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THERMOMECHANICS OF MARTENSITIC PHASE TRANSITIONS IN ELASTOPLASTIC MATERIALS

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Introduction

For the description of phase transitions (PT) in elastic materials the principle of the minimum of free energy is usually used. But for media with dissipation the corresponding principle is lacking. For elastic materials with hysteresis and elastoplastic materials PT criterion was suggested (see [2]–[4] and references) in the following form: the driving force of PT reaches some threshold value. In [5] it was obtained that for elastoplastic materials an additional threshold, related with the plastic dissipation, should be introduced and can be easily calculated. But PT criterion is only one scalar equation, which is not sufficient for the determination of all parameters, e.g. shape and orientation of nuclei, jump of strain, etc. For these purposes in [3, 5] some extremum principles were substantiated, which were also applied for the noncoherent PT. The present paper is a further development of the methods suggested in [2, 3, 5]. Both coherent (jump of the position vector $\mathbf{r}$ across the interface $[\mathbf{r}] := \mathbf{r}_2 - \mathbf{r}_1 = 0$, where subscripts 1 and 2 denote the phase before and after PT) and noncoherent ($[\mathbf{r}] \neq 0$) PT are considered; but $[\mathbf{r}]$ is geometrically small in the sense that the same points of the interface remain in contact. The conditions of nucleation, nondisappearance of nucleus and interface propagation are derived. Extremum principles for determination of all unknown parameters are obtained based on the postulate of realizability. Simple averaged description of PT is suggested. The predicted effect of shear stresses and plastic strains on PT is in qualitative agreement with experiments.
Let superscript t denotes transposition, dots mean contractions of the tensors, $\boldsymbol{\nabla}$ is the gradient operator.

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Conditions of nucleation, nondisappearance of nucleus and interface propagation

Consider a volume V of multiphase material with a boundary S in the reference configuration. Assume that on part of surface S the stress vector $\mathbf{p}$ is prescribed and on the rest part the velocity vector $\mathbf{v}$ is given, but a mixed boundary conditions (BC) are also possible. For the isothermal processes the dissipation increment N during the time Δt can be defined, using the second law of thermodynamics [5]

$$N := \int_t^{t+\Delta t} \int_S \mathbf{p} \cdot \mathbf{v} \, dS \, dt - \int_t^{t+\Delta t} \frac{d}{dt} \int_V \rho\psi \, dV \, dt \ \geq \ 0 \, , \tag{1}$$

where ρ is the mass density in the reference configuration, ψ the Helmholtz free energy per unit mass. Let us divide the volume V into three parts: the volume V_n with the boundary Σ_n, in which due to PT during the time Δt the new nuclei appeared; the volume $\int_\Sigma v_n \, d\Sigma \, \Delta t$ covered by the moving interface Σ with normal velocity v_n; the rest volume V_1 in which PT do not occur during the time Δt. Using the Gauss theorem for the volume V with the discontinuity surfaces $\Sigma + \Sigma_n$ and the formula for differentiating on a variable volume we obtain a decomposition of N into dissipation increments in each of the above volumes

$$\begin{aligned} N &= N_1 + N_n + \int_t^{t+\Delta t} \int_{\Sigma+\Sigma_n} \tilde{X}_\Sigma \, d\Sigma \, dt \, , \qquad N_1 = \int_t^{t+\Delta t} \int_{V_1} \left(\mathbf{P}^t : \dot{\mathbf{F}} - \rho\dot{\psi} \right) dt \, dV_1 \, ; \\ N_n &= \int_{\mathbf{F}_1}^{\mathbf{F}_2} \int_{V_n} \mathbf{P}^t : d\mathbf{F} \, dV_n - \int_{V_n} \rho \, (\psi_2 - \psi_1) \, dV_n \, , \qquad \tilde{X}_\Sigma = -\mathbf{p} \cdot [\mathbf{v}] - \rho[\psi] \, v_n \, , \end{aligned} \tag{2}$$

where $\mathbf{P}$ and $\mathbf{F}$ denote the first Piola–Kirchhgoff nonsymmetric stress tensor and deformation gradient, and we took into account $[\mathbf{p}] = 0$. Due to the mutual independence of each of three integrals in Eq. (2), each of them is nonnegative.

For elastic materials without dissipation conditions $N_n = 0$ and $\tilde{X}_\Sigma = 0 \quad \forall \mathbf{r} \in \Sigma$ can be considered as equilibrium nucleation and interface propagation conditions, because they describe PT at zero dissipation. For PT in elastoplastic materials and in elastic materials with the hysteresis these conditions can not be applied, because the finite dissipation occurs in course of PT.

Consider the volume V_n and assume that we can determine the actual value of the dissipation increment N_n^a in course of PT in V_n and $N_n^a = \int (k_n^e + k_n^p) \, dV_n$, where k_n^p and k_n^e are the plastic and "nonplastic" dissipation increment in a unit reference volume. The term k_n^e is related with the emission of acoustic waves, lattice friction and it is responsible for the hysteresis at PT in elastic materials [2]–[6].

