phase state at the reference stress state $\underline{\sigma} = 0$ and at the reference temperature $T = T_0$. This phase is conventionally called "austenite" (A) and is regarded as a high-temperature phase. It can be transformed in a self-accommodating martensite (M_T) by pure cooling or in a stress-induced martensite (M_σ) under pure mechanical loading.

The martensite partition in M_T and M_σ is nowadays well accepted (Brinson, 1993; Leclercq and Lexcellent, 1996; Juhasz et al., 2002). In what follows, the austenite thermomechanical properties will be indexed $\alpha = 1$, the self-accommodating martensite $\alpha = 2$ and the stress-induced martensite $\alpha = 3$.
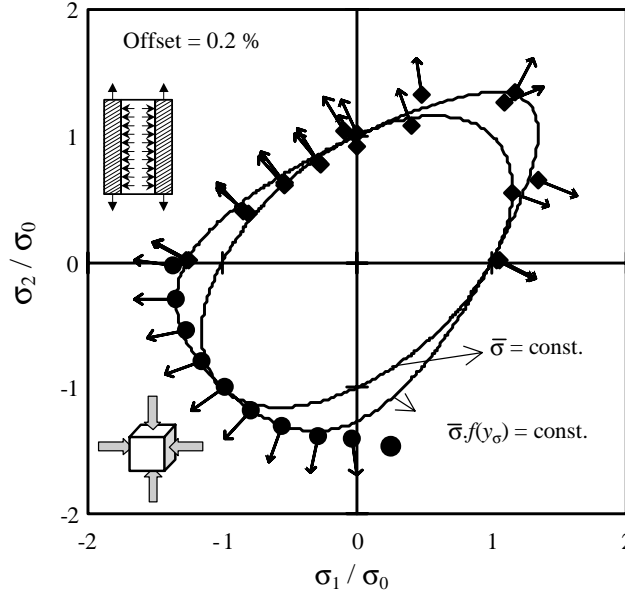
Fig. 4. Normality of the phase transformation directions to the forward yield surface.

Suppose that a non-equilibrium state of the three phases mixture RVE is described by the following variables: $\underline{\varepsilon}_a$ is the total strain tensor of each phase ($\alpha = 1, 2, 3$); T the temperature; z_T the self-accommodating martensite volume fraction; z_σ the stress-induced martensite volume fraction; H_k a set of internal variables ($k \in \aleph$).

The internal variables represent the RVE internal pattern rearrangements at the micro-scale level. Neither their number nor their physical characters will be specified here. But an example of these internal variables H_k can be the internal stress tensor $\underline{\sigma}_i$ (called also back-stress) developed under the external stress action ($\underline{\sigma}$).

Consider the following form of the specific free energy ϕ_n of a solid three phases mixture (Leclercq and Lexcellent, 1996):

$$\phi_n(\underline{\varepsilon}_a, T, z_T, z_\sigma, H_k) = (1-z)\phi_1 + z_T\phi_2 + z_\sigma\phi_3 + \Delta\phi; \quad z = z_T + z_\sigma, \quad z, z_T, z_\sigma \in [0, 1] \quad (7)$$

with

$$\phi_\alpha = u_0^\alpha - Ts_0^\alpha + \frac{1}{2\rho}(\underline{\varepsilon}_\alpha - \underline{\varepsilon}_\alpha^{\mathrm{tr}} - \underline{\varepsilon}_\alpha^{\mathrm{th}}) : \underline{\underline{L}}(\underline{\varepsilon}_\alpha - \underline{\varepsilon}_\alpha^{\mathrm{tr}} - \underline{\varepsilon}_\alpha^{\mathrm{th}}) + c_v\left[(T - T_0) - T\,\mathrm{Ln}\left(\frac{T}{T_0}\right)\right] \quad (8)$$

and

$$\Delta\phi = z(1-z)\phi_{it}(T) + z_T z_\sigma \phi_{it}^m(T) \quad (9)$$

where

$$\phi_{it}(T) = \bar{u}_0 - T\bar{s}_0, \quad \phi_{it}^m(T) = \bar{u}_0^m - T\bar{s}_0^m \quad (10)$$

The exact form of $\Delta\phi$ remains an open problem since it strongly depends on the incompatibilities between the martensite platelets and between martensite and austenite.

