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Phase Transitions in Inelastic Materials at Finite Strains: A Local Description

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Abstract. A general theory of phase transitions (PT) in the material point of simple inelastic materials with arbitrary constitutive equations is developed. The standard thermodynamical approach can be applied only after averaging of thermodynamical parameters, related to PT, over a PT duration. A PT criterion for the material point is derived, taking into account the temperature variation and dissipation due to PT, as well as internal variables. Temperature variation in the course of PT is determined with the help of the entropy balance equation under the assumption that the process is adiabatic. Based on results for the material point, new nucleation and interface propagation criteria are derived. A postulate of realizability is applied to determine all unknown parameters in PT criteria. A model problem is solved.

1. INTRODUCTION

There are following known descriptions of martensitic PT: jump conditions for a moving interface, a variation of a volume fraction of phases in a multiphase material, a condition of nucleation in a finite volume and so on [1] – [3]. But a description of PT as a thermomechanical deformation process in a *material point* is lacking. This fact does not allow us to apply the standard methods of derivation of constitutive equations, as e.g. for a material point of elastoplastic materials. Moreover, an account for *temperature variation* in the course of PT, temperature gradient and internal variables in the above approaches [1] – [3] is nontrivial without a consequent theory for the material point. In the present paper PT is regarded as a thermomechanical inelastic deformation process, accompanied by change of all thermomechanical properties. The following important property is used: a norm (or components) of the transformation deformation gradient is fixed for each of crystallographically equivalent variants of PT and cannot be larger or smaller. All other configurations (crystal structures) with another norm of transformation deformation gradient are unstable and thus impossible. Based on these statements a general theory of PT in the material point of a simple inelastic body is developed. It is shown that a standard thermodynamical approach cannot be directly applied. It can be applied after *averaging* of thermodynamical parameters, related to PT, over a PT duration. A PT *criterion* is derived with account for the temperature variation due to PT and internal variables. It is shown that the temperature gradient does not contribute to PT criterion.

Nucleation and interface propagation conditions are derived, which generalize the conditions postulated in [3, 4], for nonisothermal processes and media with internal variables. A model problem is solved. Some preliminary results were reported in [5].

Let a superscript t denote transposition, dots mean contractions of the tensors. All statements are developed with respect to the reference configuration.

2. THERMODYNAMICS OF MARTENSITIC PHASE TRANSITIONS IN A MATERIAL POINT

Let us consider an uniformly deformed material point in a process of martensitic PT. We shall

consider simple materials only, i.e. the material's response in the given point is independent of thermomechanical parameters in other points. We assume a multiplicative decomposition of a total deformation gradient $\mathbf{F}$ into elastic $\mathbf{F}_e$, thermal $\mathbf{F}_\theta$, transformational $\mathbf{F}_t$ and plastic $\mathbf{F}_p$ parts [6], i.e.

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_\theta \cdot \mathbf{F}_t \cdot \mathbf{F}_p. \quad (1)$$

We introduce the internal dimensionless parameter ξ ($0 \leq \xi \leq 1$) which is related with $\mathbf{F}_t$ and has the following properties: PT starts at $\xi = 0$ and finishes at $\xi = 1$; when ξ varies between 0 and 1, the transformation deformation gradient grows from 0 till $\mathbf{F}_{t \max}$. During this process all the thermodynamical properties of the phase 1 vary into the properties of the phase 2. It is possible to define

$$\xi := \text{tr } \mathbf{F}_t / \text{tr } \mathbf{F}_{t \max}, \quad \xi := |\mathbf{F}_t| / |\mathbf{F}_{t \max}|, \quad (2)$$

but a lot of other definitions are acceptable. The internal parameter ξ plays a similar role for the consideration of the uniformly deformed material point, as a volume fraction of martensite for the averaged description of PT.

Let us define the specific Helmholtz free energy

$$\psi = \psi(\mathbf{F}_e(\xi), \theta(\xi), \mathbf{F}_p(\xi), \mathbf{g}(\xi), \mathbf{F}_t(\xi), \xi), \quad (3)$$

where $\mathbf{g}$ is a set of internal variables. We admit the second law of thermodynamic in the form of the Clausius–Duhem inequality

$$\mathcal{D} = \mathbf{P}^t : \dot{\mathbf{F}} - \rho \dot{\psi} - \rho s \dot{\theta} - \frac{\nabla \theta}{\theta} \cdot \mathbf{h} \geq 0. \quad (4)$$

Here $\mathcal{D}$ is the rate of dissipation per unit volume, $\mathbf{P}$ the first Piola–Kirchhoff nonsymmetric stress tensor, ρ mass density in the reference configuration at $\xi = 0$, s the entropy, $\nabla \theta$ the temperature gradient, $\mathbf{h}$ the heat flux. Substituting the rate of free energy $\dot{\psi}$ and taking into account the multiplicative decomposition Eq. (1) and $\dot{\mathbf{F}}_\theta = \frac{\partial \mathbf{F}_\theta}{\partial \theta} \dot{\theta} + \frac{\partial \mathbf{F}_\theta}{\partial \xi} \dot{\xi}$ in Eq. (4) yield

$$\begin{aligned} \mathcal{D} = & \left(\mathbf{F}_\theta \cdot \mathbf{F}_t \cdot \mathbf{F}_p \cdot \mathbf{P}^t - \rho \frac{\partial \psi}{\partial \mathbf{F}_e^t} \right) : \dot{\mathbf{F}}_e + \left(\mathbf{P}^t : \mathbf{F}_e \cdot \frac{\partial \mathbf{F}_\theta}{\partial \theta} \cdot \mathbf{F}_t \cdot \mathbf{F}_p - \rho \frac{\partial \psi}{\partial \theta} - \rho s \right) \dot{\theta} + \\ & + \left(\mathbf{P}^t : \mathbf{F}_e \cdot \mathbf{F}_\theta \cdot \frac{\partial \mathbf{F}_t}{\partial \xi} \cdot \mathbf{F}_p + \mathbf{P}^t : \mathbf{F}_e \cdot \frac{\partial \mathbf{F}_\theta}{\partial \xi} \cdot \mathbf{F}_t \cdot \mathbf{F}_p - \rho \frac{\partial \psi}{\partial \mathbf{F}_t^t} : \frac{\partial \mathbf{F}_t}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi} \right) \dot{\xi} + \\ & + \left(\mathbf{P}^t : \mathbf{F}_e \cdot \mathbf{F}_\theta \cdot \mathbf{F}_t - \rho \frac{\partial \psi}{\partial \mathbf{F}_p^t} \right) : \dot{\mathbf{F}}_p - \frac{\nabla \theta}{\theta} \cdot \mathbf{h} - \rho \frac{\partial \psi}{\partial \mathbf{g}^t} : \dot{\mathbf{g}} \geq 0. \end{aligned} \quad (5)$$