Both N_n and N_n^a depend on the BC. If at given BC $N_n < N_n^a$, then PT will not take place, because for actually occurring PT $N_n = N_n^a$, as N_n^a is by definition the actual value of dissipation increment. Consequently, the necessary condition of nucleation is $N_n = N_n^a$, i.e.

$$\int_t^{t+\Delta t} \int_{\Sigma_n} \mathbf{p} \cdot \mathbf{v} \, d\Sigma_n \, dt = \int_{\mathbf{F}_1}^{\mathbf{F}_2} \int_{V_n} \mathbf{P}^t : d\mathbf{F} \, dV_n = \int_{V_n} \rho \, (\psi_2 - \psi_1) \ dV_n + \int_{V_n} (k_n^e + k_n^p) \ dV_n \ , \tag{3}$$

where $\mathbf{v}$ is the velocity on Σ_n from the side of nucleus. Note that Gauss theorem was used. Let us consider the small strain approximation and decompose $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p + \boldsymbol{\varepsilon}^f$, where $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}^e$, $\boldsymbol{\varepsilon}^p$ and $\boldsymbol{\varepsilon}^f$ are total elastic, plastic and transformation strains. In this case $\mathbf{P}^t : d\mathbf{F} = \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}$, where $\boldsymbol{\sigma}$

is the Cauchy stress tensor, $k_n^p = \int \left(\boldsymbol{\sigma} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^p}\right) : d\boldsymbol{\varepsilon}^p$ [5]. At $\frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^p} = 0$ the terms $\boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^p$ in the left and right parts of Eq. (3) eliminate each other and we obtain

$$\int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \int_{V_n} \boldsymbol{\sigma} : d\left(\boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^f\right) dV_n - \int_{V_n} \rho\,(\psi_2 - \psi_1)\, dV_n - \int_{V_n} k_n^e\, dV_n = 0\,. \qquad (4)$$

Formally Eq. (4) has the same form as for PT in elastic materials; plasticity effects on a variation of $\boldsymbol{\sigma}$ in the course of PT. At $\frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^p} \neq 0$ we have

$$\int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \int_{V_n} \left(\boldsymbol{\sigma} : d\left(\boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^f\right) + \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^p} : d\boldsymbol{\varepsilon}^p\right) dV_n - \int_{V_n} \rho\,(\psi_2 - \psi_1)\, dV_n - \int k_n^e dV_n = 0. \qquad (5)$$

If $\psi_i = 0,5\,\boldsymbol{\varepsilon}_i^e : \mathbf{E}_i : \boldsymbol{\varepsilon}_i^e + \psi_i^\theta$, $i = 1,\ 2$ and $\mathbf{E}_1 = \mathbf{E}_2$, where $\mathbf{E}_i$ are the tensors of elastic moduli of $i-$phase, ψ_i^θ the thermal part of the free energy, then

$$\int_{\boldsymbol{\varepsilon}_1^f}^{\boldsymbol{\varepsilon}_2^f} \int_{V_n} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^f\, dV_n - \int_{V_n} \rho\left(\psi_2^\theta - \psi_1^\theta\right) dV_n - \int_{V_n} k_n^e\, dV_n = 0\,, \qquad (6)$$

i.e. the elastic strains also disappear. Let us consider the finite strain case. After PT it is possible to decompose [3, 5] $\mathbf{F} = \mathbf{F}_2^e \cdot \mathbf{F}_2^p \cdot \mathbf{F}^f \cdot \mathbf{F}_1^p$, where $\mathbf{F}^e$, $\mathbf{F}^p$ and $\mathbf{F}^f$ are the elastic, plastic and transformation deformation gradients. We assume that invariance requirements under all possible elastic, plastic and transformational rigid body rotations are met using methods developed in [7]–[9] . As one of possible constitutive hypothesis we assume, that after beginning of PT $\mathbf{F}_1^p = \mathbf{const}$. Then in the course of PT

$$\mathbf{P}^t : d\mathbf{F} = \mathbf{P}^t : \left(d\mathbf{F}^e \cdot \mathbf{F}^p \cdot \mathbf{F}^f \cdot \mathbf{F}_1^p + \mathbf{F}^e \cdot d\mathbf{F}^p \cdot \mathbf{F}^f \cdot \mathbf{F}_1^p + \mathbf{F}^e \cdot \mathbf{F}^p \cdot d\mathbf{F}^f \cdot \mathbf{F}_1^p\right), \qquad (7)$$