The elastic stiffness tensor $\underline{\underline{L}}$, the thermal expansion coefficient α and the specific heat C_v are supposed independent of the phase state, i.e., whatever $\alpha = 1, 2$ or 3:

$$\underline{\varepsilon}_\alpha^{\mathrm{th}} = \alpha(T - T_0)\underline{1} = \underline{\varepsilon}^{\mathrm{th}}, \quad \underline{\varepsilon}_\alpha^{\mathrm{e}} = \underline{\underline{L}}^{-1}\underline{\sigma} = \underline{\varepsilon}^{\mathrm{e}} \quad (11)$$

Moreover

$$\underline{\varepsilon}_1^{tr} = \underline{\varepsilon}_2^{tr} = 0, \quad \underline{\varepsilon}_3^{tr} = \underline{K}(H_k) \tag{12}$$

Assuming that the total macroscopic strain tensor $\underline{\varepsilon}$ and the total intrinsic strain tensors $\underline{\varepsilon}_\alpha$ ($\alpha = 1, 2, 3$) must comply with the following relation:

$$\underline{\varepsilon} = (1 - z)\underline{\varepsilon}_1 + z_T\underline{\varepsilon}_2 + z_\sigma\underline{\varepsilon}_3 \tag{13}$$

corresponding to a series arrangement which is equivalent to the Reuss bound model for the response of an austenite–martensite composite, the Helmholtz specific free energy function of the three-phase system in constrained equilibrium (Raniecki et al., 1992) is

$$\begin{aligned}
\phi_{eq}(\underline{\varepsilon}, T, z_T, z_\sigma, H_k) &= u_0^1 - Ts_0^1 - z\pi_0^f(T) + c_v\left[(T - T_0) - T\,\text{Ln}\left(\frac{T}{T_0}\right)\right] \\
&\quad + \frac{1}{2\rho}[\underline{\varepsilon} - z_\sigma\underline{K}(H_k) - \alpha(T - T_0)\underline{1}] : \underline{\underline{L}}[\underline{\varepsilon} - z_\sigma\underline{K}(H_k) - \alpha(T - T_0)\underline{1}] \\
&\quad + z(1 - z)\phi_{it} + z_T z_\sigma \phi_{it}^m
\end{aligned} \tag{14}$$

where

$$\pi_0^f(T) = \Delta u_0 - T\Delta s_0, \quad \Delta u_0 = u_0^1 - u_0^2, \quad \Delta s_0 = s_0^1 - s_0^2 \tag{15}$$

We now introduce the concept of "optimal internal arrangement" following which the set of the internal variables H_k minimises the free energy function (14). In Raniecki and Lexcellent (1998), it has been established that the quantity $\underline{K}_{eq}(H_k)$ can be derived from a positively homogeneous function of first order $g^*(\underline{\sigma})$ such as

$$\underline{\sigma} : \underline{K}_{eq}(H_k) = \rho g^*(\underline{\sigma}) \tag{16}$$

So

$$\underline{K}_{eq}(H_k) = \rho\frac{\partial g^*(\underline{\sigma})}{\partial \underline{\sigma}} \tag{17}$$

Taking into account the definitions of the previous section for the forward transformation:

$$g^*(\underline{\sigma}) = \gamma\frac{\sigma_{ef}}{\rho} \tag{18}$$

γ being the maximum phase transformation strain in pure shearing.

Denoting $\hat{\phi}_{eq}$ the specific free energy function for an optimal internal arrangement, i.e. $\hat{\phi}_{eq} = \phi_{eq}|_{K=K_{eq}}$, the associated Gibbs' function g such as $\rho g = \rho\hat{\phi}_{eq} - \underline{\sigma} : \underline{\varepsilon}$ is

$$\begin{aligned}
\rho g &= \rho\left(u_0^1 - Ts_0^1 - z\pi_0^f(T) + c_v\left[(T - T_0) - T\,\text{Ln}\left(\frac{T}{T_0}\right)\right]\right) - \frac{1}{2}\underline{\sigma} : \underline{\underline{L}}^{-1}\underline{\sigma} - z_\sigma\underline{\sigma} : \underline{K}_{eq} - \alpha(T - T_0)\underline{\sigma} : \underline{1} \\
&\quad + \rho z(1 - z)\phi_{it} + \rho z_T z_\sigma\phi_{it}^m
\end{aligned} \tag{19}$$