The possibility of permutation of tensors in a scalar product is used, $\mathbf{P}^t : \dot{\mathbf{F}}_e \cdot \mathbf{F}_\theta \cdot \mathbf{F}_t \cdot \mathbf{F}_p = \mathbf{F}_\theta \cdot \mathbf{F}_t \cdot \mathbf{F}_p \cdot \mathbf{P}^t : \dot{\mathbf{F}}_e = \mathbf{F}_e^{-1} \cdot \mathbf{F} \cdot \mathbf{P}^t : \dot{\mathbf{F}}_e$ (decomposition (1) is taken into account). The assumption that the rate of dissipation is independent of $\dot{\mathbf{F}}_e$ and $\dot{\theta}$ results in the hyperelasticity law and the expression for entropy, as well as in the reduced dissipative inequality:

$$\mathbf{F}_e^{-1} \cdot \mathbf{F} \cdot \mathbf{P}^t = \rho \frac{\partial \psi}{\partial \mathbf{F}_e^t}; \quad s = -\frac{\partial \psi}{\partial \theta} + \frac{1}{\rho} \mathbf{P}^t : \mathbf{F}_e \cdot \frac{\partial \mathbf{F}_\theta}{\partial \theta} \cdot \mathbf{F}_t \cdot \mathbf{F}_p; \quad (6)$$

$$\mathcal{D} = \mathbf{X}_p : \dot{\mathbf{F}}_p + \mathbf{X}_g : \dot{\mathbf{g}} + \mathbf{X}_h \cdot \mathbf{h} + X_\xi \dot{\xi} \geq 0, \quad (7)$$

$$(8)$$

$$\text{where} \quad \mathbf{X}_p = \mathbf{P}^t : \mathbf{F}_e \cdot \mathbf{F}_\theta \cdot \mathbf{F}_t - \rho \frac{\partial \psi}{\partial \mathbf{F}_p^t}; \quad \mathbf{X}_g = -\rho \frac{\partial \psi}{\partial \mathbf{g}^t}; \quad \mathbf{X}_h = -\frac{\nabla \theta}{\theta} \quad (9)$$

$$\text{and} \quad X_\xi = \mathbf{P}^t : \mathbf{F}_e : \left(\frac{\partial \mathbf{F}_\theta}{\partial \xi} \cdot \mathbf{F}_t + \mathbf{F}_\theta \cdot \frac{\partial \mathbf{F}_t}{\partial \xi} \right) \cdot \mathbf{F}_p - \rho \frac{\partial \psi}{\partial \mathbf{F}_t^t} : \frac{\partial \mathbf{F}_t}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi} \quad (10)$$

are dissipative forces conjugated with dissipative rates $\dot{\mathbf{F}}_p$, $\dot{\mathbf{g}}$, $\mathbf{h}$ and $\dot{\xi}$ respectively. The simplest assumption that each rate depends on the conjugate force only leads to evolution equations

$$\dot{\mathbf{F}}_p = \mathbf{f}_p(\mathbf{X}_p, \xi); \quad \dot{\mathbf{g}} = \mathbf{f}_g(\mathbf{X}_g, \xi); \quad \mathbf{h} = \mathbf{f}_h(\mathbf{X}_h, \xi); \quad \dot{\xi} = f_\xi(X_\xi, \xi). \quad (11)$$

Eq. (11)₁ is the flow rule, Eq. (11)₂ is the evolution equation for the internal variables, Eq. (11)₃ is the generalized Fourier law and Eq. (11)₄ is the kinetic equation for PT. We consider the last equation for the description of PT only. The account for mutual influence of all thermomechanical processes can be made in a standard way.

We assume that the condition $\dot{\xi} = 0$ is valid at $X_\xi = 0$ only. Then it is possible to describe the equilibrium PT ($\dot{\xi} \rightarrow 0$) with the equation $X_\xi = 0$. This is one scalar equation, and for each ξ and $\theta(\xi)$ it is always possible to choose six components of the stress tensor $\mathbf{P}(\xi, \theta(\xi))$ to satisfy $X_\xi = 0$. If the actual stress variation follows this dependence, then the phase equilibrium is possible for arbitrary ξ . But from the experiments it follows that the phase equilibrium is impossible at $0 < \xi < 1$, only at $\xi = 0$ and $\xi = 1$ we have the stable equilibrium (see Introduction). At $0 < \xi < 1$ a nonequilibrium process proceeds which requires energy and stress fluctuations.