$k_n^p = \int_{\mathbf{F}_1^p}^{\mathbf{F}_2^p} \left(\mathbf{P}^t : \mathbf{F}^e \cdot d\mathbf{F}^p \cdot \mathbf{F}^f \cdot \mathbf{F}_1^p - \rho \frac{\partial \psi}{\partial \mathbf{F}^{pt}} : d\mathbf{F}^p\right)$ [3, 12, 9] and from Eq. (3) we obtain

$$\int_{\mathbf{F}_1}^{\mathbf{F}_2} \int_{V_n} \left(\mathbf{P}^t : d\mathbf{F}^e \cdot \mathbf{F}^p \cdot \mathbf{F}^f \cdot \mathbf{F}_1^p + \mathbf{P}^t : \mathbf{F}^e \cdot \mathbf{F}^p \cdot d\mathbf{F}^f \cdot \mathbf{F}_1^p + \rho \frac{\partial \psi}{\partial \mathbf{F}^{pt}} : d\mathbf{F}^p\right) dV_n - \\ - \int_{V_n} \rho\,(\psi_2 - \psi_1)\, dV_n - \int_{V_n} k_n^e dV_n = 0\,. \qquad (8)$$

A similar consideration gives a condition of interface propagation

$$\tilde{X}_\Sigma = -\mathbf{p} \cdot [\mathbf{v}] - \rho[\psi]\, v_n = \tilde{k}_{1\to2}^e + \tilde{k}_{1\to2}^p > 0 \qquad \forall\, \mathbf{r} \in \Sigma, \qquad t' \in [t,\ t + \Delta\, t]\,, \qquad (9)$$

where $\tilde{k}_{1\to2}^p$ and $\tilde{k}_{1\to2}^e$ are the actual value of the dissipation rate due to plastic deformation and nonplastic effects (e.g. due to intersection of interface with different types of defects and lattice friction) at the moving interface. For coherent PT due to compatibility condition [3, 5] $[\mathbf{F}] =$
$= -[\mathbf{v}]\, \mathbf{n}/v_n$, whence $[\mathbf{v}] = -[\mathbf{F}] \cdot \mathbf{n}\, v_n$, $[\mathbf{F}] = [\mathbf{F}] \cdot \mathbf{n}\,\mathbf{n}$, where $\mathbf{n}$ is the unit normal to the interface. We obtain $-\mathbf{p} \cdot [\mathbf{v}] = \mathbf{n} \cdot \mathbf{P}^t \cdot [\mathbf{F}] \cdot \mathbf{n}\, v_n = \mathbf{P}^t : ([\mathbf{F}] \cdot \mathbf{n}\,\mathbf{n})\ v_n = \mathbf{P}^t : [\mathbf{F}]\ v_n = \mathbf{P}^t : [\mathbf{F}]\, v_n$. Introducing $X_\Sigma = \tilde{X}_\Sigma / v_n$, $k_{1\to2}^e = \tilde{k}_{1\to2}^e / v_n$ and $k_{1\to2}^p = \tilde{k}_{1\to2}^p / v_n$ from Eq. (9) we have

$$X_\Sigma = \mathbf{P}^t : [\mathbf{F}] - \rho\,[\psi] = k_{1\to2}^e + k_{1\to2}^p \qquad \forall\, \mathbf{r} \in \Sigma, \qquad t' \in [t,\ t + \Delta\, t]\,. \qquad (10)$$

As $$k^p_{1\to 2} = \int_{\mathbf{F}_1}^{\mathbf{F}_2} \mathbf{P}^t : d\mathbf{F} - \rho \left(\psi_2 \left(\mathbf{F}^e_2, \mathbf{F}^p_2\right) - \psi_1 \left(\mathbf{F}^e_1, \mathbf{F}^p_1\right)\right) \,, \tag{11}$$

then substituting Eq. (11) into Eq. (10) we obtain the generalized Maxwell rule ($\dot{u}_n = v_n$)

$$\mathbf{P}^t : [\mathbf{F}] = \int_{\mathbf{F}_1}^{\mathbf{F}_2} \mathbf{P}^t : d\mathbf{F} + k^e_{1\to 2} \left(u_n\right) \,, \qquad t' \in [t, \;\; t + \Delta t] \,. \tag{12}$$

Let write Eq. (12) at time $t + \Delta t$ (subscript Δ denotes that parameter is determined at time $t + \Delta t$)

$$\mathbf{P}^t_\Delta : \left(\mathbf{F}_{2\,\Delta} - \mathbf{F}_{1\,\Delta}\right) = \int_{\mathbf{F}_{1\,\Delta}}^{\mathbf{F}_{2\,\Delta}} \mathbf{P}^t : d\mathbf{F} + k^e_{1\to 2} \left(u_{n\Delta}\right) \,. \tag{13}$$

For an infinitesimal Δt Eqs. (13) and (12) at $t' = t$ can be transformed into

$$\left(\dot{\mathbf{P}}^t + \mathbf{n} \cdot \boldsymbol{\nabla} \mathbf{P}^t v_n\right) : \left(\mathbf{F}_2 - \mathbf{F}_1\right) = \frac{\partial k^e_{1\to 2}}{\partial u_n} v_n \,, \tag{14}$$