and

$$\begin{aligned}
\underline{\varepsilon} &= -\rho\frac{\partial g}{\partial \underline{\sigma}} = \underline{\varepsilon}^e + \underline{\varepsilon}^{tr} + \underline{\varepsilon}^{th}, \quad \underline{\varepsilon}^e = \underline{\underline{L}}^{-1}\underline{\sigma}, \quad \underline{\varepsilon}^{tr} = z_\sigma\underline{K}_{eq}, \quad \underline{\varepsilon}^{th} = \alpha(T - T_0)\underline{1} \\
s &= -\frac{\partial g}{\partial T} = s_0^1 - z\Delta s_0 + \frac{\alpha}{\rho}\underline{\sigma} : \underline{1} + z(1 - z)\bar{s}_0 + z_T z_\sigma\bar{s}_0^m + c_v\,\text{Ln}\left(\frac{T}{T_0}\right) \\
\pi_\sigma^f &= -\frac{\partial g}{\partial z_\sigma} = \frac{1}{\rho}\underline{\sigma} : \underline{K}_{eq} - (1 - 2z)\phi_{it} - z_T\phi_{it}^m + \pi_0^f(T) \\
\pi_T^f &= -\frac{\partial g}{\partial z_T} = -(1 - 2z)\phi_{it} - z_\sigma\phi_{it}^m + \pi_0^f(T)
\end{aligned} \tag{20}$$

One must underline the important strain component:

$$\underline{\varepsilon}^{\mathrm{tr}} = z_\sigma \underline{K}_{\mathrm{eq}} \tag{21}$$

specifically associated with the phase transformation and which takes by time differentiation:

$$\dot{\underline{\varepsilon}}^{\mathrm{tr}} = \dot{z}_\sigma \underline{K}_{\mathrm{eq}} + z_\sigma \dot{\underline{K}}_{\mathrm{eq}} \tag{22}$$

For proportional loading ($\dot{\underline{K}}_{\mathrm{eq}} = 0$), the first right term is consistent with a normal phase transformation evolution. Hence, taking account for (17), (18) and (6) (forward transformations cases):

$$\underline{K}_{\mathrm{eq}} = \gamma \frac{\partial \sigma_{\mathrm{ef}}}{\sigma \underline{\sigma}} \quad \text{and} \quad \dot{\lambda}_{\mathrm{F}} = \gamma \dot{z}_\sigma \tag{23}$$

The second right term of Eq. (22) may be identified as the non-proportional loading contribution.

3.2. Clausius–Duhem inequality

In a classical way, the Clausius–Duhem inequality is written and gives for the intrinsic dissipation the following expression:

$$D_i = \pi_\sigma^{\mathrm{f}} \dot{z}_\sigma + \pi_{\mathrm{T}}^{\mathrm{f}} \dot{z}_{\mathrm{T}} \geqslant 0 \tag{24}$$

In the particular case of pure reorientation of self-accommodating martensite platelets $M_{\mathrm{T}} \to M_\sigma$ under a pure stress action, the conditions are:

$$\dot{z}_\sigma = -\dot{z}_{\mathrm{T}} \ (z_{\mathrm{T}} = 1 - z_\sigma) \quad \text{and} \quad D_i = \pi_{\mathrm{T}\sigma}^{\mathrm{f}} \dot{z}_\sigma \geqslant 0 \tag{25}$$

where $\pi_{\mathrm{T}\sigma}^{\mathrm{f}}$ is the thermodynamical force associated with the reorientation:

$$\pi_{\sigma\mathrm{T}}^{\mathrm{f}} = \frac{1}{\rho} \underline{\sigma} : \underline{K}_{\mathrm{eq}} - (1 - 2z_\sigma) \phi_{it}^m \tag{26}$$

Two other important cases can also be examined:

(i) pure thermal action $A \leftrightarrow M_{\mathrm{T}}$ (cooling or heating). In this case $\dot{z}_\sigma = 0$, so:

$$D_i = \pi_{\mathrm{T}}^{\mathrm{f}} \dot{z}_{\mathrm{T}} \geqslant 0 \tag{27}$$

Hence

$$\begin{aligned} A \to M_{\mathrm{T}} \quad &\text{if } \dot{z}_{\mathrm{T}} \geqslant 0 \ (\pi_{\mathrm{T}}^{\mathrm{f}} \geqslant 0) \\ M_{\mathrm{T}} \to A \quad &\text{if } \dot{z}_{\mathrm{T}} \leqslant 0 \ (\pi_{\mathrm{T}}^{\mathrm{f}} \leqslant 0) \end{aligned} \tag{28}$$