This situation seems new to us for continuum thermodynamics. In this case the standard thermodynamical approach cannot be applied. It is necessary to average the thermodynamical parameters, related with PT, over the duration of PT in order to filter off these fluctuations. We introduce the averaged dissipation rate as a dissipation work during PT divided on the duration t_p of PT

$$\mathcal{D}_\xi := \frac{1}{t_p} \int_0^{t_p} X_\xi \dot{\xi} dt = \frac{1}{t_p} \int_0^1 X_\xi d\xi = \frac{X}{t_p} = X \dot{\chi}, \quad \text{where } X := \int_0^1 X_\xi d\xi, \quad \dot{\chi} := \frac{1}{t_p} \quad (12)$$

are the averaged dissipative force and rate. The definition of dissipative rate is logical, because a variation of the parameter ξ during the time t_p is equal one. The dissipative force is defined as a conjugate variable in the expression for the rate of dissipation. For the macroscopically equilibrium process (PT) the following equation is valid

$$X = \int_{\mathbf{F}_{t1}}^{\mathbf{F}_{t2}} \left(\mathbf{F}_p \cdot \mathbf{P}^t \cdot \mathbf{F}_e \cdot \mathbf{F}_\theta - \rho \frac{\partial \psi}{\partial \mathbf{F}_t^t} \right) : d\mathbf{F}_t + \int_0^1 \left(\mathbf{F}_t \cdot \mathbf{F}_p \cdot \mathbf{P}^t \cdot \mathbf{F}_e : \frac{\partial \mathbf{F}_\theta}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi} \right) d\xi = 0. \quad (13)$$

The indices 1 and 2 denote the values before and after PT. Eq. (13) is the PT criterion for PT without dissipation.

Since practically all martensitic transformations, even in elastic materials, are accompanied with a dissipation and a hysteresis, the PT criterion has the following form

$$X = k. \quad (14)$$

Here k is an experimentally determined value of dissipation due to PT, which can depend on θ , $\dot{\chi}$, $\mathbf{F}_p$, $\mathbf{g}$, At $X < k$ PT is impossible.

Let us consider the alternative expressions for X . From Eqs. (4) and (7) it follows

$$X_\xi \dot{\xi} = \mathcal{D} - \mathbf{X}_p : \dot{\mathbf{F}}_p - \mathbf{X}_g : \dot{\mathbf{g}} - \mathbf{X}_h \cdot \mathbf{h} = \mathbf{P}^t : \dot{\mathbf{F}} - \rho \dot{\psi} - \rho s \dot{\theta} - \mathbf{X}_p : \dot{\mathbf{F}}_p - \mathbf{X}_g : \dot{\mathbf{g}}; \quad (15)$$

$$X = \int_{\mathbf{F}_1}^{\mathbf{F}_2} \mathbf{P}^t : d\mathbf{F} - \rho(\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} \rho s d\theta - \int_0^{t_p} (\mathbf{X}_p : \dot{\mathbf{F}}_p + \mathbf{X}_g : \dot{\mathbf{g}}) dt = k. \quad (16)$$

Taking into account the decomposition (1) and Eq. (9)₁ for $\mathbf{X}_p$ we obtain

$$\begin{aligned} X = & \int_{\mathbf{F}_1}^{\mathbf{F}_2} (\mathbf{P}^t : d\mathbf{F}_e \cdot \mathbf{F}_\theta \cdot \mathbf{F}_t \cdot \mathbf{F}_p + \mathbf{P}^t : \mathbf{F}_e \cdot d\mathbf{F}_\theta \cdot \mathbf{F}_t \cdot \mathbf{F}_p + \mathbf{P}^t : \mathbf{F}_e \cdot \mathbf{F}_\theta \cdot d\mathbf{F}_t \cdot \mathbf{F}_p) - \\ & - \rho(\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} \rho s d\theta + \int_{\mathbf{F}_{p1}}^{\mathbf{F}_{p2}} \rho \frac{\partial \psi}{\partial \mathbf{F}_p^t} : d\mathbf{F}_p + \int_{\mathbf{g}_1}^{\mathbf{g}_2} \rho \frac{\partial \psi}{\partial \mathbf{g}^t} : d\mathbf{g} = k. \end{aligned} \quad (17)$$

The expressions (16) and (17) are sometimes more convenient for the analysis, than Eq. (13). At $\frac{\partial \psi}{\partial \mathbf{F}_p} = 0$ Eq. (17) is more suitable for application, because in this case the plastic strain $\mathbf{F}_p$ disappears completely. Eq. (16) shows that X is the total dissipation increment minus plastic dissipation increment and the dissipation increment due to the internal variables. Eq. (16) is more appropriate, when the moving interface is considered and the Hadamard's compatibility condition for $\mathbf{F}_i$ is taken into account (see Section 4).

For elastic materials without internal variables and for isothermal processes, at $k = 0$ it follows from Eq. (16)

$$\int_{\mathbf{F}_1}^{\mathbf{F}_2} \boldsymbol{\sigma} : d\mathbf{F} = \rho (\psi_2 - \psi_1). \quad (18)$$

If PT proceeds at constant stress $\mathbf{P}_o$, then $\mathbf{P}_o^t : (\mathbf{F}_2 - \mathbf{F}_1) = \rho (\psi_2 - \psi_1)$. This is the Maxwell rule. Eq. (16) is a generalization of the Maxwell rule for dissipative materials, nonisothermal processes and for variable stresses.

At small strains $\mathbf{F} = \mathbf{I} + \boldsymbol{\varepsilon}$, $\mathbf{F}_e = \mathbf{I} + \boldsymbol{\varepsilon}_e$, $\mathbf{F}_\theta = \mathbf{I} + \boldsymbol{\varepsilon}_\theta$, $\mathbf{F}_t = \mathbf{I} + \boldsymbol{\varepsilon}_t$, $\mathbf{F}_p = \mathbf{I} + \boldsymbol{\varepsilon}_p$, where $\boldsymbol{\varepsilon} \ll \mathbf{I}$, $\boldsymbol{\varepsilon}_e \ll \mathbf{I}$, $\boldsymbol{\varepsilon}_\theta \ll \mathbf{I}$, $\boldsymbol{\varepsilon}_t \ll \mathbf{I}$, $\boldsymbol{\varepsilon}_p \ll \mathbf{I}$ are the corresponding strain tensors, $\mathbf{I}$ is a second order identity tensor, $\mathbf{P} = \boldsymbol{\sigma}$, $\mathbf{P}^t : \dot{\mathbf{F}} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}$, where $\boldsymbol{\sigma}$ is a stress tensor, reference and actual configurations coincide and Eqs. (1), (6), (9)₁, (10), (16) and (17) take the form

