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THE POSTULATE OF REALIZABILITY: FORMULATION AND APPLICATIONS TO THE POST-BIFURCATION BEHAVIOUR AND PHASE TRANSITIONS IN ELASTOPLASTIC MATERIALS—II

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Abstract—The extremum principles for the interface are derived using the postulate of realizability. They are used to derive a number of equations for the description of phase transitions (PTs): for jumps of the deformation gradient and the tensors characterizing the mutual orientation of the phases; for the deformation gradient history in the course of PT; for the normal velocity of the interface and the velocity of the relative sliding along the interface; the local criteria for the martensitic PT. The governing extremum principle for the description of a stable post-bifurcation process for a volume of elastoplastic materials with PT is derived. The local PT criteria represent the equations for some parameters across the interface. But even when they can be met, two solutions are possible: first, the solution with fixed interface, second, the solution with the moving one. The more stable solution can be chosen using the extremum principle for the whole volume, which is the global PT criterion and gives the final solution. Some examples are considered. It is shown that in the course of PT, the traction continuity condition is violated across the interface. To remove this contradiction the concept of fluctuating stresses is introduced. These stresses overcome the energy barrier and restore the traction continuity condition.

1. INTRODUCTION

In this part of the paper the postulate of realizability is applied to describe PT in elastoplastic materials at finite strains. We consider coherent PT (when the position vector is continuous, but the velocity vector and deformation gradient have jumps across the interface) and noncoherent ones (when the position vector has a jump too). In Section 2 the martensitic PT in elastic materials is considered. In Section 3 necessary conditions for coherent PT in elastoplastic media at simple shearing and in a general case are derived. They result in generalization of Maxwell convention. Using the postulate of realizability in Section 4 the extremum principle describing PT is derived. This principle determines jumps across the interface of the deformation gradient and the tensors characterizing the mutual orientation of the phases, deformation gradient history in the course of PT as well as local PT criterion. Then extremum principles for a finite volume of elastoplastic material with PT are derived. In the particular case, these principles result in global PT criteria (based on consideration of whole volume rather than interface only), which can differ from the local one. In Section 5 PT a simple shearing is examined and an example of noncoincidence of the local and global criteria is shown. In Section 6 the noncoherent PTs are briefly described. The Appendix contains some relations for points of the interface.

2. MARTENSITIC PT IN ELASTIC MATERIALS

Consider the simple shearing of an infinite slab (Fig. 1) of nonlinear elastic material with a diagram $\tau = f(\gamma)$, shown in Fig. 2, where τ and γ are shear stress and strain, respectively. At $y = h$ velocity v is prescribed. At $y = 0$ the velocity is equal to zero. The diagram shown in Fig.

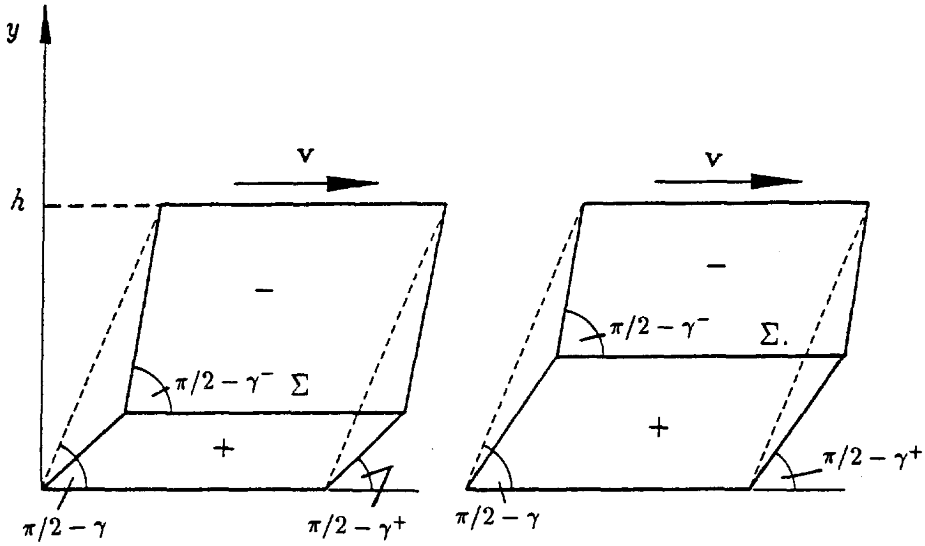


Fig. 1. Simple shearing of a slab of nonlinear elastic material.

2 is typical for materials with martensitic PT. We will not consider physical processes like crystal lattice variation, but instead we will formally describe instability in the nonlinear elastic continuum. We will label the phases corresponding to the branches *ABC* and *EFG* $(-)$ and $(+)$ respectively; branch *CDE* exhibits an unstable intermediate state. The free energy for a given material has a concave part (Fig. 3). Note that this diagram is obtained at homogeneous stress and strain distribution and all small but macroscopic volumes have to behave in accordance with this diagram [1].

Homogeneous straining along the line *ABCDEFG* for materials with the concave free energy is unstable. From the free energy minimum principle it follows that the equilibrium PT occurs at constant shear stress τ, the free energy ψ is nonconcave and the strain is nonhomogeneous (Fig. 3). At some stress τ_0, a macroscopic portion of the material is deformed from γ^- to γ^+ along line *ABCDEF* (Fig. 2). At the next total shear strain increment $\Delta\gamma$, the next portion of material undergoes PT. During the whole process of PT, the strains in the phases $(-)$ and

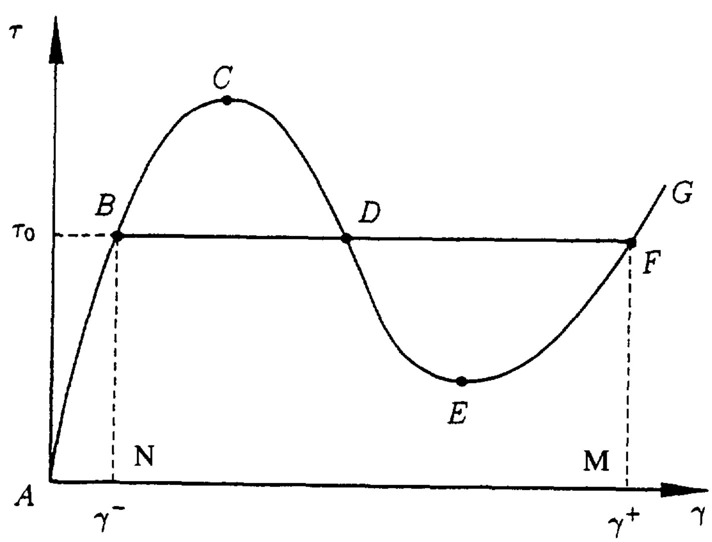


Fig. 2. Diagram of the simple shearing of nonlinear elastic material.

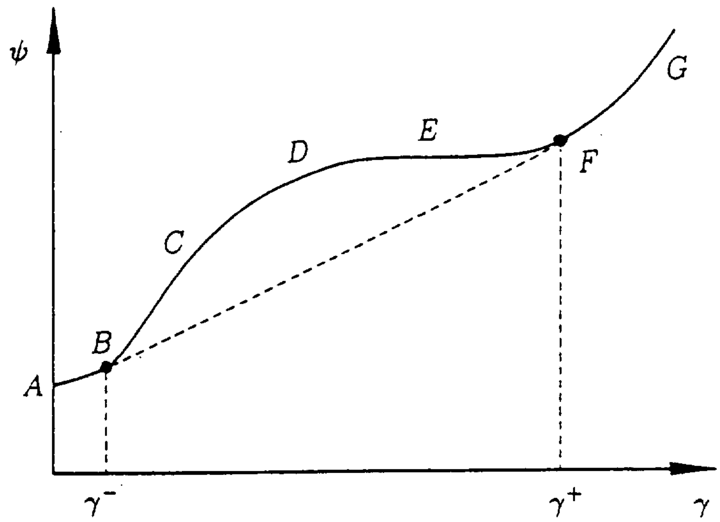


Fig. 3. Free energy vs shear strain for the diagram shown in Fig. 2.

(+) are fixed and equal to γ^- and γ^+, the stress is constant $\tau = \tau_0$ and $\Delta\gamma$ is related to the increment Δc of the volume fraction of a new phase.

Across the interface Σ the rate of dissipation takes the form (see Appendix)

$$\mathscr{D}_\Sigma = [\tau(\gamma^+ - \gamma^-) - \rho(\psi(\gamma^+) - \psi(\gamma^-))]v_n \geq 0 \tag{2.1}$$

where v_n is the normal velocity of the interface and ρ the mass density in the reference configuration V. For the thermodynamical equilibrium processes $\mathscr{D}_\Sigma = 0$ and we find the equilibrium stress

$$\tau_0 = \rho(\psi(\gamma^+) - \psi(\gamma^-))/(\gamma^+ - \gamma^-). \tag{2.2}$$

This is well known Maxwell convention. Geometrically speaking, it means that the areas (BCD) and (DEF) are the same (Fig. 1) [(BCD) denotes the area enclosed by the straight line BC and the curve BCD, and similarly for (BCD)]. In reality, terms $\tau(\gamma^+ - \gamma^-)$ and $\rho(\psi(\gamma^+) - \psi(\gamma^-))$ are equal to area $(BFNM)$ and $(BCDEFNM)$, respectively, and their equality results in the equality of areas (BCD) and (DEF). The volume fraction c of the phase (+) is determined from expression $\gamma = c\gamma^+ + (1-c)\gamma^-$, i.e. $c = (\gamma - \gamma^-)/(\gamma^+ - \gamma^-)$. Thus, all points of the materials are deformed along the line $ABCDEFG$. This deformation does not proceed simultaneously in all points, but heterogeneously, at each γ-increment at the different points in the volume. Macroscopically, this behaviour results in curve $ABDFG$ and corresponds to the free energy minimum principle, i.e. it is thermodynamically more profitable than homogeneous deformation.

Note two important details. Firstly, in the course of PT, the violation of the traction continuity across the interface Σ takes place. In the (−)-phase $\tau = \tau_0$, but at the (+)-phase the shear stress varies according to line $BCDEF$ and there is continuity at the points B, D and F only (Fig. 2).

Secondly, the fluctuations are needed in order to overcome the energy barrier (BCD) at macroscopic stress τ and move along the curve $BCDEF$. The material borrows energy (BCD) from the system and at the next instant returns the same energy (DEF) to it. The fluctuations could be both the thermoactivated and caused by stress concentrations on different types of defects. Necessity of perturbations was mentioned in the similar problem by Ericksen [2].

Let us introduce fluctuating shear stress $\tau_f = f(\gamma) - \tau^-$, $\gamma \in [\gamma^-, \gamma^+]$ [1]. This fluctuating stress acts for a very short time in a small, but macroscopic volume, undergoing PT and does not contribute to the macroscopic stress. For the equilibrium processes the time average value of τ_f is equal to zero. Consequently, after these assumptions we restore shear stress continuity across Σ: macroscopic shear stress $\tau^- = \tau^+ \ \forall \gamma \in [\gamma^-, \gamma^+]$ and the fluctuating shear stress overcomes the energy barrier (BCD).

3. SOME NECESSARY CONDITIONS FOR COHERENT PHASE TRANSITIONS IN ELASTOPLASTIC MATERIALS

In this section some necessary conditions for the coherent PT in elastoplastic materials will be derived. Some relations for the points of the interface are given in the Appendix. Sufficient conditions will be determined in the next section, using the postulate of realizability.

3.1 Simple shearing

Rigid-plastic materials. Let us start with the rigid-plastic material having a deformation diagram at the simple shearing, shown in Fig. 4. Assume that at some stress τ we have onset of PT and jump of shear strain γ from γ^- until γ^+ in some portion of the material. The rate of dissipation, related to the interface movement, will be (see equation (A8) in the Appendix)

$$\mathscr{D}_\Sigma = \tau(\gamma^+ - \gamma^-)v_n = X_\Sigma v_n. \tag{3.1}$$

But material in a PT region deforms in accordance with diagram $\tau = f(\gamma)$, and this deformation must give the dissipation work $\bar{W} = (W(\gamma^+) - W(\gamma^-))\Delta v$, where $W(\gamma) = \int_0^\gamma \tau \, d\gamma$ is the dissipated work per unit volume at the deformation from zero until shear strain γ; $\Delta v = v_n \Sigma \Delta t$ is a volume covered by surface Σ during time Δt (Fig. 5). The expression $W(\gamma^+) - W(\gamma^-)$ is equal to the area below the curve $\tau = f(\gamma)$ on the interval (γ^-, γ^+). The rate of dissipation per unit area is

$$\mathscr{D}_\Sigma^T = \bar{W}/(\Sigma \Delta t) = (W(\gamma^+) - W(\gamma^-))v_n = X_\Sigma^T v_n. \tag{3.2}$$

We have two expressions for the rate of dissipation. Equation (3.2) shows the value of the

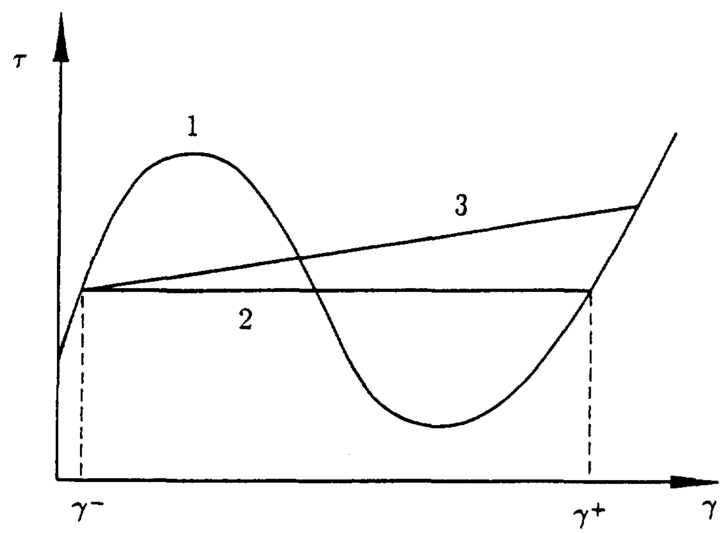


Fig. 4. Diagram of the simple shearing for rigid-plastic material with phase transition: 1—homogeneous straining; 2—phase equilibrium line at $k = 0$; 3—phase equilibrium line at $k > 0$.