(ii) pure stress action $A \leftrightarrow M_\sigma$ (pseudoelasticity or superelasticity). In this case $\dot{z}_{\mathrm{T}} = 0$, so:

$$D_i = \pi_\sigma^{\mathrm{f}} \dot{z}_\sigma \geqslant 0 \tag{29}$$

Hence

$$\begin{aligned} A \to M_\sigma \quad &\text{if } \dot{z}_\sigma \geqslant 0 \ (\pi_\sigma^{\mathrm{f}} \geqslant 0) \\ M_\sigma \to A \quad &\text{if } \dot{z}_\sigma \leqslant 0 \ (\pi_\sigma^{\mathrm{f}} \leqslant 0) \end{aligned} \tag{30}$$

3.3. Heat equation

From the thermodynamics first principle, the heat q exchanged per unit of mass is given (in it derivative expression) by

$$\dot{q} = \rho \dot{u} - \underline{\sigma} : \dot{\underline{\varepsilon}} \tag{31}$$

where u is the phase mixture specific internal energy such as

$$\rho u = \rho g + \rho T s + \underline{\sigma} : \underline{\varepsilon} \tag{32}$$

From the previous equations, it comes:

$$\rho c_v \dot{T} - \dot{q} = \rho(\Delta u_0 - (1 - 2z)\bar{u}_0)\dot{z} - T\alpha\underline{\dot{\sigma}} : \underline{1} + \gamma\sigma_{\text{ef}}\dot{z}_\sigma - \rho(z_T\dot{z}_\sigma + \dot{z}_T z_\sigma)\bar{u}_0^m \tag{33}$$

3.4. Model parameters identification

Following a proposed idea by Brocca et al. (2002) in the case of one dimensional situations (tension or compression) and its extension by Juhasz et al. (2002) for proportional loading, a ''Clausius–Clapeyron'' diagram can be built as the effective stress σ_{ef} versus temperature T (Fig. 5). This diagram is based on experimental observations: at low stresses, it becomes hypothetical to distinguish self-accommodating martensite and stress-induced martensite. In order to overcome this problem for forward transformations in the (σ_{ef}, T) space, a self-accommodating martensite domain is defined at low stresses for $T \leqslant M_{\text{f}}^0$ in addition to two domains A (austenite) and M_σ (stress-induced martensite).

For the model parameters identification:

(i) The measurement of M_{s}^0 and A_{s}^0, which are the values of forward and reverse transformation-start temperatures at stress free state respectively, delivers two data:

$$\begin{aligned}
\pi_{\text{T}}^{\text{f}}(\underline{\sigma} = \underline{0}, T = M_{\text{s}}^0, z_{\text{T}} = 0, z_\sigma = 0) &= (\Delta u_0 - \bar{u}_0) - (\Delta s_0 - \bar{s}_0)M_{\text{s}}^0 = 0 \quad \text{for } A \rightarrow M_{\text{T}} \\
\pi_{\text{T}}^{\text{f}}(\underline{\sigma} = \underline{0}, T = A_{\text{s}}^0, z_{\text{T}} = 1, z_\sigma = 0) &= (\Delta u_0 + \bar{u}_0) - (\Delta s_0 + \bar{s}_0)A_{\text{s}}^0 = 0 \quad \text{for } M_{\text{T}} \rightarrow A
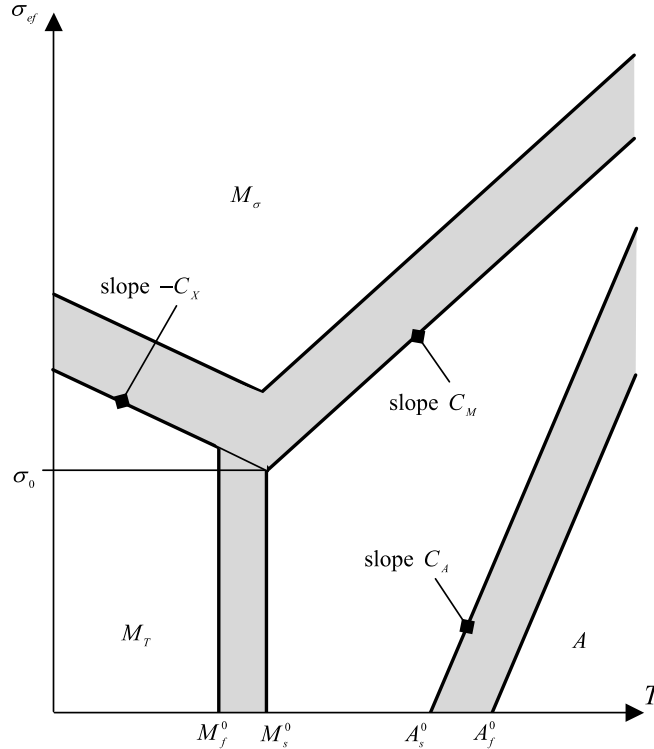\end{aligned} \tag{34}$$

Fig. 5. ''Clausius–Clapeyron'' diagram in the (σ_{ef}, T) plane.