We have taken into account that $\boldsymbol{a}_\Delta = \boldsymbol{a} + \left(\dot{\boldsymbol{a}} + \mathbf{n} \cdot \boldsymbol{\nabla}\, \boldsymbol{a}\, v_n\right) \Delta t$, for $\boldsymbol{a} = \mathbf{P}^t$, $\mathbf{F}_2$ and $\mathbf{F}_1$, where the term $\boldsymbol{\nabla}\boldsymbol{a}$ appears due to the fact that the tensor $\boldsymbol{a}_\Delta$ is determined on the Σ_Δ surface, i.e. at point $\mathbf{r} + v_n\, \mathbf{n}\, \Delta t$ ($\mathbf{r} \in \Sigma\,(t)$). Consequently, Eqs. (12) at $t' = t$ and (14) are the necessary conditions for the coherent interface propagation.
It is not necessary that Eqs. (12) and (13) are valid for the points of Σ_n, because after nucleation the interface Σ_n can be fixed. But we should be sure that Σ_n does not move back and nucleus does not disappear. The condition of nondisappearance of nucleus is a violation of the propagation condition, when $v_n < 0$ and PT $2 \to 1$ occurs, i.e.

$$\tilde{X}_\Sigma = -\mathbf{p} \cdot [\mathbf{v}] - \rho\, [\psi]\, v_n < \tilde{k}^e_{2\to 1} + \tilde{k}^p_{2\to 1} \qquad \forall\, \mathbf{r} \,\in\, \Sigma_n \,, \qquad t' \,\in\, [t\,, \;\; t + \Delta\, t] \tag{15}$$

or for coherent PT, introducing $k^e_{2\to 1} = -\tilde{k}^e_{2\to 1}/v_n \; > \; 0$, $k^p_{2\to 1} = -\tilde{k}^p_{2\to 1}/v_n \; > \; 0$, we have

$$X_\Sigma = \mathbf{P}^t : [\mathbf{F}] - \rho\, [\psi] > -k^e_{2\to 1} - k^p_{2\to 1} < 0 \,. \tag{16}$$

<u>**The postulate of realizability**</u>

To determine all unknown parameters $\mathbf{b}$ (position, shape and orientation of nucleus, $\boldsymbol{\varepsilon}^f$, $\boldsymbol{\varepsilon}_2$ and $\boldsymbol{\varepsilon}_1$ and so on) let us use the postulate of realizability [5]:

If starting from the state with $N_n\,(\mathbf{b}^*) \; < \; N^a_n\,(\mathbf{b}^*)$ (or $\tilde{X}_\Sigma\,(\mathbf{b}^*) \; < \; \tilde{k}^e\,(\mathbf{b}^*) + \tilde{k}^p\,(\mathbf{b}^*)$) for all possible PT parameters $\mathbf{b}^*$ (i.e. PT does not occur) in the course of variation of BC the condition $N_n\,(\mathbf{b}) = N^a_n\,(\mathbf{b})$ (or $\tilde{X}_\Sigma\,(\mathbf{b}) = \tilde{k}^e\,(\mathbf{b}) + \tilde{k}^p\,(\mathbf{b})$) is fulfilled the first time for some of parameters $\mathbf{b}$, then nucleation (or interface propagation) will occur with this $\mathbf{b}$ (if condition $\tilde{X}_\Sigma\,(\mathbf{b}) = \tilde{k}^e\,(\mathbf{b}) + \tilde{k}^p\,(\mathbf{b})$ is not violated in the course of interface propagation).

If, in the course of variation of BC condition $N_n(\mathbf{b}) = N^a_n\,(\mathbf{b})$ (or $\tilde{X}_\Sigma\,(\mathbf{b}) = \tilde{k}^e\,(\mathbf{b}) + \tilde{k}^p\,(\mathbf{b})$) is met for one or several $\mathbf{b}$, then for arbitrary other $\mathbf{b}^*$ inequality $N_n\,(\mathbf{b}^*) \; < \; N^a_n\,(\mathbf{b}^*)$ (or $\tilde{X}_\Sigma(\mathbf{b}^*) \; <$ $< \; \tilde{k}^e\,(\mathbf{b}^*) + \tilde{k}^p\,(\mathbf{b}^*)$) should be held, as in the opposite case for this $\mathbf{b}^*$ condition $N_n = N^a_n$ (or