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p + \boldsymbol{\varepsilon}_\theta + \boldsymbol{\varepsilon}_t; \quad (19)$$

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e}; \quad s = \frac{\boldsymbol{\sigma}}{\rho} : \frac{\partial \boldsymbol{\varepsilon}_\theta}{\partial \theta} - \frac{\partial \psi}{\partial \theta}; \quad (20)$$

$$\mathbf{X}_p = \boldsymbol{\sigma} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_p}; \quad \mathbf{X}_\xi = \boldsymbol{\sigma} : \frac{\partial (\boldsymbol{\varepsilon}_t + \boldsymbol{\varepsilon}_\theta)}{\partial \xi} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_t} : \frac{\partial \boldsymbol{\varepsilon}_t}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi}; \quad (21)$$

$$X = \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon} - \rho (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} \rho s d\theta - \int_0^{t_p} (\mathbf{X}_p : \dot{\mathbf{F}}_p + \mathbf{X}_g : \dot{\mathbf{g}}) dt = k; \quad (22)$$

$$X = \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma} : d(\boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_\theta + \boldsymbol{\varepsilon}_t) - \rho (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} \rho s d\theta + \int_{\mathbf{g}_1}^{\mathbf{g}_2} \rho \frac{\partial \psi}{\partial \mathbf{g}^t} : d\mathbf{g} + \int_{\boldsymbol{\varepsilon}_{p1}}^{\boldsymbol{\varepsilon}_{p2}} \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_p} : d\boldsymbol{\varepsilon}_p = k. \quad (23)$$

Assume that both phases have the same elasticity tensor $\mathbf{E}$ and

$$\rho \psi_i = 0,5 \boldsymbol{\varepsilon}_{e1} : \mathbf{E} : \boldsymbol{\varepsilon}_{e1} + \rho \psi_i^\theta = \rho \psi_i^e + \rho \psi_i^\theta, \quad i = 1, 2, \quad (24)$$

where ψ_i^e and ψ_i^θ are the elastic and thermal parts of free energy. Since

$$\int_{\boldsymbol{\varepsilon}_{e1}}^{\boldsymbol{\varepsilon}_{e2}} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}_e = \mathbf{E} \cdots \int_{\boldsymbol{\varepsilon}_{e1}}^{\boldsymbol{\varepsilon}_{e2}} \boldsymbol{\varepsilon}_e d\boldsymbol{\varepsilon}_e = 0,5 \boldsymbol{\varepsilon}_{e2} : \mathbf{E} : \boldsymbol{\varepsilon}_{e2} - 0,5 \boldsymbol{\varepsilon}_{e1} : \mathbf{E} : \boldsymbol{\varepsilon}_{e1} = \rho (\psi_2^e - \psi_1^e), \quad (25)$$

it follows then from Eq. (23)

$$X = \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma} : d(\boldsymbol{\varepsilon}_\theta + \boldsymbol{\varepsilon}_t) - \rho (\psi_2^\theta - \psi_1^\theta) - \int_{\theta_1}^{\theta_2} \rho s d\theta + \int_{\mathbf{g}_1}^{\mathbf{g}_2} \rho \frac{\partial \psi}{\partial \mathbf{g}^t} : d\mathbf{g} + \int_{\boldsymbol{\varepsilon}_{p1}}^{\boldsymbol{\varepsilon}_{p2}} \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_p} : d\boldsymbol{\varepsilon}_p = k. \quad (26)$$

Since $\boldsymbol{\varepsilon}_\theta = \boldsymbol{\alpha} (\theta - \theta_o)$, where $\boldsymbol{\alpha} = \boldsymbol{\alpha} (\xi, \theta - \theta_o)$ is the thermal expansion tensor and θ_o is the reference temperature, we shall assume that for isothermal processes $\theta = \theta_o$ and we obtain $\boldsymbol{\varepsilon}_\theta = 0$. Consequently, for $\frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_p} = \frac{\partial \psi}{\partial \mathbf{g}} = 0$ and isothermal processes we have

$$X = \int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}_t - \rho (\psi_2^\theta - \psi_1^\theta) = k. \quad (27)$$

There is one *general* problem: for calculation of integrals in Eq. (16) it is necessary to determine the stress variation (as well as $\mathbf{F}_p, \mathbf{g}, \theta$) during PT (variation of $\mathbf{F}_t$).

3. DETERMINATION OF TEMPERATURE

For the determination of a temperature variation in the course of PT we can use an entropy balance equation

$$\rho \theta \dot{s} = \mathcal{D} + \operatorname{div} \mathbf{h} + \frac{\nabla \theta}{\theta} \cdot \mathbf{h}. \quad (28)$$

Substitution of expression (7) for the rate of dissipation $\mathcal{D}$ in Eq. (28) yields

$$\rho \theta \dot{s} = \operatorname{div} \mathbf{h} + \mathbf{X}_p : \dot{\mathbf{F}}_p + \mathbf{X}_g : \dot{\mathbf{g}} + X_\xi \dot{\xi}. \quad (29)$$

According to Eq. (6)₂ $s = s(\theta, \mathbf{P}, \mathbf{g}, \mathbf{F}_p, \mathbf{F}_t, \xi)$. Substitution of this expression and Eq. (11)₃ for the heat flux into Eq. (29) leads to the temperature evolution equation

$$\begin{aligned} \rho \nu \dot{\theta} = & \operatorname{div} \mathbf{f}_h \left(-\frac{\nabla \theta}{\theta} \right) + \left(\mathbf{X}_p - \rho \frac{\partial s}{\partial \mathbf{F}_p^t} \theta \right) : \dot{\mathbf{F}}_p + \left(\mathbf{X}_g - \rho \frac{\partial s}{\partial \mathbf{g}} \theta \right) : \dot{\mathbf{g}} + \\ & + \left(X_\xi - \rho \frac{\partial s}{\partial \xi} \theta - \rho \frac{\partial s}{\partial \mathbf{F}_t^t} : \frac{\partial \mathbf{F}_t}{\partial \xi} \right) \dot{\xi} - \theta \frac{\partial s}{\partial \mathbf{P}^t} : \dot{\mathbf{P}}, \quad \nu := \theta \frac{\partial s}{\partial \theta}, \end{aligned} \quad (30)$$

where ν is the specific heat. Due to the divergence term the temperature in the given point can be defined after formulation and solution of a boundary-value problem. Taking into account a very short duration of PT ($10^{-6} - 10^{-11}$ s), the *adiabatic* process can be assumed (similar to the processes in shock waves). In this case $\operatorname{div} \mathbf{h} = 0$ and Eq. (30) determines the temperature evolution in each material point *independently*, i.e. without solution of a boundary-value problem.