(ii) Concerning the pseudo-elastic behaviour, the yield states at which the forward and the reverse transformations are initiated, are such as putting: $\underline{\sigma} : \underline{K}_{eq} = \gamma \sigma_{ef}$:

$$\pi_\sigma^f(\sigma_{ef}, T, z_T = 0, z_\sigma = 0) = \pi_\sigma^f(\sigma_0, T = M_s^0, z_T = 0, z_\sigma = 0) \quad \text{for } A \to M_\sigma \tag{35}$$

Hence

$$\sigma_{ef} - \sigma_0 - \frac{\rho(\Delta s_0 - \bar{s}_0)}{\gamma}(T - M_s^0) = 0 \tag{36}$$

or by derivation:

$$\frac{d\sigma_{ef}}{dT} = \frac{\rho(\Delta s_0 - \bar{s}_0)}{\gamma} = C_M \tag{37}$$

C_M being obtained from different isothermal curves in the pseudo-elasticity range and

$$\pi_\sigma^f(\sigma_{ef}, T, z_T = 0, z_\sigma = 1) - \pi_\sigma^f(0, T = A_s^0, z_T = 0, z_\sigma = 1) = 0 \quad \text{for } M_\sigma \to A \tag{38}$$

Hence

$$\sigma_{ef} - \frac{\rho(\Delta s_0 + \bar{s}_0)}{\gamma}(T - A_s^0) = 0 \tag{39}$$

or by derivation:

$$\frac{d\sigma_{ef}}{dT} = \frac{\rho(\Delta s_0 + \bar{s}_0)}{\gamma} = C_A \tag{40}$$

C_A being also determined experimentally.

(iii) About the reorientation process, the yield state at which the reorientation process is initiated is governed by the following conditions:

$$\pi_{\sigma T}^f(\sigma_{ef}, T, z_\sigma = 0, z_T = 1) - \pi_{\sigma T}^f(\sigma_0, T = M_s^0, z_\sigma = 0, z_T = 1) = 0 \quad \text{for } M_T \to M_\sigma \tag{41}$$

Hence

$$\sigma_{ef} - \sigma_0 + \frac{\rho}{\gamma}\bar{s}_0^m(T - M_s^0) = 0 \tag{42}$$

or by derivation:

$$\frac{d\sigma_{ef}}{dT} = -\frac{\rho}{\gamma}\bar{s}_0^m = -C_X \tag{43}$$

Moreover, at any starting point of the reorientation process, $\pi_{\sigma T}^f = 0$, hence:

$$\pi_{\sigma T}^f(\sigma_0, T = M_s^0, z_T = 1, z_\sigma = 0) = \sigma_0 - \frac{\rho}{\gamma}(\bar{u}_0^m - M_s^0\bar{s}_0^m) = 0 \tag{44}$$

The seven equations (35), (38), (41), (44) and (45) are sufficient to estimate the six model parameters Δu_0, Δs_0, $\bar{u}_0$, $\bar{s}_0$, $\bar{u}_0^m$ and $\bar{s}_0^m$.

3.5. System evolution and kinetics

The instability of the thermodynamic equilibrium implies that it does not exist any thermodynamic relation giving the hysteresis loop branches equations. Nevertheless, such equations are needed to determine the evolution laws of z_σ and z_r. These laws have to be combined with the behaviour relations in order to completely define the system behaviour.

Let us assume that there exist five constitutive functions ψ_F^σ, ψ_F^T, ψ_R^σ, ψ_R^T and $\psi^{\sigma T}$ that are, respectively, linked to the forward phase transformation (F: austenite $\rightarrow$ martensite) the reverse one (R: martensite $\rightarrow$ austenite) and to the reorientation process of the self-accommodating martensite. The superscripts σ and T refer to the martensite type involved during the process. The functions ψ_F and ψ_R, which are available for each kind of martensite, in addition to $\psi^{\sigma T}$, which is devoted to the reorientation, complete the behaviour constitutive equations.