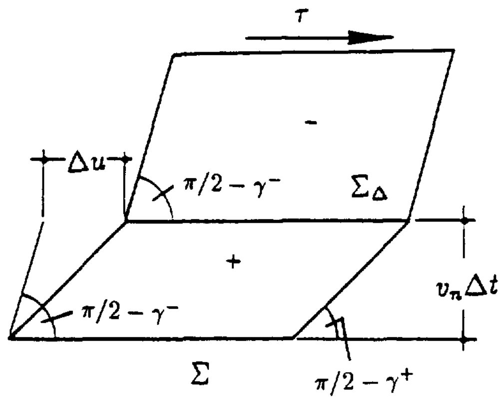


Fig. 5. Volume $\Delta v = v_n \Sigma\, \Delta t$, covered by the Σ-surface during the time increment Δt at simple shearing.

power which have to be dissipated at the Σ-surface movement. Equation (3.1) exhibits the power of the external stress τ, if the Σ-surface with strain jump $(\gamma^+ - \gamma^-)$ moves with rate v_n; for rigid-plastic materials all of this power will be dissipated. Evidently, if

$$X_\Sigma < X_\Sigma^{\mathrm{T}}, \quad \text{i.e.} \quad \tau(\gamma^+ - \gamma^-) < (W(\gamma^+) - W(\gamma^-)), \tag{3.3}$$

then the Σ-surface movement is impossible, if a Σ-surface exists, or the first jump of strain is impossible in the opposite case. To prove this, consider the energy balance equation for the volume $\Delta v = v_n \, \mathrm{d}\Sigma \, \Delta t$ (Fig. 5):

$$\int_{\Sigma_\Delta} \tau \, \Delta u \, \mathrm{d}\Sigma - \bar{W} = \Delta K, \tag{3.4}$$

where $\Delta u = (\gamma^+ - \gamma^-) v_n \, \Delta t$ is the displacement increment on the surface Σ_Δ (surface Σ fixed), $K \geq 0$ is the kinetic energy of the volume Δv; $\Delta K = K(t + \Delta t) - K(t) = K(t + \Delta t) \geq 0$ due to the assumption of $K(t) = 0$. From equation (3.4) it follows

$$[\tau(\gamma^+ - \gamma^-) - (W(\gamma^+) - W(\gamma^-))] v_n \, \mathrm{d}\Sigma \, \Delta t = K(t + \Delta t) \geq 0. \tag{3.5}$$

Consequently, for PT which has actually occurred quasistatically ($K = 0$)

$$\tau(\gamma^+ - \gamma^-) = (W(\gamma^+) - W(\gamma^-)). \tag{3.6}$$

Thus, equation (3.6) is a necessary condition for the jump of the shear strain (instability, PT), and inequality (3.3) is a sufficient condition for the absence of strain jump. To prove the sufficient condition for PT and the necessary condition for stability, we need a principle describing post-bifurcation behaviour. Consequently, we have the Maxwell rule as a candidate for the determination of the bifurcation point and the phase equilibrium diagram (Fig. 1).

Note that superscript T in equation (3.2) denotes "threshold", i.e. $\mathscr{D}_\Sigma^{\mathrm{T}}$ and X_Σ^{T} are the threshold value of the rate of dissipation and dissipation force which it is necessary to reach for the Σ-surface movement. Note that the concept of threshold-type dissipation force which resists the interface movement at the martensitic PT was considered in [3–5]. For the elastic materials this force is related with intersections of the interface Σ with different types of defects—point defects, dislocations and especially with grain and subgrain boundaries. Only under the presence of this force we do succeed in describing stable two-phase thermodynamic equilibrium for elastic materials with PT [3, 4]. For elastoplastic materials when both sources of force X^{T}

appear (the jump of the plastic strain and the intersections of the Σ-surface with defects) they have to be summed up. In this case $X_\Sigma^T = W(\gamma^+) - W(\gamma) + k(c)$ and condition $X_\Sigma = X_\Sigma^T$ results (Fig. 4) in

$$\tau(\gamma^+ - \gamma^-) = W(\gamma^+) - W(\gamma^-) + k(c), \tag{3.7}$$

where k is the threshold value of the dissipation force, which resists the interface movement and is not related to plastic strain; it may depend on the interface displacement u_n and its history, but for simple shear (and at the averaged description) it is more convenient to consider k as a function of the volume fraction c and its history. Some analytical approximations of k for polycrystals are given in [6] and for monocrystals in [7]. Note that equation (3.7) could be obtained by making use of the energy balance equation [as in equation (3.4)].

Elastoplastic materials. For the simple shear problem the total, elastic and plastic deformation gradients are equal, respectively, to $\mathbf{F} = \mathbf{I} + \gamma\mathbf{mn}$, $\mathbf{F}_e = \mathbf{I} + \gamma_e\mathbf{mn}$, $\mathbf{F}_p = \mathbf{I} + \gamma_p\mathbf{mn}$, where $\mathbf{m}$ and $\mathbf{n}$ are the shear directions and normal to the shear plane, respectively. From the multiplicative decomposition $\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p$, taking into account for $\mathbf{n} \cdot \mathbf{m} = 0$, it follows that $\mathbf{F} = \mathbf{I} + \gamma\mathbf{mn} = \mathbf{I} + (\gamma_e + \gamma_p)\mathbf{mn}$; $\gamma = \gamma_e + \gamma_p$. Assuming that $\psi = \psi(\gamma_e, \gamma_p)$, let us determine the rate of plastic dissipation $\mathscr{D} = \tau\dot{\gamma} - \rho\dot{\psi}$ and dissipation work in a volume Δv $\bar{W} = (\int_{\gamma^-}^{\gamma^+} \mathscr{D}\,\mathrm{d}t + k(c))\,\Delta v$, whence

$$X_\Sigma^T = \frac{\bar{W}}{\Delta v} = \int_{\gamma^-}^{\gamma^+} f(\gamma)\,\mathrm{d}\gamma - \rho(\psi(\gamma_e^+, \gamma_p^+) - \psi(\gamma_e^-, \gamma_p^-)) + k(c). \tag{3.8}$$

Expression (A8) in the Appendix results in $X_\Sigma = \tau(\gamma^+ - \gamma^-) - \rho(\psi(\gamma^+) - \psi(\gamma^-))$ and from the necessary condition for PT $X_\Sigma = X_\Sigma^T$ we get

$$\tau(\gamma^+ - \gamma^-) = \int_{\gamma^-}^{\gamma^+} f(\gamma)\,\mathrm{d}\gamma + k(c), \tag{3.9}$$

i.e. the generalized Maxwell convention. The same result may be obtained using energy balance considerations. The results of this section are new ones.

3.2 *General case*

The second law of thermodynamics for a finite volume of the elastoplastic multiphase materials with moving interface Σ has the form

$$\int_S \mathbf{p} \cdot \mathbf{v}\,\mathrm{d}S - \frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\psi(\mathbf{F}_e, \mathbf{F}_p)\,\mathrm{d}v$$
$$= \int_{\bar{v}} \mathscr{D}(\dot{\mathbf{F}}_p, \mathbf{F}_p)\,\mathrm{d}\bar{v} + \int_\Sigma \mathscr{D}_\Sigma^T(\mathbf{F}^+, \mathbf{F}^-, \mathbf{F}(s), \boldsymbol{\chi}, u_n, v_n)\,\mathrm{d}\Sigma \geq 0, \tag{3.10}$$

where $\mathbf{F}^+$ and $\mathbf{F}^-$ are the deformation gradients from the side of positive and negative direction of normal $\mathbf{n}$ to the interface, respectively, $\mathbf{F}(s)$ is the deformation gradient path between $\mathbf{F}^-$ and $\mathbf{F}^+$; tensor (or a set of tensors) $\boldsymbol{\chi}$ characterizes the mutual orientation of the new and the partent phases; $\mathscr{D}_\Sigma^T$ is a threshold value of dissipated power due to the interface motion; $\bar{v} = v - \Sigma$ means the volume v without interfaces; $\mathscr{D}_\Sigma^T$ depends on the whole history of u_n, ψ and $\mathscr{D}$ depend on history of $\mathbf{F}$. The first two terms in equation (3.10) represent, according to the second law of thermodynamics, the rate of dissipation in a volume v. Equation (3.10) shows only that this rate of dissipation consists of two parts: one of them is concentrated across Σ and the second term is distributed in the points of $\bar{v}$.

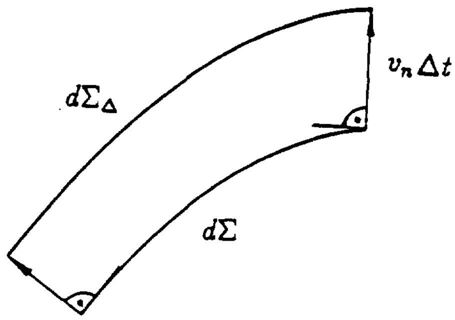


Fig. 6. Volume $dv = v_n \, d\Sigma \, \Delta t$, covered by the Σ-surface during the time increment Δt in the general case.

Consider an infinitesimal volume $dv = v_n \, \Delta t \, d\Sigma$ (Fig. 6), covered by the Σ-surface during the time Δt. Calculating the dissipated work $\bar{W}$ in a volume Δv and $X_\Sigma^T = \bar{W}/\Delta v$ we have

$$X_\Sigma^T = \int_{\mathbf{F}^-}^{\mathbf{F}^+} \mathbf{P}'(\mathbf{F}(s), \chi) : d\mathbf{F} - \rho(\psi(\mathbf{F}_e^+, \mathbf{F}_p^+, \chi) - \psi(\mathbf{F}_e^-, \mathbf{F}_p^-)) + k(u_n). \tag{3.11}$$

The integral in equation (3.11) is calculated along the deformation path $\mathbf{F}(s)$. We shall assume the tensor χ is varied (has jump) only as the interface sweeps by; in the points of the volume $\bar{v}$ it is fixed (this variation was taken into account in [4]).

From equations (3.10) and (3.11) and the results of the Appendix it follows

$$\int_v (\mathbf{P}' : \dot{\mathbf{F}} - \rho\dot{\psi} - \mathscr{D}(\dot{\mathbf{F}}_p, \mathbf{F}_p)) \, dv + \int_\Sigma (X_\Sigma - X_\Sigma^T) v_n \, d\Sigma = 0 \tag{3.12}$$

where

$$X_\Sigma = \mathbf{P}' : [\mathbf{F}] - \rho[\psi] = \mathbf{n} \cdot \mathbf{P}' \cdot [\mathbf{F}] \cdot \mathbf{n} - \rho(\psi(\mathbf{F}_e^+, \mathbf{F}_p^+, \chi) - \psi(\mathbf{F}_e^-, \mathbf{F}_p^-)). \tag{3.13}$$

At $\dot{\mathbf{F}}_p \neq \mathbf{0}$ and $v_n \neq 0$ equation (3.12) gives the same definition of $\mathscr{D}$ in the points of the volume $\bar{v}$, as equation (2.32) from Part I [8] for media without PT and

$$X_\Sigma = X_\Sigma^T \quad \text{or} \quad \mathbf{P}' : [\mathbf{F}] = \int_{\mathbf{F}^-}^{\mathbf{F}^+} \mathbf{P}'(\mathbf{F}(s), \chi) : d\mathbf{F} + k(u_n). \tag{3.14}$$

Equation (3.14) represents the generalized Maxwell rule for inelastic materials. It contains the stress work independently of the fact of whether work is dissipated or not. Equation (3.14) can also be obtained from the energy balance principles for the volume dv.

Equation (3.14) is one of the necessary conditions of the PT ($v_n \neq 0$). For actually occurring PT, the analogous conditions has to be met at time $t + \Delta t$ across the surface Σ_Δ

$$\mathbf{P}'_\Delta : (\mathbf{F}_\Delta^+ - \mathbf{F}_\Delta^-) = \int_{\mathbf{F}_\Delta^-}^{\mathbf{F}_\Delta^+} \mathbf{P}'(\mathbf{F}(s), \chi_\Delta) : d\mathbf{F} + k(u_{n\Delta}). \tag{3.15}$$

For an infinitesimal time increment Δt and the existence of all the derivatives which are necessary, equation (3.15) transforms into

$$(\dot{\mathbf{P}}' + \mathbf{n} \cdot \nabla \mathbf{P}' v_n) : (\mathbf{F}^+ - \mathbf{F}^-) = \frac{\partial k}{\partial u_n} v_n. \tag{3.16}$$

We have taken into account that $\mathbf{A}_\Delta = \mathbf{A} + (\dot{\mathbf{A}} + \mathbf{n} \cdot \nabla \mathbf{A} v_n) \Delta t$ for $\mathbf{A} = \mathbf{P}'$, $\mathbf{F}^+$ and $\mathbf{F}^-$, respectively, and

$$\int_{\mathbf{F}_\Delta^-}^{\mathbf{F}_\Delta^+} \mathbf{P}' : d\mathbf{F} = \int_{\mathbf{F}^-}^{\mathbf{F}^+} \mathbf{P}' : d\mathbf{F} + \int_{\mathbf{F}^+}^{\mathbf{F}_\Delta^+} \mathbf{P}' : d\mathbf{F} - \int_{\mathbf{F}^-}^{\mathbf{F}_\Delta^-} \mathbf{P}' : d\mathbf{F}$$

$$= \int_{\mathbf{F}^-}^{\mathbf{F}^-} \mathbf{P}' : d\mathbf{F} + \mathbf{P}' : (\dot{\mathbf{F}}^+ + \mathbf{n} \cdot \nabla \mathbf{F}^+ v_n) \Delta t - \mathbf{P}' : (\dot{\mathbf{F}}^- + \mathbf{n} \cdot \nabla \mathbf{F}^- v_n) \Delta t. \tag{3.17}$$

The term $\nabla\mathbf{A}$ appears due to the fact that the tensor $\mathbf{A}_\Delta$ is determined on the Σ_Δ surface, i.e. at point $\mathbf{r}_\tau + v_n\mathbf{n}\,\Delta t$, where $\mathbf{r}_\tau$ belong to Σ. At a homogeneous stress field in equation (3.16) $\nabla\mathbf{P} = \mathbf{0}$. If $\partial k/\partial u_n = 0$ then $\dot{\mathbf{P}}':(\mathbf{F}^+ - \mathbf{F}^-) = 0$. Equations (3.14) and (3.16) are the necessary conditions for the interface propagation. Equation (3.13) is well-known, but equations (3.11), (3.14)–(3.16) are the new ones.

4. THE GOVERNING PRINCIPLE FOR THE DESCRIPTION OF THE POST-BIFURCATION PROCESS FOR ELASTOPLASTIC MATERIALS WITH PT

4.1 Application of the postulate of realizability to determine the parameters across the interface

It is evident that the parameters $\mathbf{F}^+$, $\mathbf{F}^-$, $\boldsymbol{\chi}$ and the paths $\mathbf{F}(s)$ are not determined uniquely by condition (3.15). Usually the several crystallographically equivalent variants of the PT with various $\boldsymbol{\chi}$ tensors are possible, and each of them could give various $\mathbf{F}^+$, $\mathbf{F}^-$ and $\mathbf{F}(s)$; but even for fixed $\boldsymbol{\chi}$ or for isotropic phases, when $\boldsymbol{\chi}$ is not a state parameter, tensors $\mathbf{F}^+$, $\mathbf{F}^-$ and $\mathbf{F}(s)$ may be ambiguous due to, for example, nonuniqueness of the flow rule or complex geometry of the yield surface and free energy. Let us use the postulate of realizability to determine these parameters. It is evident that if

$$X_\Sigma(\mathbf{F}^{+*}, \mathbf{F}^-, \boldsymbol{\chi}^*) < X_\Sigma^{\mathrm{T}}(\mathbf{F}^{+*}, \mathbf{F}^{-*}, \mathbf{F}^*(s), \boldsymbol{\chi}^*) \quad \forall \mathbf{F}^{+*}, \mathbf{F}^{-*}, \mathbf{F}^*(s) \text{ and } \boldsymbol{\chi}^*, \tag{4.1}$$

then $v_n = 0$ and PT is impossible. The proof is trivial: for an actually occurring PT equation (3.14) is valid, which is in contradiction with inequality (4.1).