A general scheme of application of PT criterion (16) and temperature evolution equation (30) is following. All material properties, constitutive equations (11) and transformation strain $\mathbf{F}_t(\xi)$ should be given as function of ξ . Then assume that at some stress $\mathbf{P}_s$ and temperature θ_s PT in the given point starts. Stress variation $\mathbf{P}(\xi)$, as well as $\mathbf{F}_p(\xi)$, $\mathbf{g}(\xi)$, are determined by solution of a boundary value-problem or using some simplified models (e.g. [2]). The temperature can be determined by solution of Eq. (30). In the general case mechanical and thermal equations are *coupled* and should be considered together. After determination of all parameters for $0 \leq \xi \leq 1$ the criterion (14) allows us to determine (iteratively or explicitly) the temperature θ_s at the given $\mathbf{P}_s$ or one of the components of the stress tensor $\mathbf{P}_s$ with the remaining five components of $\mathbf{P}_s$ and the temperature θ_s given.

Let us consider some specifications and simplifications of Eq. (30) at small strain. Assume the validity of Eq. (24) for the free energy with equal elastic properties of both phases and the following explicit expression for a thermal part of free energy [7]

$$\psi_1^\theta = \psi_{oi} - s_{oi} (\theta - \theta_o) - \nu_i \theta (\ln \theta / \theta_o - 1) - \nu_i \theta_o, \quad i = 1, 2. \quad (31)$$

Here $\nu_i > 0$ are the specific heats, s_{oi} and ψ_{oi} are the constants. If the thermal expansion coefficient is independent of θ , then from Eq. (20)₂ it follows

$$\rho s = \rho s_o(\xi) + \rho \nu(\xi) \ln \frac{\theta}{\theta_o} + \boldsymbol{\sigma} : \boldsymbol{\alpha}(\xi) \quad \text{and} \quad \theta \frac{\partial s}{\partial \theta} = \nu(\xi), \quad (32)$$

i.e. the accepted Eq. (30)₂ for the specific heat in a general nonlinear situation, coincides in this case with the specific heat in the expression for ψ^θ . This is a reason for using a logarithmic term in Eq. (31).

Functions $s_o(\xi)$, $\nu(\xi)$ and $\alpha(\xi)$ are usually unknown and we assume a linear approximation

$$s_o = (1 - \xi) s_{o1} + \xi s_{o2}, \quad \nu = (1 - \xi) \nu_1 + \xi \nu_2, \quad \alpha(\xi) = (1 - \xi) \alpha_1 + \xi \alpha_2. \quad (33)$$

Then Eq. (30) can be transformed into the form

$$\begin{aligned} \rho \nu(\xi) \dot{\theta} = & (X_\xi - \rho \theta \Delta s_o - \rho \Delta \nu \theta \ln \theta / \theta_o - \sigma : \Delta \alpha \theta) \dot{\xi} - \\ & - \dot{\sigma} : \alpha(\xi) \theta + X_p : \dot{\epsilon}_p + X_g : \dot{g}, \end{aligned} \quad (34)$$

where $\Delta \mathbf{b} := \mathbf{b}_2 - \mathbf{b}_1$. If $\psi_o = (1 - \xi) \psi_{o1} + \xi \psi_{o2}$ and ψ_{oi} are independent of $\mathbf{g}$ and ϵ_p , then $X_g = 0$ and $X_p = \sigma$. In this case Eq. (13) is the most convenient form of X . PT criterion results in

$$\begin{aligned} \int_{\epsilon_{i1}}^{\epsilon_{i2}} \sigma : d\epsilon_i + \int_0^1 \sigma : \Delta \alpha (\theta - \theta_o) d\xi + \rho (\Delta s_o - \Delta \nu) \int_0^1 \theta d\xi + \\ + \rho \Delta \nu \int_0^1 \theta \ln \frac{\theta}{\theta_o} d\xi = k + \rho \Delta \psi_o + \rho (\Delta s_o - \Delta \nu) \theta_o. \end{aligned} \quad (35)$$

Eq. (35) shows that the thermal expansion tensors of each phase do not effect on PT criterion, only their difference contributes to the driving force. For an isothermal process at $\theta = \theta_o$ Eq. (35) coincides with Eq. (27) at $(\psi_2^\theta - \psi_1^\theta) = \Delta \psi_o$.

For isotropic $\alpha = \alpha I$ we have $\sigma : \Delta \alpha = 3 \sigma_o \Delta \alpha$, $\dot{\sigma} : \alpha = 3 \dot{\sigma}_o \alpha$, where σ_o is a mean pressure and for fixed σ_o , for elastic materials and constant $X_\xi = k$ Eq. (34) is independent of the stress variation

$$\rho ((1 - \xi) \nu_1 + \xi \nu_2) \dot{\theta} = (k - \rho \theta \Delta s_o - \rho \Delta \nu \theta \ln \theta / \theta_o - 3 \sigma_o \Delta \alpha \theta) \dot{\xi}. \quad (36)$$