Concerning the forward phase transformation ($A \rightarrow M_\sigma$) or ($A \rightarrow M_T$) and the reorientation process of self-accommodating martensite ($M_T \rightarrow M_\sigma$):

$$\psi_F^\sigma(\underline{\sigma}, T, z_\sigma, z_T) = \pi_\sigma^f - k_F^\sigma, \quad \psi_F^T(T, z_\sigma, z_T) = \pi_T^f - k_F^T, \quad \psi^{\sigma T}(\underline{\sigma}, T, z_\sigma) = \pi_{\sigma T}^f - k^{\sigma T} \tag{45}$$

The functions k_F^σ, k_F^T and $k^{\sigma T}$ are derived from the kinetics forms proposed by metallurgists as Koistinen and Marburger (1959).

For instance, one can propose with the help of the consistency conditions $\dot{\psi}_F^\sigma = 0$, $\dot{\psi}_F^T = 0$ and $\dot{\psi}^{\sigma T} = 0$:

$$\dot{z}_\sigma = (1 - z_\sigma)\left[\frac{\gamma a_F^\sigma}{\rho \Delta s_0} \dot{\sigma}_{ef} - b_F^\sigma a_F^\sigma \dot{T} \exp\left[-b_F(T - M_s^0)\right]\right] \quad \text{for } A \rightarrow M_\sigma$$

$$\dot{z}_T = (1 - z_T)a_F^T \dot{T} \quad \text{for } A \rightarrow M_T \tag{46}$$

$$\dot{z}_\sigma = (1 - z_\sigma)\frac{\gamma a^{\sigma T}}{\rho \Delta s_0} \dot{\sigma}_{ef} \quad \text{for } M_T \rightarrow M_\sigma$$

a_F^σ, a_F^T, $a^{\sigma T}$, b_F^σ and b_F being material constants.

Concerning the reverse phase transformation ($M_\sigma \rightarrow A$); ($M_T \rightarrow A$):

$$\psi_R^\sigma(\underline{\sigma}, T, z_\sigma, z_T) = -\pi_\sigma^f + k_R^\sigma, \quad \psi_R^T(T, z_\sigma, z_T) = -\pi_T^f + k_R^T \tag{47}$$

A unique yield function can be built in the deviatoric stresses plane for all the possible reverse transformations by considering proportional loading paths or radial loading $\underline{\sigma} = c(t)\underline{\sigma}_0$, $\underline{\sigma}_0$ being a constant tensor and $c(t)$ a positive time-dependent function. Taking account for the yield criterion form for the forward phase transformation, it comes:

$$\psi_R^\sigma(\underline{\sigma}, T, z_\sigma, z_T) = -\sigma_{ef} + \sigma_0^{MA}(T, z_\sigma, z_T) \tag{48}$$

σ_0^{MA} being the threshold stress during the reverse phase transformation $M_\sigma \rightarrow A$.

The use of the maximum dissipation principle in order to derive the complementary evolution laws requires a convex constraint region (elastic domain) to assure their uniqueness. However, in the particular case of the reverse phase transformation, the elastic domain is not convex, what suggests the building of a non-associated constitutive frame by using of a constitutive function $\kappa(\underline{\sigma}, T, z_\sigma, z_T)$ verifying:

$$\begin{aligned}
\kappa(\underline{\sigma}, T, z_\sigma, z_T) < 0 \quad \text{when } \psi_R^\sigma(\underline{\sigma}, T, z_\sigma, z_T) < 0 \\
\kappa(\underline{\sigma}, T, z_\sigma, z_T) = 0 \quad \text{when } \psi_R^\sigma(\underline{\sigma}, T, z_\sigma, z_T) = 0
\end{aligned} \tag{49}$$

Such a function can be chosen as the support straight to the convex domain delimited by the yield function $\psi_R^\sigma(\underline{\sigma}, T, z_\sigma, z_T)$. Hence:

$$\kappa(\underline{\sigma}, T, z_\sigma, z_T) = -\underline{\sigma} : \frac{\varepsilon^{tr}}{\varepsilon_{ef}^{tr}} + \sigma_0^{MA}(T, z_\sigma, z_T) \tag{50}$$

and then (refer to (17)):

$$\dot{\underline{\varepsilon}}^{tr} = \gamma \dot{z}_\sigma \frac{\varepsilon^{tr}}{\varepsilon_{ef}^{tr}} \quad \text{i.e. } \underline{K}_{eq} = \rho \frac{\partial}{\partial \underline{\sigma}}\left(-\frac{\gamma}{\rho}\kappa\right) \tag{51}$$

As previously done, $\dot{z}_\sigma$ derive from the consistency condition $\dot{\psi}_R^\sigma = 0$:

$$\dot{z}_\sigma = z_\sigma \left[\frac{\gamma a_R^\sigma}{\rho \Delta s_0} \dot{\sigma}_{ef} - b_R^\sigma a_R^\sigma \dot{T} \exp\left[-b_R(T - A_s^0)\right] \right] \tag{52}$$

a_R^σ, b_R^σ and b_R being material constants.