$\tilde{X}_\Sigma = \tilde{k}^e + \tilde{k}^p$) had to be met before it was satisfied for $\mathbf{b}$. Consequently, we obtain the extremum principles

$$N_n(\mathbf{b}^*) - N_n^a(\mathbf{b}^*) < 0 = N_n(\mathbf{b}) - N_n^a(\mathbf{b}) ; \tag{17}$$

$$\tilde{X}_\Sigma(\mathbf{b}^*) - \tilde{k}^e(\mathbf{b}^*) - \tilde{k}^p(\mathbf{b}^*) < 0 = \tilde{X}_\Sigma(\mathbf{b}) - \tilde{k}^e(\mathbf{b}) - \tilde{k}^p(\mathbf{b}) \tag{18}$$

for determination of all unknown parameters $\mathbf{b}$. From principle (17) using Eq. (4) we obtain

$$\int_{\boldsymbol{\varepsilon}_1^*}^{\boldsymbol{\varepsilon}_2^*} \int_{V_n^*} \boldsymbol{\sigma}^* : d\left(\boldsymbol{\varepsilon}^{e*} + \boldsymbol{\varepsilon}^{f*}\right) dV_n - \int_{V_n^*} \rho\,(\psi_2^* - \psi_1^*)\, dV_n - \int_{V_n^*} k_n^{e*}\, dV_n < 0 =$$
$$\int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \int_{V_n} \boldsymbol{\sigma} : d\left(\boldsymbol{\varepsilon}^{e} + \boldsymbol{\varepsilon}^{f}\right) dV_n - \int_{V_n} \rho\,(\psi_2 - \psi_1)\, dV_n - \int_{V_n} k_n^{e}\, dV_n = 0 . \tag{19}$$

For points of coherent interface using Eq. (12) we obtain

$$\mathbf{P}^{t*} : (\mathbf{F}_2^* - \mathbf{F}_1^*) - \int_{\mathbf{F}_1^*}^{\mathbf{F}_2^*} \mathbf{P}^t\,(\mathbf{F}^*(s), \boldsymbol{\chi}^*) : d\mathbf{F} - k_{1\to 2}^e\,(u_n, \mathbf{F}_1^*, \mathbf{F}_2^*, \mathbf{F}^*(s), \boldsymbol{\chi}^*) < 0 =$$
$$= \mathbf{P}^t : (\mathbf{F}_2 - \mathbf{F}_1) - \int_{\mathbf{F}_1}^{\mathbf{F}_2} \mathbf{P}^t\,(\mathbf{F}(s), \boldsymbol{\chi}) : d\mathbf{F} - k_{1\to 2}^e\,(u_n, \mathbf{F}_1, \mathbf{F}_2, \mathbf{F}(s), \boldsymbol{\chi}) , \tag{20}$$

where $\mathbf{F}(s)$ is the deformation gradient path between $\mathbf{F}_2$ and $\mathbf{F}_1$, tensor $\boldsymbol{\chi}$ characterizes the mutual orientation of phases. The dependence of k on $\mathbf{F}_1$, $\mathbf{F}_2$, $\mathbf{F}(s)$ and $\boldsymbol{\chi}$ should be taken into account in Eq. (14). If k is independent of $\mathbf{F}(s)$ and $\boldsymbol{\chi}$, then at fixed $\mathbf{P}$, $\mathbf{F}_2$ and $\mathbf{F}_1$ from principle (20) the principle of minimum work follows:

$$\int_{\mathbf{F}_1}^{\mathbf{F}_2} \mathbf{P}^t\,(\mathbf{F}^*(s)\,, \ \boldsymbol{\chi}^*) : d\mathbf{F} \to min. \tag{21}$$

Corresponding principles for points of noncoherent interfaces are given in detail in [5].

Averaged description of martensitic phase transitions

Let PT austenite $(A) \to$ martensite (M) occur due to permanent nucleation of M particles. For determination of $\boldsymbol{\sigma}_n$ and $\boldsymbol{\varepsilon}_n$ variation in the course of PT let use developed in [1, 2] method. It allows to determine explicitly stress and strain in each (isotropic or anisotropic) phase of n–phase material under the assumption of homogeneity of stress and strain in each phase. For compactness we shall consider isotropic phases with equal elastic moduli and neglect the volumetric transformation strain. In this case from Eq. (6) it follows

$$X_n \;=\; \int_{\mathbf{e}_1^f}^{\mathbf{e}_2^f} \mathbf{S}_n : d\,\mathbf{e}_n^f - \rho\left(\psi_2^\theta - \psi_1^\theta\right) \;=\; k_n^e\,, \tag{22}$$

where $\mathbf{S}_n$ and $\mathbf{e}_n^f$ are deviators of $\boldsymbol{\sigma}_n$ and $\boldsymbol{\varepsilon}_n^f \left(= \mathbf{e}_n^f\right)$ in nucleus. Using results of [1, 2] for the mixture $A + M+$ nucleus we obtain

$$\mathbf{S}_A \;=\; \mathbf{S} + c\,P\,(\mathbf{e}_M^r - \mathbf{e}_A^r)\,; \qquad \mathbf{S}_M \;=\; \mathbf{S} - (1-c)\;P\;(\mathbf{e}_M^r - \mathbf{e}_A^r)\,; \tag{23}$$

$$\mathbf{S}_n = \mathbf{S} - P\left(\mathbf{e}^r_n - \mathbf{e}^r\right); \qquad \mathbf{e}^r = c\mathbf{e}^r_M + (1-c)\,\mathbf{e}^r_A, \tag{24}$$

