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THEORY OF MARTENSITIC PHASE TRANSFORMATIONS IN INELASTIC MATERIALS IN LOCAL DESCRIPTION

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1. Introduction

A number of descriptions of phase transitions (PT) have been proposed: a jump condition 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, 2]. But a description of PT as a thermomechanical deformation process in a *material point* is lacking. This fact does not allow to apply 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, 2] is difficult without a proper theory for the material point. In the present paper a general theory of PT in the material point of a simple inelastic body is developed. It is found that a standard thermodynamical approach can not 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 the PT criterion.

Nucleation and interface propagation conditions are derived, which generalize the conditions, postulated in [2, 3], for nonisothermal processes and media with internal variables. A model problem is solved. Some preliminary results were reported in [4].

2. Thermodynamics of martensitic phase transitions in a material point

Introduction of an internal time. Let us consider a uniformly deformed infinitesimal volume (material point) in a process of martensitic PT. We will consider simple materials only, i.e. a material response in the given point is independent of thermomechanical parameters in other points. We assume an additive decomposition of a total strain tensor $\boldsymbol{\varepsilon}$ into elastic $\boldsymbol{\varepsilon}_e$, plastic $\boldsymbol{\varepsilon}_p$, thermal

$\boldsymbol{\varepsilon}_\theta$ and transformational $\boldsymbol{\varepsilon}_t$ parts, i.e.

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p + \boldsymbol{\varepsilon}_\theta + \boldsymbol{\varepsilon}_t \,. \tag{1}$$

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

$$\xi \ := \ tr\, \boldsymbol{\varepsilon}_t / tr\, \boldsymbol{\varepsilon}_{t\,max} \qquad \text{or} \qquad \xi \ := |\, dev\, \boldsymbol{\varepsilon}_t \,| \,/\, |\, dev\, \boldsymbol{\varepsilon}_{t\,max} \,|, \tag{2}$$

although other definitions are also possible. Definition $(2)_1$ is natural for dilatational PT (dev $\boldsymbol{\varepsilon}_t = 0$), definition $(2)_2$ suits for the case $tr\, \boldsymbol{\varepsilon}_t = 0$. The internal time ξ plays a role for the consideration of the uniformly deformed material point, similar to that of a volume fraction of martensite for the averaged description of PT.

Let us define the specific Helmholtz free energy

$$\psi = \psi \left(\boldsymbol{\varepsilon}_e (\xi),\ \theta (\xi),\ \boldsymbol{\varepsilon}_p (\xi),\ \boldsymbol{g} (\xi),\ \boldsymbol{\varepsilon}_t (\xi),\ \xi \right) \,, \tag{3}$$

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

$$\mathcal{D} = \boldsymbol{\sigma} \,\boldsymbol{:}\, \dot{\boldsymbol{\varepsilon}} - \rho \,\dot{\psi} - \rho\, s\, \dot{\theta} - \frac{\boldsymbol{\nabla}\, \theta}{\theta} \boldsymbol{\cdot} \boldsymbol{h} \ge 0 \,. \tag{4}$$

Here $\mathcal{D}$ is the rate of dissipation per unit volume, ρ mass density at $\xi = 0$, s the entropy, $\boldsymbol{\nabla}\, \theta$ the temperature gradient, $\boldsymbol{h}$ the heat flux. The substitution of the rate of free energy

$$\dot{\psi} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} \boldsymbol{:} \dot{\boldsymbol{\varepsilon}}_e + \frac{\partial \psi}{\partial \theta} \dot{\theta} + \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_p} \boldsymbol{:} \dot{\boldsymbol{\varepsilon}}_p + \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_t} \boldsymbol{:} \dot{\boldsymbol{\varepsilon}}_t + \frac{\partial \psi}{\partial \boldsymbol{g}^t} \boldsymbol{:} \dot{\boldsymbol{g}} + \frac{\partial \psi}{\partial \xi} \dot{\xi} \tag{5}$$

with taking into account the additive decomposition of $\boldsymbol{\varepsilon}$ and $\dot{\boldsymbol{\varepsilon}}_\theta = \frac{\partial \boldsymbol{\varepsilon}_\theta}{\partial \theta} \dot{\theta} + \frac{\partial \boldsymbol{\varepsilon}_\theta}{\partial \xi} \dot{\xi}$ in Eq. (4) yields