The condition $\dot{\psi}_R^T = 0$ allows us to obtain $\dot{z}_T$.

As the model is built starting from the experimental determination of yield surfaces ($A \rightarrow M_\sigma$, the Figs. 1, 2 and 4 exhibit a strong asymmetry between tension and compression (see the dotted line representing symmetry on Fig. 1).

When the important property of asymmetry between tension and compression is not taken into account, it is natural to define the effective phase transformation strain ε_{ef}^{tr} as the von Mises equivalent strain as it was done by Juhasz et al. (2002) or Helm and Haupt (2003). However, when the tension–compression asymmetry is taken into account, it can be stated that for proportional loading:

$$\varepsilon_{ef}^{tr} = \gamma z_\sigma = \frac{\bar{\varepsilon}^{tr}}{\left(f^2(y_\sigma) + 9\left(\frac{df}{dy_\sigma}\right)^2 (1 - y_\sigma^2)\right)^{1/2}}, \quad \bar{\varepsilon}^{tr} = \left(\frac{2}{3} T \underline{\varepsilon}^{tr} \underline{\varepsilon}^{tr}\right)^{1/2} \tag{53}$$

With this definition, ε_{ef}^{tr} depends on stresses trough y_σ (2). To overcome this problem, y_σ must be expressed as a function of the phase transformation strain tensor $\underline{\varepsilon}^{tr}$ for every proportional loading. Nevertheless, an analytical expression of this function cannot be easily derived but the following approximation can be used (Bouvet, 2002) (Fig. 6a):

$$\frac{1}{\left(f^2(y_\sigma) + 9\left(\frac{df}{dy_\sigma}\right)^2 (1 - y_\sigma^2)\right)^{1/2}} = \frac{f(-y_\varepsilon)}{f(-1)}, \quad y_\varepsilon = 4\frac{\det(\underline{\varepsilon}^{tr})}{(\bar{\varepsilon}^{tr})^3} \tag{54}$$

The difference between the right-hand member and the left-hand one does not exceed 2.5% whatever a varying with the range [0, 1] (Fig. 6b).

$$\dot{z}_T = -a_R^T z_T \dot{T} \tag{55}$$
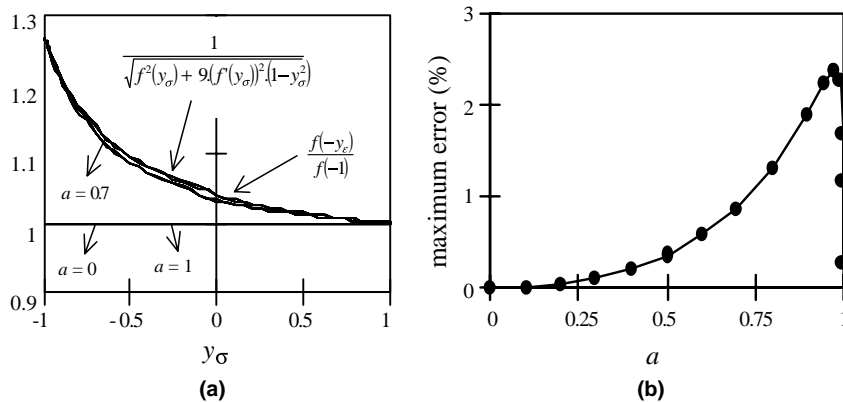
a_R^T being also a material constant.

Fig. 6. Approximation function for effective phase transformation strain computation.

3.6. Effective phase transformation strain

Whatever phase transformation ($A \to M_\sigma$ or $M_\sigma \to A$), $\gamma \dot{z}_\sigma$, defines the equivalent or effective transformation strain rate $\dot{\varepsilon}_{ef}^{tr}$ such as

$$\underline{\sigma} : \underline{\dot{\varepsilon}}^{tr} = \sigma_{ef} \dot{\varepsilon}_{ef}^{tr} \tag{56}$$

at the loading point.

3.7. Summary of the model

Table 1 gives the summary of the model.