where $\mathbf{S}$ and $\mathbf{e}^r$ are averaged over the mixture stress and inelastic strain; $\mathbf{e}^r = \mathbf{e}^p + \mathbf{e}^f$, subscripts A and M mean averaged over A and M values, c is the volume fraction of M, P the constant depending on elastic moduli. Expressions (23) for $\mathbf{S}_A$ and $\mathbf{S}_M$ are the same as in two–phase mixture [2, 3] (due to infinitesimal volume fraction c_n of nucleus). At $\mathbf{S} = 0$ expressions of $\mathbf{S}_A$, $\mathbf{S}_M$ and $\mathbf{S}_n$ characterize the internal (eigen) stresses in A, M and nucleus. At $\mathbf{e}^r_n = \mathbf{e}^r_A$ we have $\mathbf{S}_n = \mathbf{S}_A$, at $\mathbf{e}^r_n = \mathbf{e}^r_M$ we obtain $\mathbf{S}_n = \mathbf{S}_M$, i.e. the expression for $\mathbf{S}_n$ has no contradictions. After substituting $\mathbf{S}_n$ from Eq. (24) into Eq. (22) and integrating we obtain $\left(\mid \mathbf{A} \mid = (\mathbf{A} : \mathbf{A})^{1/2}\right)$

$$\begin{aligned} X_n &= \left(\mathbf{S} + P\mathbf{e}^f\right) : \left(\mathbf{e}^f_2 - \mathbf{e}^f_1\right) - 0,5\,P\left(\mid \mathbf{e}^f_2 \mid^2 - \mid \mathbf{e}^f_1 \mid^2\right) - \\ &- P\int_{\mathbf{e}^f_1}^{\mathbf{e}^f_2} \left(\mathbf{e}^p_n - \mathbf{e}^p\right) : d\mathbf{e}^f_n - \rho\left(\psi^\theta_2 - \psi^\theta_1\right) = k^e_n. \end{aligned} \tag{25}$$

Eq. (25) is a general expression for PT criterion in elastoplastic materials, which can be applied for $A \to M$ and $M \to A$ PT or reorientation of M particles. At $\mathbf{e}^p = \mathbf{e}^p_n = 0$ it coincide with one obtained in [12] for elastic materials. For elastoplastic materials some information concerning plastic flow in phases should be used. Assume that tensor $\mathbf{S}$ received some increment. Using plasticity theory of two–phase materials [2, 3] and fixing $\mathbf{e}^f_i$ we can determine $\mathbf{S}_A$, $\mathbf{S}_M$, $\mathbf{e}^p_A$, $\mathbf{e}^p_M$ and $\mathbf{e}^p$. Then we consider appearance of new nucleus and assume $\mathbf{e}^p = \mathbf{const}$, because at $c_n \to 0$ stresses $\mathbf{S}_A$ and $\mathbf{S}_M$ are fixed in the course of nucleation (also $\mathbf{e}^f = \mathbf{const}$ due to $c_n \to 0$). Consequently,

$$\begin{aligned} X_n = \left(\mathbf{S} + P\mathbf{e}^r\right) : \left(\mathbf{e}^f_2 - \mathbf{e}^f_1\right) - 0,5\,P\left(\mid \mathbf{e}^f_2 \mid^2 - \mid \mathbf{e}^f_1 \mid^2\right) - \\ -P\int_{\mathbf{e}^f_1}^{\mathbf{e}^f_2} \mathbf{e}^p_n : d\mathbf{e}^f_n - \rho\left(\psi^\theta_2 - \psi^\theta_1\right) = k^e_n. \end{aligned} \tag{26}$$

Consider the case of nucleation without additional plastic strain in nucleus, $\mathbf{e}^p_n = \mathbf{e}^p_1 = \mathbf{const}$ and

$$X_n = \mathbf{S}_{eq} : \left(\mathbf{e}^f_2 - \mathbf{e}^f_1\right) - 0,5\,P\left(\mid \mathbf{e}^f_2 \mid^2 - \mid \mathbf{e}^f_1 \mid^2\right) - \rho\left(\psi^\theta_2 - \psi^\theta_1\right) = k^e_n, \tag{27}$$

where $\mathbf{S}_{eq} = \mathbf{S} + P\left(\mathbf{e}^r - \mathbf{e}^p_1\right)$. At PT $A \to M$ we have $\mathbf{e}^f_A = \mathbf{e}^f_1 = 0$, $\mathbf{e}^p_1 = \mathbf{e}^p_A$, $\mathbf{S}_{eq} = \mathbf{S} + P\left(\mathbf{e}^r - \mathbf{e}^p_A\right) = \mathbf{S}_A$ (as $\mathbf{e}^r - \mathbf{e}^p_A = \mathbf{e}^r - \mathbf{e}^r_A = c\mathbf{e}^r_M + (1-c)\,\mathbf{e}^r_A - \mathbf{e}^r_A = c\left(\mathbf{e}^r_M - \mathbf{e}^r_A\right)$) and

$$X_n = \mathbf{S}_A : \mathbf{e}^f_2 - 0,5\,P \mid \mathbf{e}^f_2 \mid - \rho\left(\psi^\theta_M - \psi^\theta_A\right) = k^e_n. \tag{28}$$