According to the postulate of realizability, PT will occur the first time when equation (3.14) is met. Consequently, for real values of the varied parameters equation (3.14) is valid, for all possible ones—inequality (4.1) is true. We obtain the extremum principle

$$X_\Sigma(\mathbf{F}^{+*}, \mathbf{F}^{-*}, \boldsymbol{\chi}^*) - X_\Sigma^{\mathrm{T}}(\mathbf{F}^{+*}, \mathbf{F}^{-*}, \mathbf{F}^*(s), \boldsymbol{\chi}^*) < 0 = X_\Sigma(\mathbf{F}^+, \mathbf{F}^-, \boldsymbol{\chi}) - X_\Sigma^{\mathrm{T}}(\mathbf{F}^+, \mathbf{F}^-, \mathbf{F}(s), \boldsymbol{\chi}). \tag{4.2}$$

Making use of equations (3.13) and (3.11) for X_Σ and X_Σ^T we have

$$\mathbf{P}':(\mathbf{F}^{+*} - \mathbf{F}^{-*}) - \int_{\mathbf{F}^{-*}}^{\mathbf{F}^{+*}} \mathbf{P}'(\mathbf{F}^*(s), \boldsymbol{\chi}^*):\mathrm{d}\mathbf{F} - k(u_n) < 0$$

$$= \mathbf{P}':(\mathbf{F}^+ - \mathbf{F}^-) - \int_{\mathbf{F}^-}^{\mathbf{F}^+} \mathbf{P}'(\mathbf{F}(s), \boldsymbol{\chi}):\mathrm{d}\mathbf{F} - k(u_n). \tag{4.3}$$

Principle (4.3) has to be considered jointly with the equations for the yield surface, the free energy and the flow rule. At fixed $\mathbf{F}^{+*} = \mathbf{F}^+$ and $\mathbf{F}^{-*} = \mathbf{F}^-$ from principle (4.3) it follows

$$\int_{\mathbf{F}^-}^{\mathbf{F}^+} \mathbf{P}'(\mathbf{F}^*(s), \boldsymbol{\chi}^*):\mathrm{d}\mathbf{F} \to \min, \tag{4.4}$$

i.e. the principle of the minimum of work. It is easy to take into account dependence of k on $\mathbf{F}^+$, $\mathbf{F}^-$, $\boldsymbol{\chi}$ and $\mathbf{F}(s)$. The counterparts of the principles (4.2)–(4.3) at time $t + \Delta t$ read

$$X_{\Sigma\Delta}(\mathbf{F}_\Delta^{+*}, \mathbf{F}_\Delta^{-*}, \boldsymbol{\chi}_\Delta^*) - X_{\Sigma\Delta}^{\mathrm{T}}(\mathbf{F}_\Delta^{+*}, \mathbf{F}_\Delta^{-*}, \mathbf{F}^*(s), \boldsymbol{\chi}_\Delta^*) < 0$$

$$= X_{\Sigma\Delta}(\mathbf{F}_\Delta^+, \mathbf{F}_\Delta^-, \boldsymbol{\chi}_\Delta) - X_{\Sigma\Delta}^{\mathrm{T}}(\mathbf{F}_\Delta^+, \mathbf{F}_\Delta^-, \mathbf{F}(s), \boldsymbol{\chi}_\Delta); \tag{4.5}$$

$$\mathbf{P}_\Delta':(\mathbf{F}_\Delta^{+*} - \mathbf{F}_\Delta^{-*}) - \int_{\mathbf{F}_\Delta^{-*}}^{\mathbf{F}_\Delta^{+*}} \mathbf{P}'(\mathbf{F}^*(s), \boldsymbol{\chi}_\Delta^*):\mathrm{d}\mathbf{F} - k(u_{n\Delta}) < 0$$

$$= \mathbf{P}_\Delta':(\mathbf{F}_\Delta^+ - \mathbf{F}_\Delta^-) - \int_{\mathbf{F}_\Delta^-}^{\mathbf{F}_\Delta^+} \mathbf{P}'(\mathbf{F}(s), \boldsymbol{\chi}_\Delta):\mathrm{d}\mathbf{F} - k(u_{n\Delta}). \tag{4.6}$$

4.2 Application of the postulate of realizability for a finite volume of elastoplastic material with phase transition

For all admissible fields $\mathbf{v}^*$, $\dot{\mathbf{F}}^*$, $\dot{\mathbf{F}}_p^*$, $\mathbf{F}_e^*$ and v_n^* we have

$$\int_S \mathbf{p}\cdot\mathbf{v}^*\,\mathrm{d}S - \frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\psi^*\,\mathrm{d}v - \int_{\bar v} \mathbf{X}:\dot{\mathbf{F}}_p^*\,\mathrm{d}\bar v - \int_\Sigma X_\Sigma([\mathbf{F}^*],\boldsymbol{\chi}^*)v_n^*\,\mathrm{d}\Sigma = 0, \tag{4.7}$$

where

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\psi^*(\mathbf{F}_e,\mathbf{F}_p)\,\mathrm{d}v = \int_{\bar v}\rho\dot\psi^*\,\mathrm{d}\bar v + \int_\Sigma \rho[\psi^*]v_n^*\,\mathrm{d}\Sigma$$

$$= \int_{\bar v}\rho\dot\psi^*(\mathbf{F}_e,\mathbf{F}_p)\,\mathrm{d}\bar v + \int_\Sigma \rho(\psi(\mathbf{F}_e^{+*},\mathbf{F}_p^{+*},\boldsymbol{\chi}^*) - \psi(\mathbf{F}_e^{-*},\mathbf{F}_p^{-*}))v_n^*\,\mathrm{d}\Sigma \tag{4.8}$$

$\dot\psi^*(\mathbf{F}_e,\mathbf{F}_p)$ is determined by equation (4.10) from Part I [8]. We assume that $\mathbf{P}$ and $\mathbf{X}$ meet the yield criteria and $X_\Sigma \le X_\Sigma^T$. Remember, that at PT tensors $\mathbf{F}^{+*}$, $\mathbf{F}_e^{+*}$, $\mathbf{F}_p^{+*}$, $\mathbf{F}_e^{-*}$, $\mathbf{F}_p^{-*}$ and $\boldsymbol{\chi}^*$ depend on the conditions of transition. The proof of equation (4.7) is simple:

$$\int_S \mathbf{p}\cdot\mathbf{v}^*\,\mathrm{d}S - \frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\psi^*\,\mathrm{d}v = \int_{\bar v}\mathbf{P}':\dot{\mathbf{F}}^*\,\mathrm{d}\bar v - \int_\Sigma \mathbf{p}\cdot[\mathbf{v}^*]\,\mathrm{d}\Sigma - \int_{\bar v}\rho\dot\psi^*\,\mathrm{d}\bar v - \int_\Sigma\rho[\psi^*]v_n^*\,\mathrm{d}\Sigma$$

$$= \int_{\bar v}(\mathbf{P}':\dot{\mathbf{F}}^* - \rho\dot\psi^*)\,\mathrm{d}\bar v + \int_\Sigma(\mathbf{P}':[\mathbf{F}^*] - \rho[\psi^*])v_n^*\,\mathrm{d}\Sigma$$

$$= \int_{\bar v}\mathbf{X}:\dot{\mathbf{F}}_p^*\,\mathrm{d}\bar v + \int_\Sigma X_\Sigma(\mathbf{F}^{+*},\mathbf{F}^{-*},\boldsymbol{\chi}^*)v_n^*\,\mathrm{d}\Sigma. \tag{4.9}$$

We used equations (2.32) from Part I and (3.13), the results of the Appendix and $[\mathbf{v}^*] = -[\mathbf{F}^*]\cdot\mathbf{n}v_n^*$. As

$$\mathbf{X}\cdot\dot{\mathbf{F}}_p^* < \mathscr{D}(\dot{\mathbf{F}}_p^*,\mathbf{F}_p) \quad \forall\dot{\mathbf{F}}_p^* \ne \dot{\mathbf{F}}_p, \quad \dot{\mathbf{F}}_p^* \ne \mathbf{0}, \tag{4.10}$$

$$X_\Sigma(\mathbf{F}^{+*},\mathbf{F}^{-*},\boldsymbol{\chi}^*) < X_\Sigma^T(\mathbf{F}^{+*},\mathbf{F}^{-*},\mathbf{F}^*(s),\boldsymbol{\chi}^*), \tag{4.11}$$

for all parameters which are not equal to the real ones, then from equations (3.10), (4.7)–(4.11) the extremum principle follows

$$\int_S \mathbf{p}\cdot\mathbf{v}\,\mathrm{d}S - \frac{\mathrm{d}}{\mathrm{d}t}\int_v\rho\psi\,\mathrm{d}v - \int_{\bar v}\mathscr{D}(\dot{\mathbf{F}}_p,\mathbf{F}_p)\,\mathrm{d}\bar v - \int_\Sigma X_\Sigma^T(\mathbf{F}^+,\mathbf{F}^-,\mathbf{F}(s),\boldsymbol{\chi},u_n)v_n\,\mathrm{d}\Sigma$$

$$= 0 > \int_S \mathbf{p}\cdot\mathbf{v}^*\,\mathrm{d}S - \frac{\mathrm{d}}{\mathrm{d}t}\int_v\rho\psi^*\,\mathrm{d}v - \int_{\bar v}\mathscr{D}(\dot{\mathbf{F}}_p^*,\mathbf{F}_p)\,\mathrm{d}\bar v$$

$$- \int_\Sigma X_\Sigma^T(\mathbf{F}^{+*},\mathbf{F}^{-*},\mathbf{F}^*(s),\boldsymbol{\chi}^*,u_n)v_n^*\,\mathrm{d}\Sigma. \tag{4.12}$$

This principle could be obtained also using the postulate of realizability directly for the finite volume v without implementation of the consequence from this postulate for points of volume $\bar{v}$ and the surface Σ. An equivalent expression for principle (4.12) has the form

$$\int_S \mathbf{p}\cdot\mathbf{v}\,\mathrm{d}S-\int_{\bar{v}}(\rho\dot{\psi}+\mathscr{D}(\dot{\mathbf{F}}_{\mathrm{p}},\mathbf{F}_{\mathrm{p}}))\,\mathrm{d}\bar{v}-\int_\Sigma\int_{\mathbf{F}^-}^{\mathbf{F}^+}(\mathbf{P}'(\mathbf{F}(s),\boldsymbol{\chi}):\mathrm{d}\mathbf{F}+k(u_{\mathrm{n}}))v_{\mathrm{n}}\,\mathrm{d}\Sigma$$

$$=0>\int_S \mathbf{p}\cdot\mathbf{v}^*\,\mathrm{d}S-\int_{\bar{v}}(\rho\dot{\psi}^*+\mathscr{D}(\dot{\mathbf{F}}^*_{\mathrm{p}},\mathbf{F}_{\mathrm{p}}))\,\mathrm{d}\bar{v}$$

$$-\int_\Sigma\int_{\mathbf{F}^{-*}}^{\mathbf{F}^{+*}}(\mathbf{P}(\mathbf{F}^*(s),\boldsymbol{\chi}^*):\mathrm{d}\mathbf{F}+k(u_{\mathrm{n}}))v^*_{\mathrm{n}}\,\mathrm{d}\Sigma. \quad (4.13)$$

We used the same manipulation as at the transition from principle (4.2) to (4.3) and equation (4.8). At time $t+\Delta t$ the counterparts of principles (4.12) and (4.13) read

$$\int_S \mathbf{p}_\Delta\cdot\mathbf{v}_\Delta\,\mathrm{d}S-\frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\psi(\mathbf{F}_{\mathrm{e}\Delta},\mathbf{F}_{\mathrm{p}\Delta},\mathbf{F}^+_\Delta,\mathbf{F}^-_\Delta,\boldsymbol{\chi}_\Delta)\,\mathrm{d}v-\int_{\bar{v}}\mathscr{D}(\dot{\mathbf{F}}_{\mathrm{p}\Delta},\mathbf{F}_{\mathrm{p}\Delta})\,\mathrm{d}\bar{v}$$

$$-\int_{\Sigma_\Delta}X^{\mathrm{T}}_\Sigma(\mathbf{F}^+_\Delta,\mathbf{F}^-_\Delta,\mathbf{F}(s),\boldsymbol{\chi}_\Delta,u_{\mathrm{n}\Delta})v_{\mathrm{n}\Delta}\,\mathrm{d}\Sigma_\Delta$$

$$=0>\int_S \mathbf{p}_\Delta\cdot\mathbf{v}^*_\Delta\,\mathrm{d}S-\frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\psi^*(\mathbf{F}_{\mathrm{e}\Delta},\mathbf{F}_{\mathrm{p}\Delta},\mathbf{F}^+_\Delta,\mathbf{F}^-_\Delta,\boldsymbol{\chi}_\Delta)\,\mathrm{d}v$$

$$-\int_{\bar{v}}\mathscr{D}(\dot{\mathbf{F}}^*_{\mathrm{p}\Delta},\mathbf{F}_{\mathrm{p}\Delta})\,\mathrm{d}\bar{v}-\int_{\Sigma_\Delta}X^{\mathrm{T}}_\Sigma(\mathbf{F}^{+*}_\Delta,\mathbf{F}^{-*}_\Delta,\mathbf{F}^*(s),\boldsymbol{\chi}^*_\Delta,u_{n\Delta})v^*_{\mathrm{n}\Delta}\,\mathrm{d}\Sigma_\Delta; \quad (4.14)$$

$$\int_S \mathbf{p}_\Delta\cdot\mathbf{v}_\Delta\,\mathrm{d}S-\int_{\bar{v}}(\rho\dot{\psi}(\mathbf{F}_{\mathrm{e}\Delta},\mathbf{F}_{\mathrm{p}\Delta})+\mathscr{D}(\dot{\mathbf{F}}_{\mathrm{p}\Delta},\mathbf{F}_{\mathrm{p}\Delta}))\,\mathrm{d}\bar{v}$$

$$-\int_{\Sigma_\Delta}\int_{\mathbf{F}^-_\Delta}^{\mathbf{F}^+_\Delta}(\mathbf{P}'(\mathbf{F}(s),\boldsymbol{\chi}):\mathrm{d}\mathbf{F}+k(u_{\mathrm{n}\Delta}))v_{\mathrm{n}\Delta}\,\mathrm{d}\Sigma_\Delta$$

$$=0>\int_S \mathbf{p}_\Delta\cdot\mathbf{v}^*_\Delta\,\mathrm{d}S-\int_{\bar{v}}(\rho\dot{\psi}^*(\mathbf{F}_{\mathrm{e}\Delta},\mathbf{F}_{\mathrm{p}\Delta})+\mathscr{D}(\dot{\mathbf{F}}^*_{\mathrm{p}},\mathbf{F}_{\mathrm{p}}))\,\mathrm{d}\bar{v}$$

$$-\int_{\Sigma_\Delta}\int_{\mathbf{F}^{-*}_\Delta}^{\mathbf{F}^{+*}_\Delta}(\mathbf{P}'(\mathbf{F}^*(s),\boldsymbol{\chi}^*):\mathrm{d}\mathbf{F}+k(u_{\mathrm{n}\Delta}))v^*_{\mathrm{n}\Delta}\,\mathrm{d}\Sigma_\Delta. \quad (4.15)$$