Table 1
Summary of the model

R.V.E. behaviour

Choice of the free energy function ϕ and of the associated Gibbs function g

$$\rho g = \rho \left(u_0^1 - T s_0^1 - z \pi_0^f(T) + c_v \left[(T - T_0) - T \operatorname{Ln}\left(\frac{T}{T_0}\right) \right] \right)$$
$$- \frac{1}{2} \underline{\sigma} : \underline{\underline{L}}^{-1} \underline{\sigma} - z_\sigma \underline{\sigma} : \underline{K}_{eq} - \alpha(T - T_0)\underline{\sigma} : \underline{1} + \rho z(1-z)\phi_{it} + \rho z_T z_\sigma \phi_{it}^m \tag{1}$$

Internal variables:
- Stress induced martensite fraction z_σ
- Thermal induced martensite fraction z_T

$$\sigma_{ef} = \bar{\sigma} f(y_\sigma), \quad \bar{\sigma} = \left(\frac{3}{2} \operatorname{dev}\underline{\sigma} : \operatorname{dev}\underline{\sigma}\right)^{1/2}, \quad y_\sigma = \frac{27}{2} \frac{\det(\operatorname{dev}\underline{\sigma})}{\bar{\sigma}^3}$$

$$\underline{\varepsilon} = -\rho \frac{\partial g}{\partial \underline{\sigma}}, \quad \pi_\sigma^f = -\frac{\partial g}{\partial z_\sigma}, \quad \pi_T^f = -\frac{\partial g}{\partial z_T},$$

$$\underline{\varepsilon} = \underline{\varepsilon}^e + \underline{\varepsilon}^{tr} + \underline{\varepsilon}^{th}, \quad \underline{\varepsilon}^e = \underline{\underline{L}}^{-1}\underline{\sigma}, \quad \underline{\varepsilon}^{tr} = \gamma z_\sigma \frac{\partial \sigma_{ef}}{\partial \underline{\sigma}}, \quad \underline{\varepsilon}^{th} = \alpha(T - T_0)\underline{1}$$

Forward phase transformation $A \to M_\sigma$ or $A \to M_T$ and $M_T \to M_\sigma$

$$\psi_F^\sigma(\underline{\sigma}, T, z_\sigma, z_T) = \pi_\sigma^f = k_F^\sigma, \quad \psi_F^T(T, z_\sigma, z_T) = \pi_T^f - k_F^T, \quad \psi^{\sigma T}(\underline{\sigma}, T, z_\sigma) = \pi_{\sigma T}^f - k^{\sigma T}$$

efficient choice of k_F^σ, k_F^T and $k^{\sigma T}$ and consistency equations $\dot{\psi}_F^\sigma = 0$, $\dot{\psi}_F^T = 0$ and $\dot{\psi}^{\sigma T} = 0$ determines the kinetics

$$\dot{z}_\sigma = \text{for } A \to M_\sigma, \quad \dot{z}_T = \text{for } A \to M_T, \quad \dot{z}_\sigma = \text{for } M_T \to M_\sigma$$

Reverse phase transformation $M_\sigma \to A$ $M_T \to A$

$$\psi_R^\sigma = -\sigma_{ef} + \sigma_0^{MA}(T, z_\sigma, z_T) \quad \psi_R^T = -\pi_T^f + k_R^T$$
$$\underline{\dot{\varepsilon}}^{tr} = \gamma \dot{z}_\sigma \frac{\underline{\varepsilon}^{tr}}{\varepsilon_{ef}^{tr}} \quad \dot{\psi}_R^\sigma = 0 \to \dot{z}_\sigma =$$
$$\dot{\psi}_R^T = 0 \to \dot{z}_T =$$

Effective phase transformation strain ε_{ef}^{tr} defined as $\sigma_{ef}\dot{\varepsilon}_{ef}^{tr} = \underline{\sigma} : \underline{\dot{\varepsilon}}^{tr}$

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4. Conclusion

The originality of the present work comes from

(i) The experimental determination of the initiation surfaces of phase transformation to built the model as it was done for classical elastoplasticity models.
(ii) A consistent constitutive frame for the reverse phase transformation has been derived within the context of the generalized standard materials theory using non-associated approach.
(iii) A general definition of the effective phase transformation strain.

Modelling anisothermal SMA behaviour under proportional loading seems to be a solved problem, at least for the forward transformation. On the opposite of Juhasz et al. (2002), the choice of the equivalent or effective stress σ_{ef} accounting for the tension–compression asymmetry does not allow to substitute as an internal variable the stress-induced martensite volume fraction z_σ by an equivalent phase transformation strain in the von Mises sense. Besides, the introduction of a back-stress tensor as internal variable by Helm and Haupt (2003), is an interesting idea for non-proportional modelling. An important forthcoming work could concern the best understanding of the cyclic behaviour and the associated two-way shape memory effect for an SMA efficient use in technological applications.

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