$$\begin{aligned} \mathcal{D} \ = \ & \left(\boldsymbol{\sigma} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} \right) \boldsymbol{:} \dot{\boldsymbol{\varepsilon}}_e - \rho \left(s + \frac{\partial \psi}{\partial \theta} - \frac{\boldsymbol{\sigma}}{\rho} \boldsymbol{:} \frac{\partial \boldsymbol{\varepsilon}_\theta}{\partial \theta} \right) \dot{\theta} + \left(\boldsymbol{\sigma} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_p} \right) \boldsymbol{:} \dot{\boldsymbol{\varepsilon}}_p - \rho \frac{\partial \psi}{\partial \boldsymbol{g}^t} \boldsymbol{:} \dot{\boldsymbol{g}} - \frac{\boldsymbol{\nabla} \theta}{\theta} \boldsymbol{\cdot} \boldsymbol{h} + \\ + \ & \left(\boldsymbol{\sigma} \boldsymbol{:} \frac{\partial \left(\boldsymbol{\varepsilon}_t + \boldsymbol{\varepsilon}_\theta \right)}{\partial \xi} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_t} \boldsymbol{:} \frac{\partial \boldsymbol{\varepsilon}_t}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi} \right) \dot{\xi} \ge 0 \,. \end{aligned} \tag{6}$$

Here a superscript t denote transposition, dots mean contractions of the tensors.

The assumption that the rate of dissipation is independent of $\dot{\boldsymbol{\varepsilon}}_e$ and $\dot{\theta}$ results in the hyperelasticity law and expression for entropy, as well as in a reduced dissipative inequality:

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} \,; \qquad s = \frac{\boldsymbol{\sigma}}{\rho} \boldsymbol{:} \frac{\partial \boldsymbol{\varepsilon}_\theta}{\partial \theta} - \frac{\partial \psi}{\partial \theta} \,; \tag{7}$$

$$\mathcal{D} = \boldsymbol{X}_p \boldsymbol{:} \dot{\boldsymbol{\varepsilon}}_p + \boldsymbol{X}_g \boldsymbol{:} \dot{\boldsymbol{g}} + \boldsymbol{X}_h \boldsymbol{\cdot} \boldsymbol{h} + X_\xi\, \dot{\xi} \ge 0 \,, \tag{8}$$

$$\text{where} \qquad \boldsymbol{X}_p = \boldsymbol{\sigma} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_p} \,; \qquad \boldsymbol{X}_g = - \rho \frac{\partial \psi}{\partial \boldsymbol{g}^t} \,; \qquad \boldsymbol{X}_h = - \frac{\nabla \theta}{\theta} \qquad \text{and} \tag{9}$$

$$X_\xi = \boldsymbol{\sigma} \boldsymbol{:} \frac{\partial \left(\boldsymbol{\varepsilon}_t + \boldsymbol{\varepsilon}_\theta \right)}{\partial \xi} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_t} \boldsymbol{:} \frac{\partial \boldsymbol{\varepsilon}_t}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi} \tag{10}$$

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

$$\dot{\boldsymbol{\varepsilon}}_p = \boldsymbol{f}_p \left(\boldsymbol{X}_p \,,\ \xi \right) \,; \qquad \dot{\boldsymbol{g}} = \boldsymbol{f}_g \left(\boldsymbol{X}_g \,,\ \xi \right) \,; \qquad \boldsymbol{h} = \boldsymbol{f}_h \left(\boldsymbol{X}_h \,,\ \xi \right) \,; \qquad \dot{\xi} = f_\xi \left(X_\xi ,\ \xi \right) \,. \tag{11}$$

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 allowance for mutual influences of all thermomechanical processes can be made in a standard way.

Averaging over the characteristic time. We assume that the condition $\dot{\xi} = 0$ is valid at $X_\xi = 0$ only. Then it is possible to describe the equilibrium PT $\left(\dot{\xi} \to 0\right)$ with the equation $X_\xi = 0$, i.e.

$$X_\xi = \boldsymbol{\sigma} : \frac{\partial\left(\boldsymbol{\varepsilon}_t + \boldsymbol{\varepsilon}_\theta\right)}{\partial \xi} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_t} : \frac{\partial \boldsymbol{\varepsilon}_t}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi} = 0 \,. \tag{12}$$

Eq. (12) allows to determine the equilibrium stress variation $\boldsymbol{\sigma}\left(\xi,\ \theta(\xi)\right)$ in the course of PT. If the actual stress variation follows this dependence, then 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 $\xi = 1$ do we have the stable equilibrium. At $0 < \xi < 1$ a nonequilibrium process proceeds, which requires energy and stress fluctuations.