If we have at time t several possible solutions, then using the postulate of realizability we could choose the unique one. For this solution principles (4.14) and (4.15) are valid, but for other arbitrary solutions which we will label with 0 we have

$$\exists\mathbf{v}^*\text{ for which }\int_{S_{\mathrm{v}}}\mathbf{p}^0_\Delta\cdot\mathbf{v}\,\mathrm{d}S+\int_{S_{\mathrm{p}}}\mathbf{p}_\Delta\cdot\mathbf{v}^*_\Delta\,\mathrm{d}S-\frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\psi^*(\mathbf{F}^0_{\mathrm{e}\Delta},\mathbf{F}^0_{\mathrm{p}\Delta})\,\mathrm{d}v$$

$$-\int_{\bar{v}}\mathscr{D}(\dot{\mathbf{F}}^*_{\mathrm{p}\Delta},\mathbf{F}^0_{\mathrm{p}\Delta})\,\mathrm{d}\bar{v}-\int_{\Sigma_\Delta}X^{\mathrm{T}}_\Sigma(\mathbf{F}^{+*}_\Delta,\mathbf{F}^{-*}_\Delta,\mathbf{F}^*(s),\boldsymbol{\chi}^*_\Delta,u^0_{\mathrm{n}\Delta})v^*_{\mathrm{n}\Delta}\,\mathrm{d}\Sigma^0_\Delta>0; \quad (4.16)$$

$$\exists\mathbf{v}^*\text{ for which }\int_{S_{\mathrm{v}}}\mathbf{p}^0_\Delta\cdot\mathbf{v}\,\mathrm{d}S+\int_{S_{\mathrm{p}}}\mathbf{p}_\Delta\cdot\mathbf{v}^*_\Delta\,\mathrm{d}S-\int_{\bar{v}}(\rho\dot{\psi}^*(\mathbf{F}^0_{\mathrm{e}\Delta},\mathbf{F}^0_{\mathrm{p}\Delta})+\mathscr{D}(\dot{\mathbf{F}}^*_{\mathrm{p}\Delta},\mathbf{F}^0_{\mathrm{p}\Delta}))\,\mathrm{d}\bar{v}$$

$$-\int_{\Sigma^0_\Delta}\int_{\mathbf{F}^{-*}_\Delta}^{\mathbf{F}^{+*}_\Delta}(\mathbf{P}'(\mathbf{F}^*(s),\boldsymbol{\chi}^*_\Delta):\mathrm{d}\mathbf{F}+k(u^0_{n\Delta})v^*_{\mathrm{n}})\,\mathrm{d}\Sigma^0_\Delta>0. \quad (4.17)$$

If we use $\mathbf{v}^*_\Delta = \mathbf{v}^0_\Delta$ in principles (4.14) and (4.15), and $\mathbf{v}^*_\Delta = \mathbf{v}_\Delta$ in inequalities (4.16) and (4.17), than we get the generalization of principles (98) form Part I [8] for media with PT:

$$\int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS + \int_{S_v} \mathbf{p}^0_\Delta \cdot \mathbf{v}_\Delta \, dS - \frac{d}{dt}\int_v \rho\psi(\mathbf{F}^0_{e\Delta}, \mathbf{F}^0_{p\Delta}, \mathbf{F}^+_\Delta, \mathrm{F}^-_\Delta, \boldsymbol{\chi}_\Delta)\, dv$$
$$- \int_{\bar v} \mathscr{D}(\dot{\mathbf{F}}_{p\Delta}, \mathbf{F}^0_{p\Delta})\, d\bar v - \int_{\Sigma^0_\Delta} X^{\mathrm{T}}_\Sigma(\mathbf{F}^+_\Delta, \mathbf{F}^-_\Delta, \mathbf{F}(s), \boldsymbol{\chi}_\Delta, u^0_{n\Delta}) v_{n\Delta}\, d\Sigma^0_\Delta > 0$$
$$= \int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS + \int_{S_v} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS - \frac{d}{dt}\int_v \rho\psi(\mathbf{F}_{e\Delta}, \mathbf{F}_{p\Delta}, \mathbf{F}^+_\Delta, \mathbf{F}^-_\Delta, \boldsymbol{\chi}_\Delta)\, dv$$
$$- \int_{\bar v} \mathscr{D}(\dot{\mathbf{F}}_{p\Delta}, \mathbf{F}_{p\Delta})\, d\bar v - \int_{\Sigma_\Delta} X^{\mathrm{T}}_\Sigma(\mathbf{F}^+_\Delta, \mathbf{F}^-_\Delta, \mathbf{F}(s), \boldsymbol{\chi}_\Delta, u_{n\Delta}) v_{n\Delta}\, d\Sigma_\Delta$$
$$= \int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}^0_\Delta \, dS + \int_{S_v} \mathbf{p}^0_\Delta \cdot \mathbf{v}_\Delta \, dS - \frac{d}{dt}\int_v \rho\psi^0(\mathbf{F}^0_{e\Delta}, \mathbf{F}^0_{p\Delta}, \mathbf{F}^{+0}_\Delta, \mathbf{F}^{-0}_\Delta, \boldsymbol{\chi}^0_\Delta)\, dv$$
$$- \int_{\bar v} \mathscr{D}(\dot{\mathbf{F}}^0_{p\Delta}, \mathbf{F}^0_{p\Delta})\, d\bar v - \int_{\Sigma^0_\Delta} X^{\mathrm{T}}_\Sigma(\mathbf{F}^{+0}_\Delta, \mathbf{F}^{-0}_\Delta, \mathbf{F}^0(s), \boldsymbol{\chi}^0_\Delta, u^0_{n\Delta}) v^0_{n\Delta}\, d\Sigma^0_\Delta$$
$$> \int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}^0_\Delta \, dS + \int_{S_v} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS - \frac{d}{dt}\int_v \rho\psi^0(\mathbf{F}_{e\Delta}, \mathbf{F}_{p\Delta}, \mathbf{F}^{+0}_\Delta, \mathbf{F}^{-0}_\Delta, \boldsymbol{\chi}^0_\Delta)\, dv$$
$$- \int_{\bar v} \mathscr{D}(\dot{\mathbf{F}}^0_{p\Delta}, \mathbf{F}_{p\Delta})\, d\bar v - \int_{\Sigma_\Delta} X^{\mathrm{T}}_\Sigma(\mathbf{F}^{+0}_\Delta, \mathbf{F}^{-0}_\Delta, \mathbf{F}^0(s), \boldsymbol{\chi}^0_\Delta, u_{n\Delta}) v^0_{n\Delta}\, d\Sigma_\Delta \tag{4.18}$$

or

$$\int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS + \int_{S_v} \mathbf{p}^0_\Delta \cdot \mathbf{v}_\Delta \, dS - \int_{\bar v} (\rho\dot\psi(\mathbf{F}^0_{e\Delta}, \mathbf{F}^0_{p\Delta}) + \mathscr{D}(\dot{\mathbf{F}}_{p\Delta}, \mathbf{F}^0_{p\Delta}))\, d\bar v$$
$$- \int_{\Sigma^0_\Delta} \int_{\mathbf{F}^-_\Delta}^{\mathbf{F}^+_\Delta} (\mathbf{P}'(\mathbf{F}(s), \boldsymbol{\chi}_\Delta) : d\mathbf{F} + k(u^0_{n\Delta})) v_{n\Delta}\, d\Sigma^0_\Delta > 0$$
$$= \int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS + \int_{S_v} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS - \int_{\bar v} (\rho\dot\psi(\mathbf{F}_{e\Delta}, \mathbf{F}_{p\Delta}) + \mathscr{D}(\dot{\mathbf{F}}_{p\Delta}, \mathbf{F}_{p\Delta}))\, d\bar{\mathrm{v}}$$
$$- \int_{\Sigma_\Delta} \int_{\mathbf{F}^-_\Delta}^{\mathbf{F}^+_\Delta} (\mathbf{P}'(\mathbf{F}(s), \boldsymbol{\chi}_\Delta) : d\mathbf{F} + k(u_{n\Delta})) v_{n\Delta}\, d\Sigma_\Delta$$
$$= \int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}^0_\Delta \, dS + \int_{S_v} \mathbf{p}^0_\Delta \cdot \mathbf{v}_\Delta \, dS - \int_{\bar v} (\rho\dot\psi^0(\mathbf{F}^0_{e\Delta}, \mathbf{F}^0_{p\Delta}) + \mathscr{D}(\dot{\mathbf{F}}^0_{p\Delta}, \mathbf{F}^0_{p\Delta}))\, d\bar v$$
$$- \int_{\Sigma^0_\Delta} \int_{\mathbf{F}^{-0}_\Delta}^{\mathbf{F}^{+0}_\Delta} (\mathbf{P}'(\mathbf{F}^0)(s), \boldsymbol{\chi}^0_\Delta) : d\mathbf{F} + k(u^0_{n\Delta})) v^0_{n\Delta}\, d\Sigma^0_\Delta$$
$$> \int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}^0_\Delta \, dS + \int_{S_v} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS - \int_{\bar v} (\rho\dot\psi^0(\mathbf{F}_{e\Delta}, \mathbf{F}_{p\Delta}) + \mathscr{D}(\dot{\mathbf{F}}^0_{p\Delta}, \mathbf{F}_{p\Delta}))\, d\bar v$$
$$- \int_{\Sigma_\Delta} \int_{\mathbf{F}^{-0}_\Delta}^{\mathbf{F}^{+0}_\Delta} (\mathbf{P}'(\mathbf{F}^0(s), \boldsymbol{\chi}^0_\Delta) : d\mathbf{F} + k(u_{n\Delta})) v^0_{n\Delta}\, d\Sigma_\Delta. \tag{4.19}$$

The method of application of principles (4.18) and (4.19) is similar to the case of the absence of PT. If for volume $\bar v$ we use the principles of Section 4.3 instead of the ones of Section 4.2 at

Part I [8] (i.e. we admit jumps of $\mathbf{F}_{e\Delta}$ and $\mathbf{P}_\Delta$ from the unstable solution to the stable one), then we obtain instead of principles (4.19)

$$\int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS + \int_{S_v} \mathbf{p}^0_\Delta \cdot \mathbf{v}_\Delta \, dS - \int_{\bar{v}} \mathbf{P}'_\Delta(\dot{\mathbf{F}}_{p\Delta}, \mathbf{F}^0_{p\Delta}) : \dot{\mathbf{F}}_\Delta \, dv$$

$$- \int_{\Sigma^0_\Delta} \int_{\mathbf{F}^-_\Delta}^{\mathbf{F}^+_\Delta} (\mathbf{P}'(\mathbf{F}(s), \boldsymbol{\chi}_\Delta) : d\mathbf{F} + k(u^0_{n\Delta}))v_{n\Delta} \, d\Sigma^0_\Delta > 0$$

$$= \int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS + \int_{S_v} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS - \int_{\bar{v}} \mathbf{P}'_\Delta(\dot{\mathbf{F}}_{p\Delta}, \mathbf{F}_{p\Delta}) : \dot{\mathbf{F}}_\Delta \, d\bar{v}$$

$$- \int_{\Sigma_\Delta} \int_{\mathbf{F}^-_\Delta}^{\mathbf{F}^+_\Delta} (\mathbf{P}'_\Delta(\mathbf{F}(s), \chi_\Delta) : d\mathbf{F} + k(u_{n\Delta}))v_{n\Delta} \, d\Sigma_\Delta$$

$$= \int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}^0_\Delta \, dS + \int_{S_v} \mathbf{p}^0_\Delta \cdot \mathbf{v}_\Delta \, dS - \int_{\bar{v}} \mathbf{P}^{0\prime}_\Delta(\dot{\mathbf{F}}^0_{p\Delta}, \mathbf{F}^0_{p\Delta}) : \dot{\mathbf{F}}_\Delta \, d\bar{v}$$

$$- \int_{\Sigma^0} \int_{\mathbf{F}^{-0}_\Delta}^{\mathbf{F}^{+0}_\Delta} (\mathbf{P}'(\mathbf{F}^0(s), \boldsymbol{\chi}^0_\Delta) : d\mathbf{F} + k(u^0_{n\Delta}))v^0_{n\Delta} \, d\Sigma^0_\Delta$$

$$> \int_{S_p} \mathbf{p}_\Delta \cdot \mathbf{v}^0_\Delta \, dS + \int_{S_v} \mathbf{p}_\Delta \cdot \mathbf{v}_\Delta \, dS - \int_{\bar{v}} \mathbf{P}^{0t}_\Delta (\dot{\mathbf{F}}^0_{p\Delta}, \mathbf{F}_{p\Delta}) : \dot{\mathbf{F}}^0_\Delta \, d\bar{v}$$

$$- \int_{\Sigma} \int_{\mathbf{F}^{-0}_\Delta}^{\mathbf{F}^{+0}_\Delta} (\mathbf{P}'(\mathbf{F}^0(s), \boldsymbol{\chi}^0_\Delta) : d\mathbf{F} + k(u_{n\Delta}))v^0_{n\Delta} \, d\Sigma_\Delta. \quad (4.20)$$

It is easy to receive equations (4.26)–(4.29), (4.32) and (4.33) of Part I [8], if in definitions of stress vectors $\bar{\mathbf{p}}^0_\Delta$, $\bar{\mathbf{p}}_\Delta$, $\tilde{\mathbf{p}}^0_\Delta$ and $\tilde{\mathbf{p}}_\Delta$ we include power, related with the interface motions, from the corresponding lines of equation (4.20).

If the local criteria of the PT (3.14) and (3.16) are met at some points on the Σ-surface, it does not mean that the PT in fact will occur, because we have to satisfy the global criteria. At least two different solutions at time t are possible: with PT ($v_n \neq 0$) and without it ($v_n = 0$) and using the principle (4.20) we can choose one "more profitable" variant. If we obtain $v_n \neq 0$, it means that not only local criteria, but also the global one for PT are met. In this case, PT will really occur.