Let us apply the postulate of realizability for determination of $\mathbf{e}^f_2$. Assume that $\mid \mathbf{e}^f_2 \mid$ could not exceed some value $a\,(c)$, but due to e.g. twinning it is possible that $\mid \mathbf{e}^f_2 \mid \leq a$. Consequently from the principle (17) it follows

$$\mathbf{S}_A : \mathbf{e}^{f^*}_2 - 0,5\,P \mid \mathbf{e}^{f^*}_2 \mid^2 \leq 0 = \mathbf{S}_A : \mathbf{e}^f_2 - 0,5\,P \mid \mathbf{e}^f_2 \mid^2 \quad \text{at} \quad \mid \mathbf{e}^f_2 \mid \leq a\,; \tag{29}$$

$$\mathbf{e}^f_2 = (1/P)\,\mathbf{S}_A \quad \text{at} \quad \mid \mathbf{e}^f_2 \mid < a\,; \quad \mathbf{e}^f_2 = a\,\mathbf{S}_A / \mid \mathbf{S}_A \mid \quad \text{at} \quad \mid \mathbf{e}^f_2 \mid = a\,. \tag{30}$$

Substituting Eq. (30) in Eq. (28) we obtain explicit expression of $A \to M$ PT criterion

$$(1/2P) \mid \mathbf{S}_A \mid^2 = \left(\psi^\theta_M - \psi^\theta_A\right) + k_{A\to M} \quad \text{at} \quad \mid \mathbf{S}_A \mid < P\,a\,; \tag{31}$$

$$a \mid \mathbf{S}_A \mid = a^2\, P/2 + \left(\psi^\theta_M - \psi^\theta_A\right) + k_{A\to M} \quad \text{at} \quad \mid \mathbf{S}_A \mid \geq P\,a\,. \tag{32}$$

Eqs. (28)–(32) have the same form, as corresponding equations for elastic materials [12], but $\mathbf{S}_A$ depends on plastic strain. As $\mathbf{S}_A = \mathbf{S} + P\mathbf{e}^f + cP\left(\mathbf{e}^p_M - \mathbf{e}^p_A\right)$, then difference $\mathbf{e}^p_M - \mathbf{e}^p_A$, which increase $\mid \mathbf{S}_A \mid$, will improve PT conditions (increase X_n) and vice versa.

Consider PT with additional plastic strain in nucleus. Consider the simple (radial) loading, when the direction of the stress vector (tensor) $\mathbf{S}$ in R^5 is fixed, $\mathbf{m} = \mathbf{S}/\mid \mathbf{S} \mid = \mathbf{const}$, and directions of all other tensors ($\mathbf{e}^f_n$, $\mathbf{e}^p_n$, $\mathbf{e}^r$, ...) are the same. We shall say conventionally that some tensor $\mathbf{A}$ is increased (decreased) if value $\mathbf{A} : \mathbf{m}$ is increased (decreased). Assume that both phases are perfectly plastic and with the yield limits at tension σ_{YA} and σ_{YM} respectively, von Mises yield condition is valid $\mid \mathbf{S} \mid = \sqrt{2/3}\,\sigma_Y$ and twinning is impossible. Then in the course of PT $\mathbf{e}^f_n$ grows from zero to $\mid \mathbf{e}^f_2 \mid = a$. It follows from Eq.(24) that $\mathbf{S}_n$ is decreased from value $\mathbf{S}_A$ till zero, then $\mathbf{S}_n$ changes its sign and reaches the yield limit, after which the plastic deformation occurs in the opposite to $\mathbf{S}$ direction. From the yield condition $\mathbf{S}_n = -\mathbf{Y}_M$, where $\mathbf{Y}_M = \sqrt{2/3}\,\sigma_{YM}\mathbf{m}$, we obtain that plastic flow starts at $\mathbf{e}^f_n = \mathbf{e}^f_Y := \left(\mathbf{Y}_M + \mathbf{S}_A\right)/P$ and in the course of plastic flow $\mathbf{e}^p_n + \mathbf{e}^f_n = \mathbf{e}^f_Y + \mathbf{e}^p_A$, i.e. $\mathbf{e}^p_n = \mathbf{e}^f_Y + \mathbf{e}^p_A - \mathbf{e}^f_n$. Then

$$\begin{aligned}\int_0^{\mathbf{e}^f_2} \mathbf{e}^p_n : d\mathbf{e}^f_n &= \int_0^{\mathbf{e}^f_Y} \mathbf{e}^p_A d\mathbf{e}^f_n + \int_{\mathbf{e}^f_Y}^{\mathbf{e}^f_2} \left(\mathbf{e}^f_Y + \mathbf{e}^p_A - \mathbf{e}^f_n\right) d\mathbf{e}^f_n = \\ &= \left(\mathbf{e}^f_Y + \mathbf{e}^p_A\right) : \mathbf{e}^f_2 - 0,5\left(\mid \mathbf{e}^f_Y \mid^2 + \mid \mathbf{e}^f_2 \mid^2\right).\end{aligned} \tag{33}$$