Choosing a proper θ_o we can meet the condition of smallness of $(\theta / \theta_o - 1)$ and consequently $\ln \theta / \theta_o \simeq \theta / \theta_o - 1$. In this case the temperature can be determined analytically, but the obtained equation is rather sophisticated for analysis. In the case $\Delta \nu = 0$ we have

$$d\theta = (A + B\theta) d\xi \quad \text{or} \quad \theta = \left(\frac{A}{B} + \theta_s \right) \exp(B\xi) - \frac{A}{B}, \quad (37)$$

where $A = \frac{1}{\rho \nu} k$, $B = -\frac{1}{\rho \nu} (\rho \Delta s_o + 3 \sigma_o \Delta \alpha)$. PT criterion at $\Delta \nu = 0$ reads as

$$\int_{\epsilon_{i1}}^{\epsilon_{i2}} \sigma : d\epsilon_i = \rho \nu B \int_0^1 \theta d\xi + k + U, \quad (38)$$

where $U = \rho (\Delta \psi_o + \Delta s_o \theta_o) + 3 \sigma_o \Delta \alpha \theta_o$, or taking into account Eq. (37)

$$\int_{\epsilon_{i1}}^{\epsilon_{i2}} \sigma : d\epsilon_i = \rho \nu \left(\frac{A}{B} + \theta_s \right) (\exp B - 1) + U. \quad (39)$$

At small B we have $\exp B\xi = 1 + B\xi$ and

$$\theta = \theta_s + (A + B\theta_s) \xi; \quad \int_{\epsilon_{i1}}^{\epsilon_{i2}} \sigma : d\epsilon_i = (\rho \nu B \theta_s + k) (1 + 0.5 B) + U. \quad (40)$$

Simple analytical results can be obtained as well at variable pressure, if we assume $\alpha_1 = \alpha_2 = 0$. In this case in Eqs. (35) and (36) $\Delta\alpha = 0$, and at $\Delta\nu = 0$ Eqs. (37) - (40) are valid at

$$A = k/\rho\nu, \quad B = -\Delta s_o/\nu, \quad A/B = -k/\rho\Delta s_o, \quad U = \rho(\Delta\psi_o + \Delta s_o\theta_o). \quad (41)$$

4. CONDITIONS FOR NUCLEATION AND INTERFACE PROPAGATION

Consider a volume V of multiphase material with a boundary S . Let on one part of surface S the stress vector $\mathbf{p}$ be prescribed and on the other part the velocity vector $\mathbf{v}$ be given, but mixed boundary conditions are also possible. Assume that in some volume V_n with the fixed boundary Σ_n , due to PT during the time Δt , the new nuclei appeared.

For each point of nuclei V_n PT criterion (16) should be meet. Integrating this criterion over the volume V_n we obtain the necessary condition of *nucleation*

$$\int_{V_n} X dV_n = \int_{V_n} k dV_n, \quad (42)$$

or in explicit form

$$\begin{aligned} \int_{V_n} \int_{\mathbf{F}_1}^{\mathbf{F}_2} \mathbf{P}^t : d\mathbf{F} dV_n &= \int_t^{t+\Delta t} \int_{\Sigma_n} \mathbf{p} \cdot \mathbf{v} d\Sigma_n dt = \int_{V_n} \rho (\psi_2 - \psi_1) dV_n + \int_{V_n} \int_{\theta_1}^{\theta_2} \rho s d\theta dV_n + \\ &+ \int_{V_n} \int_t^{t+\Delta t} (X_p : \dot{\mathbf{F}}_p + X_g : \dot{\mathbf{g}}) dt dV_n + \int_{V_n} k dV_n, \end{aligned} \quad (43)$$

where $\mathbf{v}$ is the velocity on Σ_n from the side of nucleus. Note that Gauss theorem was used. Eq. (43) is a necessary condition for nucleations, because from the point of view of a stable post-bifurcation deformation process in the whole volume V_n , at the same boundary data increment another process (e.g., nucleation in another volume, interface propagation and so on) can be more stable [8, 9].

Assume that the volume V_n is obtained by *interface* Σ propagation with a normal velocity v_n during time Δt , i.e. it is bounded by surfaces Σ_t and $\Sigma_{t+\Delta t}$ at time t and $t + \Delta t$ respectively, as well as by two lateral infinitesimal surfaces with the heights $v_n \Delta t$. Let us transform the stress work integral in Eq. (43).

On the moving coherent interface the position vector and the traction vector $\mathbf{p}$ are continuous, $\mathbf{p}_2 = \mathbf{p}_1$, and due to compatibility condition [6, 8, 9]

$$[\mathbf{F}] = -[\mathbf{v}] \mathbf{n} / v_n, \quad \text{whence} \quad [\mathbf{v}] = -[\mathbf{F}] \cdot \mathbf{n} v_n \quad \text{and} \quad [\mathbf{F}] = [\mathbf{F}] \cdot \mathbf{n} \mathbf{n}. \quad (44)$$

Here $\mathbf{n}$ is the unit normal to the interface, $[\mathbf{a}] := \mathbf{a}_2 - \mathbf{a}_1$. Then neglecting all the terms of order Δt^2 we obtain

$$\begin{aligned} \int_t^{t+\Delta t} \int_{\Sigma} \mathbf{p} \cdot \mathbf{v} d\Sigma dt &= \left(\int_{\Sigma_{t+\Delta t}} \mathbf{p}_1 \cdot \mathbf{v}_1 d\Sigma_{t+\Delta t} - \int_{\Sigma_t} \mathbf{p}_2 \cdot \mathbf{v}_2 d\Sigma_t \right) \Delta t = - \int_{\Sigma_t} [\mathbf{p} \cdot \mathbf{v}] \Delta t d\Sigma_t, \\ -[\mathbf{p} \cdot \mathbf{v}] &= -\mathbf{p} \cdot [\mathbf{v}] = \mathbf{n} \cdot \mathbf{P}^t \cdot [\mathbf{F}] \cdot \mathbf{n} v_n = \mathbf{P}^t : [\mathbf{F}] \cdot \mathbf{n} \mathbf{n} v_n = \mathbf{P}^t : [\mathbf{F}] v_n, \end{aligned} \quad (45)$$

i.e. work-producing components of stress tensor are fixed in the course of PT. Substitution of Eq. (45) into Eq. (43) with account for $dV_n = v_n \Delta t d\Sigma_t$ results in