Let us designate the solution of the boundary value problem with PT by the superscript "ph" and without PT by the superscript "w". If the PT occurs, then

$$\int_S \mathbf{p}^{ph}_\Delta \cdot \mathbf{v}^w_\Delta \, dS - \int_v \mathbf{P}^{w\prime}_\Delta(\dot{\mathbf{F}}^w_{p\Delta}, \mathbf{F}^{ph}_{p\Delta}) : \dot{\mathbf{F}}^w_\Delta \, dv < 0 \quad (4.21)$$

and

$$\int_S \mathbf{p}^w_\Delta \cdot \mathbf{v}^{ph}_\Delta \, dS - \int_{\bar{v}} \mathbf{P}^{pht}_\Delta(\dot{\mathbf{F}}^{ph}_{p\Delta}, \mathbf{F}^w_{p\Delta}) : \dot{\mathbf{F}}^{ph}_\Delta \, d\bar{v} - \int_{\Sigma_\Delta} \int_{\mathbf{F}^-_\Delta}^{\mathbf{F}^+_\Delta} (\mathbf{P}'(\mathbf{F}(s), \boldsymbol{\chi}) : d\mathbf{F} + k(u_{n\Delta}))v_{n\Delta} \, d\Sigma_\Delta > 0. \quad (4.22)$$

Principle (4.21) is a particular case of the last line in the principle (4.20) when we assume that at time t the solution with PT is realized and check a possible solution without PT. Note that the Σ-surface in principle (4.21) corresponds to time $t + \Delta t$ (i.e. it is shifted due to transition), but it is fixed in the given case and there is not a jump of $\mathbf{v}^w$ across it. Principle (4.22) represents particular cases of the first line in the principle (4.20) when we assume that at time t the solution without PT is realized and check the solution with PT. The position of the Σ-surface in this case is determined at time t (it is fixed in the given solution). The parameters $\mathbf{F}^+_\Delta$, $\mathbf{F}^-_\Delta$, $\mathbf{F}(s)$, $\boldsymbol{\chi}_\Delta$ and $u_{n\Delta}$ are determined from principle (4.6) and equation (3.15). If the PT does not occur, then

$$\int_S \mathbf{p}^w_\Delta \cdot \mathbf{v}^{ph}_\Delta \, dS - \int_{\bar{v}} \mathbf{P}^{pht}_\Delta(\dot{\mathbf{F}}^{ph}_{p\Delta}, \mathbf{F}^w_{p\Delta}) : \dot{\mathbf{F}}^{ph}_\Delta \, d\bar{v} - \int_{\Sigma_\Delta} \int_{\mathbf{F}^-_\Delta}^{\mathbf{F}^+_\Delta} (\mathbf{P}'(\mathbf{F}(s), \boldsymbol{\chi}) : d\mathbf{F} + k(u_{n\Delta}))v_{n\Delta} \, d\Sigma_\Delta < 0 \quad (4.23)$$

and

$$\int_S \mathbf{p}_\Delta^{ph} \cdot \mathbf{v}_\Delta^w \, dS - \int_v \mathbf{P}_\Delta^{wt}(\dot{\mathbf{F}}_{p\Delta}^w, \mathbf{F}_{p\Delta}^{ph}) : \dot{\mathbf{F}}_\Delta^w \, dv > 0. \tag{4.24}$$

4.3 Alternative variant of the description of the phase transitions

In most cases, for inelastic materials especially, the total diagram (Fig. 4) is unknown even for the one-dimensional case. Usually, the elasticity and plasticity laws and the Helmholtz free energy for both phases are known, but with respect to the natural (stress and strain free) state of each phase, which are distinguished. The deformation gradient $\mathbf{F}_T$, which transforms the natural state of the parent phase into the natural state of the second phase, describes both volumetric and shearing components. The volumetric strain in determined uniquely by the ratio of the mass densities of these phases, but the shear strain depends on the applied stress tensor and its history. Consider a simple example for the PT in the monocrystal. Assume that only two variants of $\mathbf{F}_T$ are possible $\mathbf{F}_T^1 = \mathbf{I} + \gamma_T^1 \mathbf{mn}$; $\mathbf{F}_T^2 = \mathbf{I} + \gamma_T^2 \mathbf{mn}$; $\gamma_T^1 = -\gamma_T^2$, which corresponds to the simple shear in two opposite directions (Fig. 7). But during PT, both of these strains can be realized in different subvolumes of the macroscopic volume under consideration and $\mathbf{F}_T = c_1\mathbf{F}_T^1 + c_2\mathbf{F}_T^2$, $c_1 + c_2 = 1$, where c_i is the volume fraction of the ith variant of PT. In the general case there are much more than two crystallographically equivalent variants of PT for monocrystals. For polycrystals we have an additional degrees of freedom. Consider two types of description. In the first one, we assume that it is possible to represent

$$\mathbf{F}_T = \sum c_i \mathbf{F}_T^i, \qquad \sum c_i = 1 \quad \text{or} \quad \mathbf{F}_T = \mathbf{F}_T(c_i, \chi_i), \tag{4.25}$$

where $\chi_i \in \chi$ characterize the orientations. In the second possibility, we have an infinite number of variants. In this case we assume that all possible $\mathbf{F}_T$ tensors belong to some region $\bar{\varphi}(\mathbf{F}_T) \leq 0$. For $\mathbf{F}^+$ we can establish the formula [4] $\mathbf{F}^+ = \mathbf{F}_e^+ \cdot \mathbf{F}_p^+ \cdot \mathbf{F}_T \cdot \mathbf{F}_p^-$, where $\mathbf{F}_p^+$ and $\mathbf{F}_p^-$ are the plastic deformation gradients in the (+) and (−)-phase respectively. The expressions for X_Σ (3.13) and X_Σ^T (3.11) are valid in the given case as well. But due to the fact that we know the plastic properties at $\mathbf{F}_T = \mathbf{I}$ ((−)-phase) and at the final value of $\mathbf{F}_T$ ((+)-phase), we can take the integral in the equation (3.11) at $\mathbf{F}_p^- = \text{const}$ and use the flow rule of the (+)-phase or of the mixture of both phases [4].

All the remaining principles and equations of this Chapter are valid with one peculiarity: it is necessary to use constraints (4.25) of $\bar{\varphi} \leq 0$. The usage of a constraint $\bar{\varphi} \leq 0$ is more convenient in two stages:

(1) To use the extremum principles without accounting for constraint $\bar{\varphi} \leq 0$, and then check if the result satisfies it or not;
(2) If not, we have to use the constraint $\bar{\varphi}(\mathbf{F}_T) = 0$.

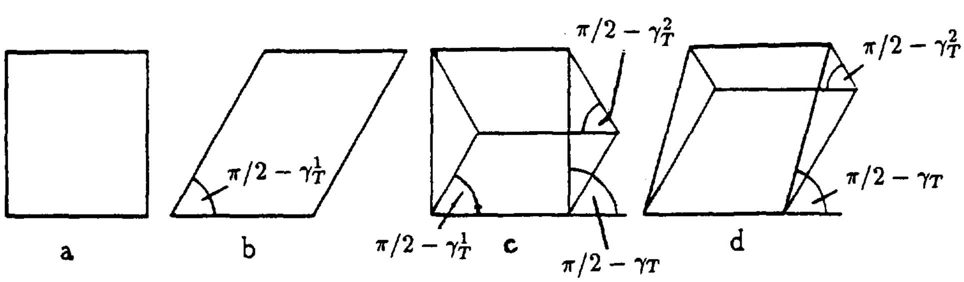


Fig. 7. Deformation gradient of the transformation shear strain γ_t for two possible variants of phase transition: (a) initial state; (b) $c_1 = 1$; (c) $c_1 = c_2 = 0.5$; (d) $c_1 > c_2$.

4.4 Comparison with some extremum principles

For discrete systems, Bažant [9] suggested criteria for the choice of the stable post-bifurcation path based on second-order work. He gave a thermodynamical substantiation of these criteria, but it is very difficult to understand it. The hypothesis adopted (see Appendix 5 in [9]), that the actual inelastic structure (irreversible) can be replaced by the tangentially equivalent elastic (reversible) structure, excludes the thermodynamic consideration, because these two systems are thermodynamically nonequivalent. That is the reason why the final formulas [(7)–(11), (13)]

$$-\theta\,\Delta S_{\text{in}} = \delta^2 W, \tag{4.26}$$

where ΔS_{in} is the internally produced entropy increment (i.e. the rate of dissipation is $\mathscr{D} = \theta(\Delta S_{\text{in}}/\Delta t)$), $\delta^2 W$ is the second-order work, are incorrect. Indeed, $\theta\,\Delta S_{\text{in}}$ could not be less than zero (according to the second law of thermodynamics), but $\Delta^2 W$ is positive for hardening materials (we recall that instability is possible at $\delta^2 W > 0$, see Fig. 4). To explore equation (4.26), Bažant uses the second law of the thermodynamics in the following form: "the structure will approach the equilibrium state, which maximizes ΔS_{in}", consequently $\Delta S_{\text{in}} \to \max$, $\delta^2 W \to \min$. But from the second law of thermodynamics it follows only that $\Delta S_{\text{in}} > 0$ for irreversible processes and $\Delta S_{\text{in}} = 0$ for reversible (equilibrium) ones. Bažant notes that "the present use of S_{in} does not represent an application of the principle of maximum entropy production". Nevertheless, if we do not consider the thermodynamic background, Bažant's criterion can be classified as a new postulate, which gives reasonable results for a number of examples considered in his paper. As was shown in [8], our extremum principle for continuous media (equation (4.23) in [8] and equation (4.20)) after some simplifying assumptions could be transformed (at least in the case considered in [8]) to the principle $\delta^2 W \to \min$.

Petryk [10] suggested the energy criteria for the definition of instability for materials with a potential dependence between the stress and the strain rates. He has also shown that a solution which is unstable in the energetic sense is also physically unstable, i.e. finite deviations from the fundamental velocity field can be caused by vanishing small perturbations. Based on these criteria, Petryk and Thermann [11] suggested a new numerical algorithm for the stable post-bifurcational branch switching of spatially discretized systems with a symmetric tangent stiffness matrix.

The approach suggested in the present paper has some features:

(1) We introduced the postulate of realizability and showed that it is a quite powerful and flexible assumption which can be considered as an essential property of dissipative systems (see below).

(2) Using the postulate of realizability, we derived the governing extremum principle for the description of stable post-bifurcation behaviour. The concept of stability, which follows from the postulate of realizability, means the following: if, under a given increment of prescribed forces and displacements, the stable solution for the velocity field is realized in the time interval $[t, t + \Delta t]$, then at time $t + \Delta t$ the power of the external forces is less than the power of the internal stresses (or the power of the external and nondissipative forces is less than the power of the dissipative forces) for all other possible solutions (velocity fields), i.e. other solutions are energetically impossible. If the unstable solution is realized in the time interval $[t, t + \Delta t]$, then at time $t + \Delta t$ for the stable solution the power of the external forces exceeds the power of the internal stresses, i.e. due to some perturbations the jump from the unstable solution to the stable one is possible with a positive increment of kinetic energy. This concept of stability seems to us physically reasonable.

(3) The governing principles derived in the paper are applicable to systems with non-associated and associated flow rules and with the nonpotential dependence between the stress

and the strain rates. They can also be applied, when a unique solution cannot be found for infinitesimal Δt.

(4) For inelastic materials with PT, we do not know the existing extremum principles and we are not even aware of any literature which considers PT from the viewpoint of choosing the stable post-bifurcation process. That is why the existence of the difference between local and global PT criteria, the expressions for the local criteria and the extremum principle describing the global criteria, as well as the relations for all the parameters ($\mathbf{F}^+, \mathbf{F}^-, \boldsymbol{\chi}, \mathbf{F}(s), v_n, [\mathbf{v}_2]$) seem new to us.

5. EXAMPLE

Phase transition at simple shearing. We now apply the results obtained in the previous sections to the simple shear problem. Let an elastoplastic material have the diagram $\tau = f(\gamma)$ shown in Fig. 8. Moreover we assume that there exists an expression $\psi(\gamma)$ for the free energy. The local criteria of PT (3.14)–(3.16) in this special case read

$$\tau(\gamma^+ - \gamma^-) = \int_{\gamma^-}^{\gamma^+} f(\gamma)\,\mathrm{d}\gamma + k(c), \qquad \tau_\Delta(\gamma_\Delta^+ - \gamma_\Delta^-) = \int_{\gamma_\Delta^-}^{\gamma_\Delta^+} f(\gamma)\,\mathrm{d}\gamma + k(c_\Delta), \tag{5.1}$$

$$\dot{\tau}(\gamma^+ - \gamma^-) = k'\dot{c}, \qquad k' := \frac{k}{\partial c} \tag{5.2}$$

(the term $\nabla\tau$ is equal to zero due to the homogeneity of τ). Assuming $k' > 0$, for $\dot{c} > 0$ we obtain from equation (5.2) $\dot{\tau}(\gamma^+ - \gamma^-) > 0$, i.e. the stress has to be increased. For prescribed γ we will obtain curve 3 in Fig. 4. Using equation (5.2) and $\dot{\gamma} = (1-c)\dot{\gamma}^- + c\dot{\gamma}^+ + \dot{c}(\gamma^+ - \gamma^-)$, the following designations for compliances $\lambda^+ := (\partial f/\partial\gamma^+)^{-1}$, $\lambda^- := (\partial f/\partial\gamma^-)^{-1}$ we can get the differential equation for this curve

$$\begin{aligned}\dot{\gamma} &= \left[c\lambda^+ + (1-c)\lambda^- + \frac{1}{k'}(\gamma^+ - \gamma^-)^2\right]\dot{\tau} = \lambda_t\dot{\tau}\\ &= \left[(c\lambda^+ + (1-c)\lambda^-)\frac{k'}{\gamma^+ - \gamma^-} + \gamma^+ - \gamma^-\right]\dot{c},\end{aligned} \tag{5.3}$$

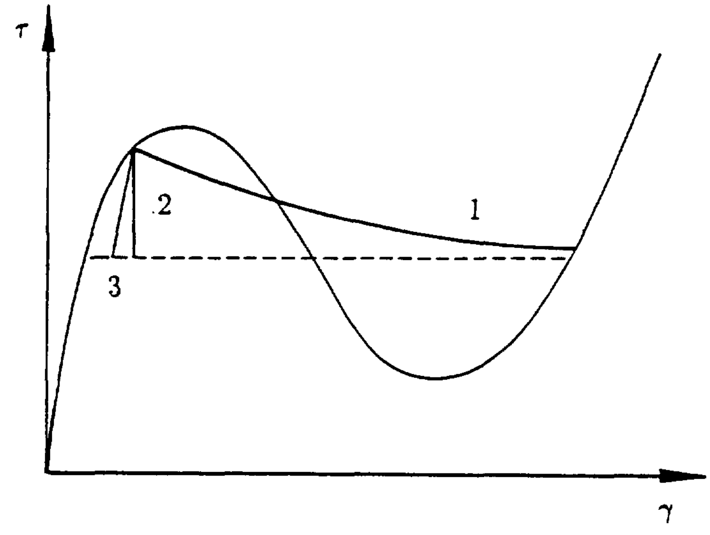


Fig. 8. Diagram of simple shearing with phase transition at $k > 0$ and different k': (a) $\lambda k' + (\gamma^+ + \gamma^-)^2 > 0$; (b) $\lambda k' + (\gamma^+ + \gamma^-)^2 = 0$; (c) $\lambda k' + (\gamma^+ + \gamma^-)^2 < 0$.

where λ_t is the overall compliance for deformation with PT. For a deformation without PT $\lambda = c\lambda^+ + (1-c)\lambda^-$. The tangential shear modulus is

$$G_t = \left(\lambda + \frac{(\gamma^+ - \gamma^-)^2}{k'}\right)^{-1} = \frac{k'}{\lambda k' + (\gamma^+ - \gamma^-)^2}.$$

At $k' = \infty$ (it corresponds to a fixed interface) $G_t = 1/\lambda = G$. At finite k' (positive or negative) and $\lambda k' + (\gamma^+ - \gamma^-)^2 > 0$ we have $G_t < G$, i.e. PT makes the tangential modulus softer. At $\lambda k' + (\gamma^+ - \gamma^-)^2 < 0$ ($k' < 0$) we obtain $G_t > G$, but this inequality does not mean an increasing tangential stiffness due to PT. An equilbrium PT is possible only at decreasing γ (Fig. 8). At a high value of $k(c)$ and $k' > 0$, when the equilibrium stress in equation (5.1) reaches its maximum value $\tau = \tau_c$ in the (−)-phase, condition (5.2) is violated (because $\dot{\tau} \leq 0$, but $k' > 0$) and the interface becomes fixed. In this case, the homogeneous strain takes place in both phases at decreasing τ (Figs 9, 10). For elastic materials, the (−)-phase deforms according to line CD, the (+)-phase according to line ED and at point D both phases have the same strain. At increasing γ the homogeneous strain in the whole volume will correspond to line DE.