Substituting this expression in Eq. (26) and making use $\mathbf{e}^f_Y = \left(\mathbf{Y}_M + \mathbf{S}_A\right)/P$ we obtain

$$X_n = -\mathbf{Y}_M : \mathbf{e}^f_2 + 0,5\,P \mid \mathbf{e}^f_Y \mid^2 - \rho\left(\psi^\theta_M - \psi^\theta_A\right) = k^e_n, \quad \text{or} \tag{34}$$

$$X_n = -\mathbf{Y}_M : \mathbf{e}^f_2 + 0,5\,\left(\mathbf{S}_A + \mathbf{Y}_M\right) : \mathbf{e}^f_Y - \rho\left(\psi^\theta_M - \psi^\theta_A\right) = k^e_n \qquad \text{and} \tag{35}$$

$$X_n = -\mathbf{Y}_M : \mathbf{e}^f_2 + \mid \mathbf{S}_A + \mathbf{Y}_M \mid^2 /2P - \rho\left(\psi^\theta_M - \psi^\theta_A\right) = k^e_n. \tag{36}$$

Let us analyze the PT criteria (34)–(36). Usually $\mid \mathbf{e}^f_2 \mid$ exceeds $\mid \mathbf{e}^f_Y \mid$ by several or even by ten times and $\mid \mathbf{S}_A \mid < \mid \mathbf{Y}_M \mid$. Consequently the first two terms in Eq. (35), which characterize mechanical contributions to the driving force X_n, are negative. But this fact does not mean that external stresses and active plastic strain produce negative contributions to X_n, because these two terms are negative at $\mathbf{S} = \mathbf{e}^p = 0$ as well. Let us consider appearance of first nucleus of martensite at $\mathbf{S} = 0$, i.e. $\mathbf{e}^r_A = \mathbf{e}^r_M = 0$. In this case Eq. (36) results in

$$X_n = X_n(0) := \mid \mathbf{Y}_M \mid^2 /2P - \mathbf{Y}_M : \mathbf{e}^f_2 - \rho\left(\psi^\theta_M - \psi^\theta_A\right) = k^e_n, \tag{37}$$

and the contributions of mechanical terms (work of internal stresses) toX_n are also negative. If the first nucleus appears at $\mathbf{e}^p_A = \mathbf{e}^p_M = 0$ and $\mathbf{S} \neq 0$, then from Eq.(36) we have

$$X_n = X_n(0) + \mid \mathbf{S} \mid^2 / (2P) + \mathbf{S} : \mathbf{Y}_M/P = k^e_n, \tag{38}$$

i.e. applied stress improve PT condition (in comparison with $X_n(0)$), which corresponds to experiments [10]. At $\mathbf{e}^r_A \neq 0$, $\mathbf{e}^r_M \neq 0$

$$X_n = X_n(0) + \mid \mathbf{S}_A \mid^2 / (2P) + \mathbf{S}_A : \mathbf{Y}_M/P = k^e_n. \tag{39}$$

The maximal value of X_n will be reached at $\mathbf{S}_A = \sqrt{2/3}\,\sigma_{YA}\,\mathbf{m}$, i.e. at plastic straining of A:

$$X_n = X_n(0) + \sigma_{YA}^2/\,(3P) + 2\sigma_{YA}\,\sigma_{YM}/\,(3P)\,. \tag{40}$$

Exact formulas for PT in the hardening materials requires more place, but rough analysis is possible making use Eqs. (37) and (40). Plastic strain, increasing both σ_{YA} and σ_{YM}, decreases $X_n(0)$, but increases the two last terms in Eq. (40). Consequently, preliminary plastic straining of A decreases $X_n(0)$ and makes PT conditions worse at $\mathbf{S} = 0$. Active plastic strains at $\mathbf{S} \neq 0$ improve PT conditions (relatively $X_n(0)$). These facts are also in agreement with experiments [10, 11].

Concluding remarks

In the paper the general thermodynamical approach for the description of PT in elastoplastic materials is suggested. Some additional aspects, related with consideration of PT as the stable post–bifurcation deformation processes in the finite volume, are considered in [5]. It is necessary to note, that value σ_{YM} is not well defined in the above equations, because plastic flow starts on some intermediate stage of PT, before formation of M. As first approximation we can use the yield condition for M in the form $\mid \mathbf{S}_M \mid = \sqrt{2/3}\,\left(\sigma_{YA}\left(1 - \mid \boldsymbol{\varepsilon}_n^f \mid\right) + \sigma_{YM} \mid \boldsymbol{\varepsilon}_n^f \mid\right) a^{-1}$.

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