$$\begin{aligned} \int_{V_n} \mathbf{n} \cdot \mathbf{P}^t \cdot [\mathbf{F}] \cdot \mathbf{n} dV_n &= \int_{V_n} \mathbf{P}^t : [\mathbf{F}] dV_n = \int_{V_n} \rho [\psi] dV_n + \int_{V_n} \int_{\theta_1}^{\theta_2} \rho s d\theta dV_n + \\ &+ \int_{V_n} \int_t^{t+\Delta t} (X_p : \dot{\mathbf{F}}_p + X_g : \dot{\mathbf{g}}) dt dV_n + \int_{V_n} k dV_n \quad \text{and} \end{aligned} \quad (46)$$

$$\mathbf{n} \cdot \mathbf{P}^t \cdot [\mathbf{F}] \cdot \mathbf{n} = \mathbf{P}^t : [\mathbf{F}] = \rho [\psi] + \int_{\theta_1}^{\theta_2} \rho s d\theta + \int_t^{t+\Delta t} (\mathbf{X}_p : \dot{\mathbf{F}}_p + \mathbf{X}_g : \dot{\mathbf{g}}) dt + k. \quad (47)$$

Transition from an integral form (46) to a local one Eq. (47) is based on the assumption, that each point of interface can move independently of another point and the surface Σ can be chosen arbitrary. If the interface can move without variation of its shape only (e.g. as a plane), i.e. the motion of interface points are not mutually independent, then only the integral form (46) is valid.

Eqs. (43) and (47) generalize equations, postulated in [2, 3], for nonisothermal processes and media with internal variables. All simplifications from the Section 2, as well as temperature evolution equation are valid. Eq. (47) is valid at time $t + \Delta t$ as well [2, 3, 8, 9]. Note that at transition from the material point to the finite volume or surface additional energy terms can appear and should be taken into account. E.g., a change of *surface* energy should be added to right side of Eqs. (43) and (47). Additional dissipation *threshold* k_Σ due to intersection of interface with dislocations, point defects, grains and subgrains boundaries should be added to k in Eq. (47).

Note, that Eqs. (43) and (47) are valid for *noncoherent* PT with small jump of displacement as well, since we are using the velocity vector $\mathbf{v}$ from the side of nucleus, i.e. the rate of relative sliding along the interface $[\mathbf{v}]^s$ is excluded from consideration and $[\mathbf{v}]$ should always meet the compatibility condition. We can define the total jump of velocity across the interface $[\mathbf{v}]^T = [\mathbf{v}] + [\mathbf{v}]^s$ and can use for the definition of $[\mathbf{v}]^s$ equations and extremum principles derived in [8, 9].

5. THE POSTULATE OF REALIZABILITY

PT criterion (42) (or its explicit forms (43), (46) and (47)) is only one scalar equation, which is not sufficient for the determination of all unknown parameters. To determine all unknown parameters $\mathbf{b}$, e.g. position, shape and orientation of nucleus, jump of $\mathbf{F}$, transformation $\mathbf{F}_t$ and plastic deformation $\mathbf{F}_p$ gradients, related with $\mathbf{F}_p$ temperature evolution, as well as functions $\mathbf{F}(\xi)$, $\mathbf{F}_t(\xi)$, $\mathbf{F}_p(\xi)$, $\theta(\xi)$ and so on, let us use the postulate of realizability [3, 4, 8, 9].

Let for the given boundary conditions

$$\int_{V_n} \mathbf{X}(\mathbf{b}^*) dV_n - \int_{V_n^*} k(\mathbf{b}^*) dV_n < 0 \quad \forall \mathbf{b}^* \quad (48)$$

for all possible PT parameters $\mathbf{b}^*$, i.e. PT does not occur. If in the course of variation of boundary conditions the condition (42) is fulfilled the first time for some of parameters $\mathbf{b}$, then PT will occur with this $\mathbf{b}$ (if condition (42) is not violated in the course of PT, e.g. interface propagation).

If, in the course of variation of boundary conditions the equality (42) is met for one or several $\mathbf{b}$, then for arbitrary other $\mathbf{b}^*$ inequality (48) should be held, as in the opposite case for this $\mathbf{b}^*$ condition (42) had to be met before it was satisfied for $\mathbf{b}$. Consequently, we obtain the extremum principle

$$\int_{V_n} \mathbf{X}(\mathbf{b}) dV_n - \int_{V_n} k(\mathbf{b}) dV_n = 0 > \int_{V_n^*} \mathbf{X}(\mathbf{b}^*) dV_n - \int_{V_n^*} k(\mathbf{b}^*) dV_n, \quad (49)$$

for determination of all unknown parameters $\mathbf{b}$. Explicit form of principle (49) looks as

$$\begin{aligned} & \int_{V_n} \int_{\mathbf{F}_1}^{\mathbf{F}_2} \mathbf{P}^t : d\mathbf{F} dV_n - \int_{V_n} \rho(\psi_2 - \psi_1) dV_n - \int_{V_n} \int_{\theta_1}^{\theta_2} \rho s d\theta dV_n - \\ & - \int_{V_n} \int_t^{t+\Delta t} (\mathbf{X}_p : \dot{\mathbf{F}}_p + \mathbf{X}_g : \dot{\mathbf{g}}) dt dV_n - \int_{V_n} k dV_n = 0 > \end{aligned}$$

$$\begin{aligned}
& \int_{V_n^*} \int_{F_1^*}^{F_2^*} \mathbf{P}^{t*} : d\mathbf{F}^* dV_n - \int_{V_n^*} \rho (\psi_2^* - \psi_1^*) dV_n - \int_{V_n^*} \int_{\theta_1^*}^{\theta_2^*} \rho s^* d\theta^* dV_n - \\
& - \int_{V_n^*} \int_t^{t+\Delta t} (\mathbf{X}_p^* : \dot{\mathbf{F}}_p^* + \mathbf{X}_g^* : \dot{\mathbf{g}}^*) dt dV_n - \int_{V_n^*} k^* dV_n
\end{aligned} \quad (50)$$