We see that a standard thermodynamical approach can not be applied, because it does not describe the experiments. It is necessary to average the thermodynamical parameters, related to PT, over some characteristic time in order to filter off these fluctuations. It is reasonable to adopt a duration of PT t_p as the characteristic time. We introduce the averaged dissipation rate due to the PT

$$\mathcal{D}_\xi := \frac{1}{t_p} \int\limits_o^{t_p} X_\xi \, \dot{\xi} \, dt = \frac{1}{t_p} \int\limits_o^{1} X_\xi \, d\xi = \frac{X}{t_p} = X \, \dot{\chi} \,, \quad \text{where} \quad X := \int\limits_o^{1} X_\xi \, d\xi \,, \qquad \dot{\chi} := \frac{1}{t_p} \tag{13}$$

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 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

$$X = \int_{\boldsymbol{\varepsilon}_{t\,1}}^{\boldsymbol{\varepsilon}_{t\,2}} \left(\boldsymbol{\sigma} - \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_t}\right) : d\boldsymbol{\varepsilon}_t + \int_0^1 \left(\boldsymbol{\sigma} : \frac{\partial \boldsymbol{\varepsilon}_\theta}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi}\right) d\xi = 0 \,. \tag{14}$$

The indices 1 and 2 denote the values before and after PT. Eq. (14) is the PT criterion for PT without dissipation.

Existence of a threshold value of the dissipative force. Let $X \neq 0$ and $\dot{\chi} = f\left(X\,,\, ...\right)$. There are only two possibility for the behaviour of the function f as $\dot{\chi} \to 0$.

1. Let the condition $\dot{\chi} = 0$ be valid at $X = 0$ only, then the macroscopically equilibrium PT $(\dot{\chi} \to 0)$ can be described with the equation $X = 0$.

2. Let

$$\begin{array}{llllll} & & \text{at} \quad \dot{\chi} = 0 & k_{2\to 1} \le X \le k_{1\to 2}\,, & & \\ \text{at} \quad \dot{\chi} > 0 & & X = k_{1\to 2} > 0\,, & \text{at} \quad \dot{\chi} < 0 & & X = k_{2\to 1} < 0\,, \end{array} \tag{15}$$

where $k_{1\to 2}$ and $k_{2\to 1}$ are the threshold values of X at the direct and the reverse PT, which can depend on θ, $\dot{\chi}$, $\boldsymbol{\varepsilon}_p$, $\boldsymbol{g}$, ... and should be determined experimentally. In this case there is *hysteresis*, i.e. direct and reverse PT begin at different values X and between these values PT is impossible. In the first case there is no hysteresis. Since practically all martensitic transformations exhibit hysteresis, we adopt the second variant. Eq. (15) means that the calculated value of the dissipation increment due to PT reaches its experimentally determined value. When X reaches k the rate $\dot{\chi}$ has a jump till $10^6 \div 10^{11}\ s^{-1}$, because $t_p \simeq 10^6 \div 10^{11}\ s$. Eq. (15) is the final expression for the PT criterion.

Remark. In the experiments the macroscopic parameters for the finite volume (not for material point) are usually determined, e.g. force, averaged stress. For plastic materials the hysteresis of this macroscopic parameter can occur at $k_{1\to 2} = k_{2\to 1} = 0$ as well, see an example in [3], and the above arguments for the existence of the dissipative threshold are invalid. For elastic materials the hysteresis of macroscopic parameters can not be obtained theoretically at $k_{1\to 2} = k_{2\to 1} = 0$ [5], but practically it always exists in the experiments. Consequently the arguments leading to the existence of the dissipative threshold are noncontradictory.