For rigid-plastic materials in this situation, the strain in the (+)-phase is fixed at decreasing stress (line EL) and equal to the strain at point E. The (−)-phase deforms in accordance with line CDE and homogeneous strain in the whole volume will occur at $\gamma > \gamma_E$.

For elastoplastic materials, the (+)-phase at decreasing and then increasing τ will be deformed in accordance with the unloading curve EL. The strain in the whole volume will also be totally homogeneous at $\gamma > \gamma_E$.

Let the slab of material have a variable cross-section $S(y)$ and assume that $\tau(y) = P/S(y)$, where P denotes the shear force. The criterion (5.1) is met the first time in the section with $S = S_{\min}$. Criterion (3.16) reads

$$(\dot{\tau} + \tau'\dot{c})(\gamma^+ - \gamma^-) = k'\dot{c}, \tag{5.4}$$

where on the interface

$$\tau' = \frac{\partial \tau}{\partial y} = P\frac{\partial}{\partial y}\left(\frac{1}{S(y)}\right) < 0,$$

because according to equation (5.1), the interface will move in the direction of increasing $S(y)$ and decreasing $\tau(y)$. From equation (5.4) we have

$$\dot{\tau}(\gamma^+ - \gamma^-) = (k' - \tau'(\gamma^+ - \gamma^-))\dot{c}, \qquad \dot{\gamma} = \left(\lambda + \frac{(\gamma^+ - \gamma^-)^2}{k' - \tau'(\gamma^+ - \gamma^-)}\right)\dot{\tau} = \lambda_t\dot{\tau}. \tag{5.5}$$

Due to $\tau' < 0$ even at $k(c) = k'(c) = 0$, from equation $(5.5)_2$ it follows $\dot{\tau} > 0$ at $\dot{c} > 0$. The conclusion that the PT decreases the stiffness is retained.

After the consideration of the local PT criteria, let us check now if the global consideration will give the same result. We will apply principles (4.21)–(4.24).

Consider the time t and some $c(t)$. Assume that at prescribed v, straining with fixed interface takes place in time $[t, t + \Delta t]$. Consider its stability under an imposed velocity field at time $t + \Delta t$, corresponding to the moving interface.

The first, second and third integral in inequality (4.22) read

$$f(\gamma_\Delta^+)v_\Delta = f(\gamma_\Delta^-)v_\Delta = \tau_\Delta v_\Delta; \qquad \tau_{0\Delta}(c\dot{\gamma}_\Delta^+ + (1-c)\dot{\gamma}_\Delta^-)l; \qquad \left(\int_{\gamma_\Delta^-}^{\gamma_\Delta^+} f(\gamma)\,\mathrm{d}\gamma + k(c_\Delta)\right)l\dot{c}_\Delta. \tag{5.6}$$

In equation $(5.6)_2$ $\tau_{0\Delta}$ is the equilibrium stress $\tau_{e\Delta}$ at the PT which is determined from equation (5.1) (if we assume that PT occurs, then the local criteria have to be met). According to equation (5.1), expression $(5.6)_3$ is equal to $\tau_{0\Delta}(\gamma_\Delta^+ - \gamma_\Delta^-)l\dot{c}_\Delta$. Expression (4.22) is equal to

$$\tau_\Delta v_\Delta - \tau_{0\Delta}(c\dot{\gamma}_\Delta^+ + (1-c)\dot{\gamma}_\Delta^- + (\gamma_\Delta^+ - \gamma_\Delta^-)\dot{c}_\Delta)l = \tau_\Delta v_\Delta - \tau_{e\Delta}v_\Delta. \tag{5.7}$$

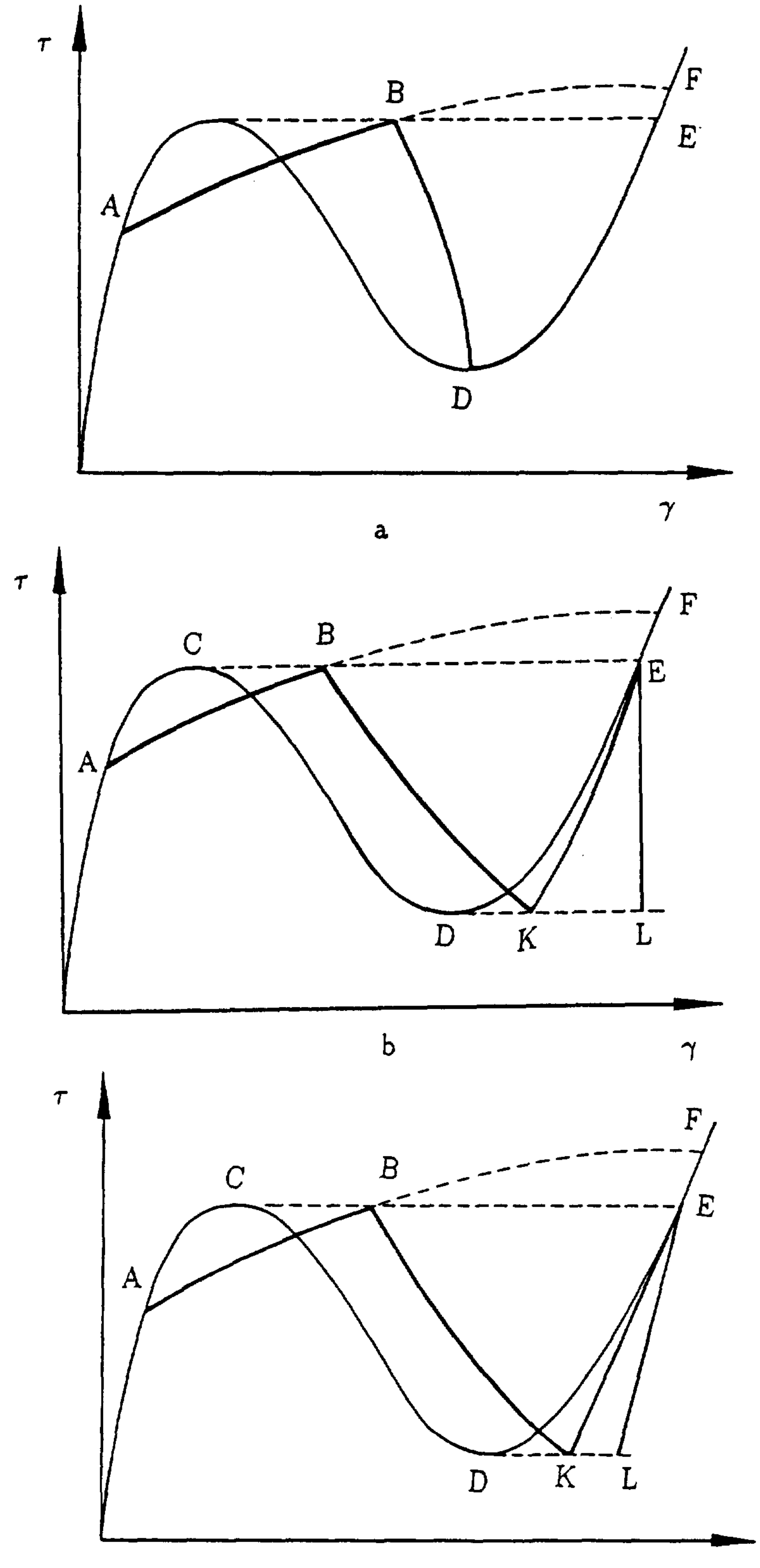


Fig. 9. Diagram of simple shearing with phase transition: (a) elastic material—*ABDEF*; (b) rigid-plastic material—*ABKEF*; (c) elastoplastic material—*ABKEF*; (d) at homogeneous straining—*ACDEF*.

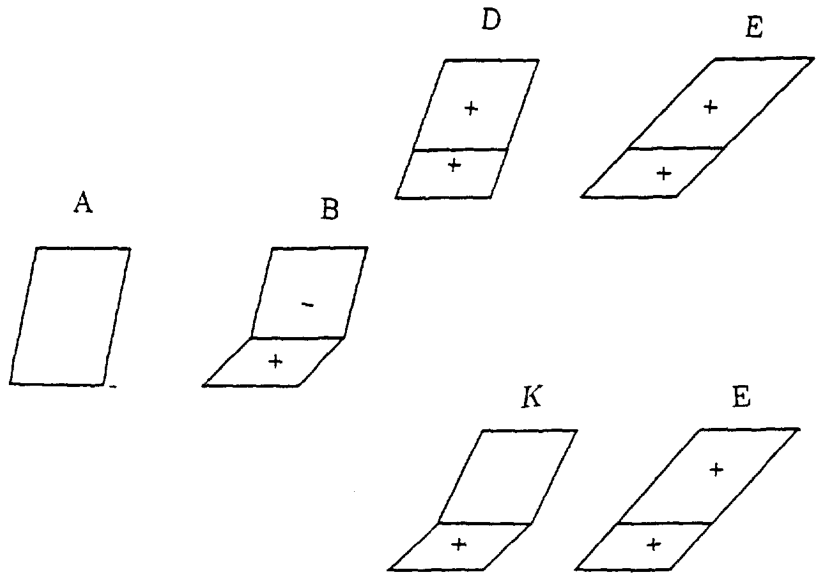


Fig. 10. Specimen geometry at different points of the τ–γ-diagram (Fig. 9) for elastic and rigid-plastic material.

If $\tau_\Delta > \tau_{0\Delta}$, i.e. the applied stress, or the stress obtained for prescribed v at a fixed interface exceeds the equilibrium value, then, according to equation (4.22), PT will occur, otherwise, according to equation (4.23), it will not occur.

To meet the criterion $\tau_\Delta > \tau_{0\Delta}$ for a prescribed velocity, it is enough to satisfy equation (5.1) at $c = 0$, because the overall tangential stiffness $G_t < G$. For prescribed increasing stress, it is also enough to satisfy equation (5.1) if $k' > 0$; if $k' < 0$, a quasi-statical stress-controlled experiment is impossible.

Consider now the situation when straining with a moving interface takes place in time $[t, t + \Delta t]$ and estimate its stability under a superposed velocity field at time $t + \Delta t$, corresponding to a fixed interface. Expression (4.21) reads now

$$\tau_{e\Delta} v_\Delta - \tau(\gamma_\Delta^w)\dot{\gamma}_\Delta l < 0 \quad \text{or} \quad \tau_{0\Delta} - \tau(\gamma_\Delta^w) < 0, \tag{5.8}$$

where $\tau(\gamma_\Delta^w)$ is the stress for straining with a fixed interface. Consequently, if at straining with a fixed interface the stress exceeds the equilibrium value $\tau_{0\Delta}$, then PT will occur, otherwise— according to equation (4.24)—will not. We obtain the same result from the local and global criteria and, in the given case, these criteria coincide.

Noncoincidence of the local and global criteria of PT. Consider the situation shown in Figs 11, 12.

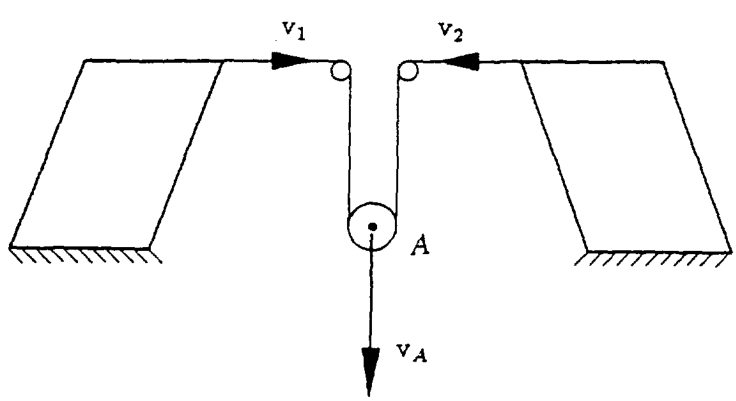
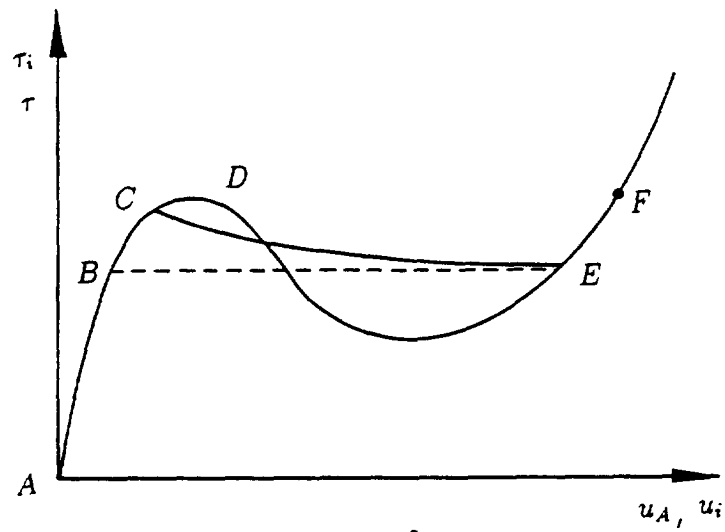
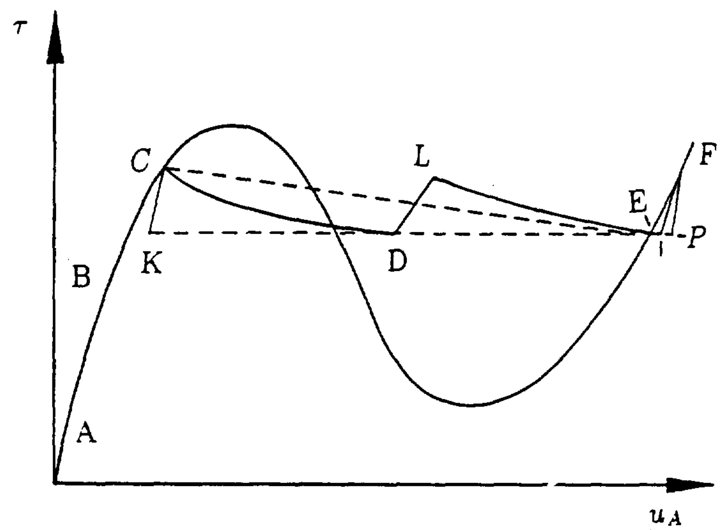


Fig. 11. Simple shearing of two specimens.



a



b

Fig. 12. (a) Diagram of simple shearing $\tau_i(u_i)$ of each slab at homogeneous strain ($ABCDLEF$) and at phase transition ($ABCEF$); diagram $\tau(u_A)$ under symmetrical straining with phase transition ($ABCEF$); (b) diagram $\tau(u_A)$ under nonsymmetrical straining ($ABCDLMF$).