for nucleation and as

$$\begin{aligned}
\mathbf{P}^t : [\mathbf{F}] &= \rho [\psi] - \int_{\theta_1}^{\theta_2} \rho s d\theta - \int_t^{t+\Delta t} (\mathbf{X}_p : \dot{\mathbf{F}}_p + \mathbf{X}_g : \dot{\mathbf{g}}) dt - k = 0 > \\
\mathbf{P}^{t*} : [\mathbf{F}^*] &= \rho [\psi^*] - \int_{\theta_1^*}^{\theta_2^*} \rho s^* d\theta^* - \int_t^{t+\Delta t} (\mathbf{X}_p^* : \dot{\mathbf{F}}_p^* + \mathbf{X}_g^* : \dot{\mathbf{g}}^*) dt - k^*
\end{aligned} \quad (51)$$

for interface propagation. In the particular case of nondissipative materials and isothermal processes, at small strains and equal elastic moduli, when PT occurs at constant stresses, the inequality (50) is equivalent to the Patel and Cohen condition $\sigma : \epsilon_t > \sigma : \epsilon_t^*$ [10].

6. MODEL PROBLEM

Let us consider the nucleation of a spherical inclusion with the radius R in an infinite elasto-perfectly plastic body under applied external pressure p . Elastic properties of parent and new phases are the same, $\alpha_1 = \alpha_2 = 0$. A similar problem is considered e.g. in [2], but our results will differ due to the new PT criterion and by taking into account the temperature variation in the nucleus.

Let $\epsilon_t = \epsilon_o I$. Then the pressure $\tilde{p}$ in a nucleus is determined by formulas [2]:

$$\text{in elastic region} \quad \tilde{p}_e = p - \frac{\epsilon_o}{C}, \quad \epsilon_o \leq \epsilon_o' := \frac{2}{3} \sigma_Y C; \quad (52)$$

$$\text{in plastic region} \quad \tilde{p}_p = p - \frac{2}{3} \sigma_Y \left(\ln \frac{3\epsilon_o}{2\sigma_Y C} + 1 \right), \quad \epsilon_o > \epsilon_o'. \quad (53)$$

Here $C = \frac{3(1-\nu)}{2E}$, E is Young's modulus, ν is Poisson's ratio, σ_Y is the yield stress of parent phase, ϵ_o' is the strain corresponding to the onset of plastic flow in the parent phase. Note that σ_Y can be positive or negative and due to the condition $\frac{3\epsilon_o}{2\sigma_Y C} > 0$ the signs of σ_Y and ϵ_o coincide.

Eqs. (37) – (39) for temperature variation and the PT criterion are valid with the constants defined by Eq. (41). Let us calculate the work integral

$$\begin{aligned}
\int_{\epsilon_{t1}}^{\epsilon_{t2}} \sigma : d\epsilon_t &= 3 \int_0^{\epsilon_o} \tilde{p} d\epsilon_o = 3 \int_0^{\epsilon_o'} \tilde{p}_e d\epsilon_o + 3 \int_{\epsilon_o'}^{\epsilon_o} \tilde{p}_p d\epsilon_o = \\
&= 3p\epsilon_o - \frac{2}{3} \sigma_Y^2 C - 2\sigma_Y \epsilon_o \ln \frac{3\epsilon_o}{2\sigma_Y C}.
\end{aligned} \quad (54)$$

Substituting Eq.(54) in Eq. (39) we obtain the PT pressure

$$p = \frac{2}{3} \sigma_Y \left(\frac{\sigma_Y C}{3\epsilon_o} + \ln \frac{3\epsilon_o}{\sigma_Y C} \right) + \frac{\rho \nu}{3\epsilon_o} \left(\frac{A}{B} + \theta_s \right) (\exp B - 1) + \frac{U}{3\epsilon_o}. \quad (55)$$

For the description of PT progress we can consider the appearance of a new martensitic nucleus in a austenite + martensite mixture. In the first approximation, neglecting the energy of internal stresses

in a mixture and assuming $\sigma_Y = c\sigma_{YM} + (1 - c)\sigma_{YA}$, where c is a volume fraction of martensite, σ_{YA} and σ_{YM} are the yield stresses of austenite and martensite, we can use Eq. (55). As for steels σ_{YM} is several times of σ_{YA} , then PT pressure should be increased significantly for the increase of the martensite fraction. At $p \equiv 0$ Eq. (55) describes temperature θ_s variation for the reaching of volume fraction c . As σ_Y increases in several times with growth of c , after some c the temperature θ_s , determined from Eq. (55), can be less than 0 K . This means that some residual austenite can not be transformed into martensite due to cooling, which is in agreement with *experiments* for steels.

If we take into account significant increase of σ_{YA} and σ_{YM} with the temperature decrease [10], then at some c Eq. (55) can have no solution with respect to θ_s , while at decreasing θ_s the increase of $\Delta\psi^\theta$ is less than increase of resistance force, related with σ_Y . This means that PT is impossible at temperature, less than some critical one, which is also in agreement with *experiments*. A similar way of explanation for the existence of martensite finish temperature, but without using the explicit expression for PT criterion (e.g. Eq. (55)), was reported in [11].

7. CONCLUDING REMARKS

A developed finite strain theory of PT in the material point of inelastic continuum allows us a consistent derivation of nucleation and interface propagation conditions for rather general situation and arbitrary inelastic materials. Thereby, the temperature variation plays a very important role. When we neglect the temperature variation, in a problem considering PT in a thin layer under prescribed normal pressure and tangential displacement [4, 12], PT occurs in an infinitesimal thin layer, and plastic shear tends to infinity. Taking into the temperature variation due to PT results in a finite width of a layer and plastic shear [12]. Note that a simplified method of taking into account the effect of a temperature increase on PT condition is described in [2]. At the next step the simplified models of transforming volume should be developed, e.g. macroscopically uniformly [3] or with constant strain gradient deformed volume [13], with account for inertia effects [6, 13], with a wave mechanism of nucleus growth and so on.

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