Two equivalent slabs, made from material with the diagram $\tau(u)$, $u = \gamma l$, according to Fig. 11, are loaded under the following conditions: $\tau = \tau_1 = \tau_2$, $v_1 + v_2 = 2v_A$, where v_A is the prescribed velocity at point A, v_1 and v_2 are the velocities prescribed for slabs 1 and 2, respectively, and τ_i are the stresses at each of them. Let $k(0) > 0$, $k' < 0$ and the diagram of straining of each slab during PT corresponds to line CDE. Two variants are possible: the symmetrical situation, when all parameters in both slabs are the same and the nonsymmetrical situation, when PT occurs only in one of the slabs. Under a symmetrical straining ($v_1 = v_2 = v_A$), the diagram $\tau(u_A)$ will be the same as for each slab.

Let at $u_A = \gamma_c l$ stress $\tau = \tau_c$ in both slabs and the local PT criterion is met. But due to some perturbations, PT started at slab 1 only. Due to the stress decreasing, PT criterion in the slab 2 is violated and it will behave in accordance with the unloading diagram CK [Fig. 12(b)]. The displacement u_A at each τ can be drawn as the semisum of coordinates of the lines CK and CDE.

When PT is the first slab is finished, $\tau_1 = \tau_E$ and under increasing u_A stress τ_1 will increase along the line EF, τ_2—along line KC. At $\tau_2 = \tau_c$ PT will start in the second slab, τ_2 will vary along the line CDE, τ_1 along the unloading line FP. At $\tau_2 = \tau_E$ PT is finished in slab 2 and the stress will increase along line EF in slab 2 and along PF in slab 1.

Let us choose a variant—symmetrical or nonsymmetrical—which is stable. The analysis is trivial. Assume that in time $[t, t + \Delta t]$ the symmetrical variant is realized, and at time $t + \Delta t$ the nonsymmetrical velocity field, consistent with $v_{A\Delta}$, is realized. The power of the external stresses is $\tau_{s\Delta} v_{A\Delta}$, the power of the internal stresses is $\tau_{n\Delta} v_{A\Delta}$, where $\tau_{s\Delta}$ and $\tau_{n\Delta}$ are the shear stresses after the symmetrical process in time $[t, t + \Delta t]$ and corresponding to the nonsymmetrical process, respectively. As $(\tau_{s\Delta} - \tau_{n\Delta}) v_\Delta > 0$ [line CB is below the line CD, Fig. 12(b)], then the symmetrical process is unstable and the nonsymmetrical one will be realized. Note that this result will be valid for slabs with diagram $ABCDE$, independently of the mechanics, leading to the decreasing branch CDE (e.g. PT, strain softening). Consequently, despite the fact that the local PT criterion was met in slab 2 at point C, the global consideration results in a stable process without PT.

6. NONCOHERENT PHASE TRANSITION

For noncoherent PT, not only the velocity vector $\mathbf{v}$, but also the position vector $\mathbf{r}$ has jumps across the interface Σ. Assuming small jump $[\mathbf{r}]$ we could use equation (A6) from the Appendix

$$\mathscr{D}_\Sigma = -\mathbf{p} \cdot [\mathbf{v}] - \rho[\psi] v_n \geq 0. \tag{6.1}$$

It is convenient to decompose $[\mathbf{v}] = [\mathbf{v}_1] + [\mathbf{v}_2]$, where $[\mathbf{v}_1]$ is the jump of $\mathbf{v}$ when $[\mathbf{r}] = \mathbf{0}$, i.e. for coherent PT; $[\mathbf{v}_1]\mathbf{n} = -[\mathbf{F}] v_n$; $[\mathbf{v}_2] = [\mathbf{v}] - [\mathbf{v}_1]$ is the jump of $\mathbf{v}$, when the surface Σ is fixed ($v_n = 0$, $[\mathbf{v}_1] = \mathbf{0}$ and $[\mathbf{v}] = [\mathbf{v}_2]$), i.e. it represents the relative sliding along the interface (Fig. 13).

Consequently, $\mathbf{p} \cdot [\mathbf{v}] = -\mathbf{P}' : [\mathbf{F}] v_n + \mathbf{p} \cdot [\mathbf{v}_2] = -\mathbf{n} \cdot \mathbf{P}' \cdot [\mathbf{F}] \cdot \mathbf{n} + \mathbf{p} \cdot [\mathbf{v}_2]$. Then the rate of dissipation across the interface $\mathscr{D}_\Sigma = (\mathbf{P}' : [\mathbf{F}] - \rho[\psi]) v_n - \mathbf{p} \cdot [\mathbf{v}_2]$ is distinguished from the corresponding expression for coherent PT by the term $-\mathbf{p} \cdot [\mathbf{v}_2]$. We get the same distinction for the threshold value $\mathscr{D}_\Sigma^{\mathrm{T}}$

$$\mathscr{D}_\Sigma^{\mathrm{T}} = \left(\int_{\mathbf{F}^-}^{\mathbf{F}^+} \mathbf{P}'(\mathbf{F}(s), \chi) : \mathrm{d}\mathbf{F} - \rho[\psi] + k(u_n) \right) v_n - \mathbf{p}([\mathbf{v}_2], v_n, \ldots) \cdot [\mathbf{v}_2]. \tag{6.2}$$

For a PT, which actually occurs it follows from the energy balance $\mathscr{D}_\Sigma = \mathscr{D}_\Sigma^{\mathrm{T}}$. If we introduce the generalized dissipative force $\mathbf{X}_\Sigma \equiv \{\mathbf{P}' : [\mathbf{F}] - \rho[\psi]; -\mathbf{p}\}$ and the generalized rates $\dot{\boldsymbol{q}} \equiv \{v_n; [\mathbf{v}_2]\}$, $\mathbf{X}_\Sigma, \dot{\mathbf{q}} \in \mathscr{R}^4$, then $\mathscr{D}_\Sigma = \mathbf{X}_\Sigma \cdot \dot{\mathbf{q}} \geq 0$ and $\mathbf{X}_\Sigma = \mathbf{X}_\Sigma(\dot{\mathbf{q}}, \mathbf{F}^+, \mathbf{F}^-, \chi)$. For time-independent martensitic

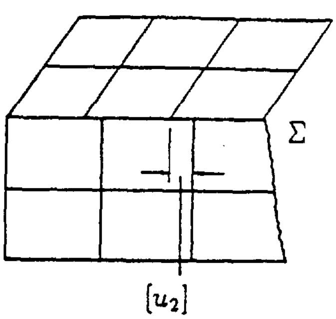


Fig. 13. Relative sliding $[u_2]$ along interface at noncoherent phase transition.

PT $\mathbf{X}_\Sigma$ is a homogeneous function of degree zero in $\dot{\mathbf{q}}$ [1, 4], and we can use the postulate of realizability. If

$$\mathbf{X}_\Sigma(\mathbf{F}^{+*}, \mathbf{F}^{-*}, \boldsymbol{\chi}^*) \cdot \dot{\mathbf{q}}^* - \mathscr{D}_\Sigma^{\mathrm{T}}(\dot{\mathbf{q}}^*, \mathbf{F}^{+*}, \mathbf{F}^{-*}, \boldsymbol{\chi}^*, \mathbf{F}^*(s)) < 0 \qquad \forall \dot{\mathbf{q}}^* \neq \mathbf{0}, \mathbf{F}^{+*}, \mathbf{F}^{-*}, \boldsymbol{\chi}^*, \mathbf{F}^*(s), \tag{6.3}$$

then $\dot{\mathbf{q}} = \mathbf{0}$ and PT will not occur, because if $\dot{\mathbf{q}} \neq \mathbf{0}$ then $\mathbf{X}_\Sigma \cdot \dot{\mathbf{q}} = \mathscr{D}_\Sigma^{\mathrm{T}}$. Using the postulate of realizability, we obtain the extremum principle:

$$\begin{aligned}\mathbf{X}_\Sigma(\mathbf{F}^{+*}, \mathbf{F}^{-*}, \boldsymbol{\chi}^*) \cdot \dot{\mathbf{q}}^* - \mathscr{D}_\Sigma^{\mathrm{T}}(\dot{\mathbf{q}}^*, \mathbf{F}^{+*}, \mathbf{F}^{-*}, \boldsymbol{\chi}^*, \mathbf{F}^*(s)) < 0 \\ = \mathbf{X}_\Sigma(\dot{\mathbf{q}}, \mathbf{F}^+, \mathbf{F}^-, \boldsymbol{\chi}) \cdot \dot{\mathbf{q}} - \mathscr{D}_\Sigma^{\mathrm{T}}(\dot{\mathbf{q}}, \mathbf{F}^+, \mathbf{F}^-, \boldsymbol{\chi}, \mathbf{F}(s)),\end{aligned} \tag{6.4}$$

whence

$$\begin{aligned}&(\mathbf{P}' : (\mathbf{F}^{+*} - \mathbf{F}^{-*}) - \rho(\psi(\mathbf{F}_\mathrm{e}^{+*}, \mathbf{F}_\mathrm{p}^{+*}, \boldsymbol{\chi}^*) - \psi(\mathbf{F}_\mathrm{e}^{-*}, \mathbf{F}_\mathrm{p}^{-*})))v_\mathrm{n}^* - \mathbf{p} \cdot [\mathbf{v}_2^*] \\ &\quad - \left(\int_{\mathbf{F}^{-*}}^{\mathbf{F}^{+*}} \mathbf{P}'(\mathbf{F}^*(s), \boldsymbol{\chi}^*) : \mathrm{d}\mathbf{F} - \rho(\psi(\mathbf{F}_\mathrm{e}^{+*}, \mathbf{F}_\mathrm{p}^{+*}, \boldsymbol{\chi}^*) - \psi(\mathbf{F}_\mathrm{e}^{-*}, \mathbf{F}_\mathrm{p}^{-*})) + k(u_\mathrm{n}, v_\mathrm{n}^*, [\mathbf{v}_2^*])\right)v_\mathrm{n}^* \\ &\quad - \mathscr{D}_2([\mathbf{v}_2^*], v_\mathrm{n}^*, \mathbf{F}^{+*}, \mathbf{F}^{-*}, \boldsymbol{\chi}^*, \mathbf{F}^*(s)) < 0 \\ &\qquad = (\mathbf{P}' : (\mathbf{F}^+ - \mathbf{F}^-) - \rho(\psi(\mathbf{F}_\mathrm{e}^+, \mathbf{F}_\mathrm{p}^+, \boldsymbol{\chi}) - \psi(\mathbf{F}_\mathrm{e}^-, \mathbf{F}_\mathrm{p}^-)))v_\mathrm{n} - \mathbf{p} \cdot [\mathbf{v}_2] \\ &\qquad\quad - \left(\int_{\mathbf{F}^-}^{\mathbf{F}^+} \mathbf{P}'(\mathbf{F}(s), \boldsymbol{\chi}) : \mathrm{d}\mathbf{F} - \rho(\psi(\mathbf{F}_\mathrm{e}^+, \mathbf{F}_\mathrm{p}^+, \boldsymbol{\chi}) - \psi(\mathbf{F}_\mathrm{e}^-, \mathbf{F}_\mathrm{p}^-)) + k(u_\mathrm{n}, v_\mathrm{n}, [\mathbf{v}_2])\right)v_\mathrm{n} \\ &\qquad\quad - \mathscr{D}_2([\mathbf{v}_2], v_\mathrm{n}, \mathbf{F}^+, \mathbf{F}^-, \boldsymbol{\chi}, \mathbf{F}(s))\end{aligned} \tag{6.5}$$

or

$$\begin{aligned}&\mathbf{P}' : (\mathbf{F}^{+*} - \mathbf{F}^{-*})v_\mathrm{n}^* - \mathbf{p} \cdot [\mathbf{v}_2^*] \\ &\quad - \left(\int_{\mathbf{F}^{-*}}^{\mathbf{F}^{+*}} \mathbf{P}'(\mathbf{F}^*(s), \boldsymbol{\chi}^*) : \mathrm{d}\mathbf{F} + k(u_\mathrm{n}, v_\mathrm{n}^*, [\mathbf{v}_2^*])\right)v_\mathrm{n}^* - \mathscr{D}_2([\mathbf{v}_2^*], v_\mathrm{n}^*, \mathbf{F}^{+*}, \mathbf{F}^{-*}, \boldsymbol{\chi}^*, \mathbf{F}^*(s)) \\ &\qquad < \mathbf{P}' : (\mathbf{F}^+ - \mathbf{F}^-)v_\mathrm{n} - \mathbf{p} \cdot [\mathbf{v}_2] \\ &\qquad\quad - \left(\int_{\mathbf{F}^-}^{\mathbf{F}^+} \mathbf{P}'(\mathbf{F}(s), \boldsymbol{\chi}) : \mathrm{d}\mathbf{F} + k(u_\mathrm{n}, v_\mathrm{n}, [\mathbf{v}_2])\right)v_\mathrm{n} - \mathscr{D}_2([\mathbf{v}_2], v_\mathrm{n}, \mathbf{F}^+, \mathbf{F}^-, \boldsymbol{\chi}, \mathbf{F}(s)),\end{aligned} \tag{6.6}$$

where $\mathscr{D}_2 = \mathbf{p}([\mathbf{v}_2], v_\mathrm{n}, \ldots) \cdot [\mathbf{v}_2]$ is a homogeneous function of degree one in v_n and $[\mathbf{v}_2]$, e.g.

$$\mathscr{D}_2 = |[\mathbf{v}_2]|\, \mathscr{D}_2\left(\frac{[\mathbf{v}_2]}{|[\mathbf{v}_2]|}, \frac{v_\mathrm{n}}{|[\mathbf{v}_2]|}, \ldots\right).$$

Function k is homogeneous of degree zero in v_n and $[\mathbf{v}_2]$, $k = k([\mathbf{v}_2]/v_\mathrm{n}, \ldots)$. From principles (6.3)–(6.6) it follows in particular

$$\mathbf{X}_\Sigma = \frac{\partial \mathscr{D}_\Sigma}{\partial \dot{\mathbf{q}}} \quad \text{or} \quad \mathbf{P}' : (\mathbf{F}^+ - \mathbf{F}^-) - \rho[\psi] = \frac{\partial \mathscr{D}_\Sigma^{\mathrm{T}}}{\partial v_\mathrm{n}}; \qquad -\mathbf{p} = \frac{\partial \mathscr{D}_\Sigma^{\mathrm{T}}}{\partial [\mathbf{v}_2]}; \tag{6.7}$$

$$\int_{\mathbf{F}^-}^{\mathbf{F}^+} \mathbf{P}'(\mathbf{F}^*(s), \boldsymbol{\chi}^*) : \mathrm{d}\mathbf{F} v_\mathrm{n} + \mathscr{D}_2([\mathbf{v}_2], v_\mathrm{n}, \mathbf{F}^+, \mathbf{F}^-, \mathbf{F}^*(s), \boldsymbol{\chi}^*) \to \min. \tag{6.8}$$

When k does not depend on $[\mathbf{v}_2]$ (and, consequently, on v_n) and $\mathscr{D}_2$ does not depend on v_n, then from equations (6.7) and (6.8) we obtain equations (3.14) and (4.5), as well as

$$-\mathbf{p} = \frac{\partial \mathscr{D}_2}{\partial [\mathbf{v}_2]}; \qquad \mathscr{D}_2[(\mathbf{v}_2], \mathbf{F}^+, \mathbf{F}^-, \mathbf{F}^*(s), \boldsymbol{\chi}^*) \to \min. \tag{6.9}$$

From equation $(6.7)_1$ the existence of the "yield surface" $\varphi(\mathbf{X}_\Sigma, \ldots) = 0$ follows (for

$\varphi(\mathbf{X}_\Sigma, \ldots) < 0$, $\dot{\mathbf{q}} = \mathbf{0}$), as well as the associated "flow rule" $\dot{\mathbf{q}} = h_\Sigma\,(\partial\varphi/\partial\mathbf{X}_\Sigma)$, where the scalar h_Σ is determined from the consistency condition $\dot{\varphi} = 0$. The counterpart of the principle (6.4) at time $t + \Delta t$ reads

$$\mathbf{X}_{\Sigma\Delta}(\mathbf{F}_\Delta^{+*}, \mathbf{F}_\Delta^{-*}, \boldsymbol{\chi}_\Delta^*) \cdot \dot{\mathbf{q}}_\Delta^* - \mathscr{D}_\Sigma^{\mathrm{T}}(\dot{\mathbf{q}}_\Delta^*, \mathbf{F}_\Delta^{+*}, \mathbf{F}_\Delta^{-*}, \boldsymbol{\chi}_\Delta^*, \mathbf{F}^*(s)) < 0$$
$$= \mathbf{X}_{\Sigma\Delta}(\dot{\mathbf{q}}_\Delta, \mathbf{F}_\Delta^{+}, \mathbf{F}_\Delta^{-}, \boldsymbol{\chi}_\Delta) \cdot \dot{\mathbf{q}}_\Delta - \mathscr{D}_\Sigma^{\mathrm{T}}(\dot{\mathbf{q}}_\Delta, \mathbf{F}_\Delta^{+}, \mathbf{F}_\Delta^{-}, \boldsymbol{\chi}_\Delta, \mathbf{F}(s)). \qquad (6.10)$$

It is not difficult to take into account the terms with $\mathbf{p} \cdot [\mathbf{v}_2]$ in the extremum principles for the finite volume in Section 4. For time-dependent behaviour ($\mathscr{D}_\Sigma^{\mathrm{T}}$ is an arbitrary function of $\dot{\mathbf{q}}$, diffusive PT [4]) using the postulate of realizability (see Appendix to Part I) we obtain the principle (6.4) with the additional condition

$$\mathscr{D}_\Sigma^{\mathrm{T}}(\dot{\mathbf{q}}^*, \mathbf{F}^{+*}, \mathbf{F}^{-*}, \boldsymbol{\chi}^*, \mathbf{F}^*(s)) = \mathscr{D}_\Sigma^{\mathrm{T}}(\dot{\mathbf{q}}, \mathbf{F}^{+}, \mathbf{F}^{-}, \boldsymbol{\chi}, \mathbf{F}(s)) \qquad (6.11)$$

and, in particular,

$$\mathbf{X}_\Sigma = \lambda_\Sigma \frac{\partial \mathscr{D}_\Sigma^{\mathrm{T}}}{\partial \dot{\mathbf{q}}}; \qquad \lambda_\Sigma = \mathscr{D}_\Sigma^{\mathrm{T}} \left(\frac{\partial \mathscr{D}_\Sigma^{\mathrm{T}}}{\partial \dot{\mathbf{q}}} \cdot \dot{\mathbf{q}} \right)^{-1}. \qquad (6.12)$$

At $v_n = 0$ the above formulas describe the stationary discontinuity surface with jumps in $\mathbf{F}$, $\mathbf{v}$ and $\mathbf{r}$.

7. ANALYSIS OF THE POSTULATE OF REALIZABILITY

The essence of the postulate of realizability is very simple: as soon as some dissipative process (plastic flow, PT) could occur from the viewpoint of thermodynamics, it will occur (or be realized), i.e. the first fulfillment of the necessary energetic condition is sufficient for the beginning of the dissipative process. This postulate was proposed by Levitas [1] and seems to us rather general and flexible. We do not postulate any extremum principles, we prove that some energetic condition is necessary for the beginning of the dissipative process and assume, that as soon as this condition is satisfied the first time for some parameters (fields), then a dissipative process will occur with these parameters. For the time-independent system this postulate is less restrictive than Drucker's postulate (as it is applicable to softening materials) and Il'yushin's one (it is applicable to rigid-plastic materials). Moreover, for more complex models, e.g. with structural changes (or with kinematical constraints) it gives a nonassociated flow rule and admits a concave yield surface; Il'yushin's and Drucker's postulate for this model cannot be applied [12, 13]. The postulate of realizability allows us to prove Ziegler's extremum principle and relations for system with arbitrary dissipation function, but some more general expressions are possible [4, 8]. In PTs theory the counterparts of the obtained extremum principles for the points of the interface are unknown for us. For PTs not only fluxes, but a number of various parameters ($\mathbf{F}^+, \mathbf{F}^-, \boldsymbol{\chi}, \mathbf{F}(\mathrm{s})$) are varied and generalized forces X_Σ, depending on these parameters, are not fixed in extremum principles [e.g. equation (6.4)], in contrast to Ziegler's extremum principles (e.g. equations (A3), (A4) in [8]). That is why even when generalized forces and fluxes are scalars, the extremum principles [e.g. equation (4.2)] give nontrivial results. Moreover, equation (4.2) gives nontrivial result even at $X_\Sigma^{\mathrm{T}} \equiv 0$, i.e. for media without dissipation. In the number of theories of inelastic strain the flow rule is accepted independently of dissipation function or yield surface (e.g. nonassociated flow rules), because the existence of additional postulates (Drucker's Il'yushin's, Hill's, Ziegler's) is not obligatory in the framework of continuum thermodynamics. But it is difficult to imagine that in PTs theory it is possible to formulate the constitutive equations for all of parameters ($\mathbf{F}^+, \mathbf{F}^-, \mathbf{F}(s), \boldsymbol{\chi}, v_n, [\mathbf{v}_2]$) of different nature without any unique principle. This fact can serve as serious argument for the existence of some general principle for dissipative processes and the postulate of realizability can be considered as one of the candidates. The next argument is that using the postulate of realizability we have derived the governing extremum principle for the description of the stable post-bifurcation deformation process for a finite volume of material with and without PTs. The concept of stability, which follows from the postulate of realizability seems to us physically reasonable.

Due to formal analogy, it is not a problem to apply the postulate of realizability to discrete and continual system with friction [12–15], systems with the cracks and damage [16], as well as to coupled above phenomena. Application can be made both on the level of derivation of constitutive equation and description of stable post-bifurcation processes.

Application of the postulate of realizability for the description of nucleation in elasto-plastic materials is given in [17], for averaging description of PTs—in [17, 18].

8. CONCLUSIONS

In this paper the extremum principles for the interface and the whole volume are derived using the postulate of realizability. They are used to derive a number of equations for the description of PT: for jumps of the deformation gradient and the tensors characterizing the mutual orientation of the phases; for the deformation gradient history in the course of PT; for the normal velocity of the interface and the velocity of the relative sliding along the interface; the local and global criteria for the martensitic PT. The local criteria represent the equations for some parameters across the interface. But even when they can be met, two solutions are possible; first, the solution with fixed interface, second, the solution with moving one. The stable solution can be chosen using the extremum principle for the whole volume. This means that the fulfilment of the local criteria is not enough for the occurrence of PT and only the global criterion will give the final solution. It seems to us that the same situation takes place for the motion of other defects with singular fields, e.g. crack tips, dislocations and point defects. Some examples are considered. It is shown that in the course of PT, the traction continuity condition is violated across the interface. To remove this contradiction the concept of fluctuating stresses is introduced. These stresses overcome the energy barrier and restore the traction continuity condition. In the future it is necessary to combine these results for PT with previously obtained ones (Levitas [4]): averaging procedure, finite strain kinematics, simplified models. The mutual influence of large plastic strain and PT is of primary importance for numerous practical applications [4].

Most of the instability problems could be solved numerically only. The enormous mesh-dependence of the numerical FEM solution is well-known (e.g. [19]) and adaptive remeshing is necessary [20]. The following method of mesh optimization at each time increment is possible. For the various meshes we obtain the various FE solutions, each of which met all the FEM equations, i.e. we have an infinite number of solutions, parameterized by nodes positions, and it is necessary to choose the best one. The best solution is the most stable one. If we consider the coordinates of the nodes of the mesh as independent variables, the discrete form of the governing extremum principle for choosing the stable deformation process will give the increment of the coordinates for each node at each time increment. From the physical point of view, this strategy seems to be very natural: if, for instance, a system with one controlled displacement at different meshes has different load–displacement curves, the most stable solution will correspond to the minimum load increment at each time step. If this approach is realized, it will be based on a natural stability criterion of mesh adaption.

The generalization of the obtained extremum principles for thermoplastic and viscoplastic materials is very important.

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APPENDIX

Some Relations for Interfaces

For coherent interfaces, the function $\mathbf{r}(\mathbf{r}_\tau, t)$ is continuous, but the velocity vector $\mathbf{v}(\mathbf{r}_\tau, t)$ and the deformation gradient $\mathbf{F}(\mathbf{r}_\tau, t)$ have jumps across the interface Σ. In this case, the compatibility condition

$$[\mathbf{F}] = -\frac{1}{v_n}[\mathbf{v}]\mathbf{n}; \qquad [\mathbf{v}] = -[\mathbf{F}]\cdot\mathbf{n}v_n; \qquad [\mathbf{F}] = \mathbf{n}\cdot[\mathbf{F}^t]\mathbf{n} = [\mathbf{F}]\cdot\mathbf{nn} \tag{A1}$$

are valid [21]. Contraction of equation $(\mathrm{A1})_1$ with the normal vector $\mathbf{n}$ gives equation $(\mathrm{A1})_2$, the substitution of equation $(\mathrm{A1})_2$ into equation $(\mathrm{A1})_1$ results in equation $(\mathrm{A1})_3$. From the equilibrium condition follows the traction continuity

$$[\mathbf{p}] = [\mathbf{P}]\cdot\mathbf{n} = 0. \tag{A2}$$

According to the second law of thermodynamics, at fixed temperature the rate of dissipation

$$\int_S \mathbf{p}\cdot\mathbf{v}\,\mathrm{d}S - \frac{\mathrm{d}}{\mathrm{d}t}\int_v \rho\psi(\mathbf{F}_e, \mathbf{F}_p)\,\mathrm{d}v \geq 0. \tag{A3}$$

To pass from the integral form of equation (A3) to the local one it is necessary to use the Gauss theorem for a volume with discontinuity surfaces.

The general scheme to apply the Gauss theorem is the following one. The volume v is divided by surfaces Σ and S into a finite number of volumes, in each of them all functions are continuous and, using the Gauss theorem, we obtain some equations. After summing up all of these equations we obtain an integral over the volume $\bar{v} = v - \Sigma$ at one side and on the other side an integral on S and an integral on Σ of the jumps of the functions (because the integration on Σ is fulfilled two times for two volumes, divided by Σ). Thus we derive

$$\int_S \mathbf{p}\cdot\mathbf{v}\,\mathrm{d}S = \int_{\bar{v}} \mathbf{P}^t : \dot{\mathbf{F}}\,\mathrm{d}\bar{v} - \int_\Sigma \mathbf{p}\cdot[\mathbf{v}]\,\mathrm{d}\Sigma. \tag{A4}$$

(Equation (A2) was applied.) Using the formulas for differentiating on a variable volume we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{v}\rho\psi\,\mathrm{d}v=\int_{\bar{v}}\rho\dot{\psi}\,\mathrm{d}\bar{v}+\int_{\Sigma}\rho[\psi]v_{n}\,\mathrm{d}\Sigma. \tag{A5}$$

From equations (A3)–(A5) it follows $\int_v (\mathbf{P}' : \dot{\mathbf{F}} - \rho\dot{\psi})\,\mathrm{d}v + \int_\Sigma \mathscr{D}_\Sigma\,\mathrm{d}\Sigma \geq 0$, where

$$\mathscr{D}_\Sigma = -\mathbf{p}\cdot[\mathbf{v}] - \rho[\psi]v_{\mathrm{n}} \tag{A6}$$

is the rate of dissipation per unit area of the interface. Using equations $(\mathrm{A1})_2$ and $(\mathrm{A1})_3$ we get

$$-\mathbf{p}\cdot[\mathbf{v}] = \mathbf{n}\cdot\mathbf{P}'\cdot[\mathbf{F}]\cdot\mathbf{n}v_{\mathrm{n}} = \mathbf{P}':([\mathbf{F}]\cdot\mathbf{nn})v_{\mathrm{n}} = \mathbf{P}':[\mathbf{F}]v_{\mathrm{n}}. \tag{A7}$$

Substituting equation (A7) into equation (A6) we obtain $\mathscr{D}_\Sigma = X_\Sigma v_{\mathrm{n}}$ where

$$X_\Sigma = \mathbf{P}':[\mathbf{F}] - \rho[\psi] = \mathbf{n}\cdot\mathbf{P}'\cdot[\mathbf{F}]\cdot\mathbf{n} - \rho(\psi(\mathbf{F}_{\mathrm{e}}^{+},\mathbf{F}_{\mathrm{p}}^{+},\chi) - \psi(\mathbf{F}_{\mathrm{e}}^{-},\mathbf{F}_{\mathrm{p}}^{-})). \tag{A8}$$

For noncoherent interfaces the position vector $\mathbf{r}$ has also a jump. We will consider a small $[\mathbf{r}]$ and neglect the difference in geometry of points $\mathbf{r}^{+}$ and $\mathbf{r}^{-}$ (like the difference between $\mathbf{r}$ and $\mathbf{r}_\tau$ is neglected at the small displacements approximation). In this case equation (A2) is valid. At finite $[\mathbf{r}]$ the traction continuity condition is valid in the actual configuration. But the points which are in the contact in the actual configuration are not in the contact in the reference one. That is why we assume the small $[\mathbf{r}]$. Equation (A6) is also valid for the noncoherent PT; all other equations in Appendix could not be used.