Alternative equivalent expressions for X. From Eqs. (5) and (7) it follows

$$\dot\psi = \frac{1}{\rho}\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}_e + \left(\frac{1}{\rho}\boldsymbol{\sigma}:\frac{\partial \boldsymbol{\varepsilon}_\theta}{\partial\theta} - s\right)\dot\theta + \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p}:\dot{\boldsymbol{\varepsilon}}_p + \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_t}:\dot{\boldsymbol{\varepsilon}}_t + \frac{\partial\psi}{\partial\boldsymbol{g}^t}:\dot{\boldsymbol{g}} + \frac{\partial\psi}{\partial\xi}\dot\xi\,. \tag{16}$$

The substitution of the expression $-\rho\frac{\partial\psi}{\partial\xi}\dot\xi - \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_t}:\dot{\boldsymbol{\varepsilon}}_t$ from Eq. (16) in $X_\xi\,\dot\xi$ yields

$$X_\xi\,\dot\xi \;=\; \boldsymbol{\sigma}:(\dot{\boldsymbol{\varepsilon}}_e + \dot{\boldsymbol{\varepsilon}}_\theta + \dot{\boldsymbol{\varepsilon}}_t) - \rho\,\dot\psi - \rho\, s\,\dot\theta + \rho\frac{\partial\psi}{\partial\boldsymbol{g}^t}:\dot{\boldsymbol{g}} + \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p}:\dot{\boldsymbol{\varepsilon}}_p \qquad \text{and} \tag{17}$$

$$X = \int\limits_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2}\boldsymbol{\sigma}:d\,(\boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_\theta + \boldsymbol{\varepsilon}_t) - \rho\,(\psi_2 - \psi_1) - \int\limits_{\theta_1}^{\theta_2}\rho s\, d\theta + \int\limits_{\boldsymbol{g}_1}^{\boldsymbol{g}_2}\rho\frac{\partial\psi}{\partial\boldsymbol{g}^t}:d\boldsymbol{g} + \int\limits_{\boldsymbol{\varepsilon}_{p\,1}}^{\boldsymbol{\varepsilon}_{p\,2}}\rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p}:d\boldsymbol{\varepsilon}_p = k\,. \tag{18}$$

An addition of the expression $\boldsymbol{\sigma}:d\boldsymbol{\varepsilon}_p$ to the first term in Eq. (18) and the subtraction $\boldsymbol{\sigma}:d\boldsymbol{\varepsilon}_p$ from the last term results in

$$X = \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2}\boldsymbol{\sigma}:d\boldsymbol{\varepsilon} - \rho\,(\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2}\rho\, s\, d\theta - \int_0^{t_p}(\boldsymbol{X}_p:\dot{\boldsymbol{\varepsilon}}_p + \boldsymbol{X}_g:\dot{\boldsymbol{g}})\; dt \;=\; k\,. \tag{19}$$

The expressions (18) and (19) are sometimes more convenient for the analysis than Eq. (14). At $\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p} = 0$ Eq. (18) is more suitable for application, because in this case the plastic strain $\boldsymbol{\varepsilon}_p$ disappears completely. Eq. (19) shows that X is the total dissipation increment minus plastic dissipation increment and the dissipation increment due to the internal variables. Eq. (19) is more appropriate when the moving interface is considered and the Hadamar compatibility condition for $\boldsymbol{\varepsilon}_i$ is taken into account (see Section 3).

For elastic materials without internal variables and for isothermal processes, at $k = 0$ it follows from Eq. (19)

$$\int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2}\boldsymbol{\sigma}:d\boldsymbol{\varepsilon} \;=\; \rho\;(\psi_2 - \psi_1)\;. \tag{20}$$

If PT proceeds at constant stress $\boldsymbol{\sigma}_o$, then $\boldsymbol{\sigma}_o:\,(\boldsymbol{\varepsilon}_2 - \boldsymbol{\varepsilon}_1) \;=\; \rho\;(\psi_2 - \psi_1)$. This is the Maxwell rule. Consequently Eq. (15) is a generalization of the Maxwell rule for dissipative materials, nonisothermal processes and for variable stresses.

Let

$$\rho\,\psi_i \;=\; 0.5\,\boldsymbol{\varepsilon}_{e\,i}:\boldsymbol{E}_i:\boldsymbol{\varepsilon}_{e\,i} + \rho\,\psi_i^\theta \;=\; \rho\,\psi_i^e \;+\; \rho\,\psi_i^\theta\;, \qquad\qquad i \;=\; 1,\;2\;, \tag{21}$$

where ψ_i^e and ψ_i^θ are the elastic and thermal parts of free energy, $\boldsymbol{E}_i$ the elasticity tensors. Since

$$\begin{aligned}\int\limits_{\boldsymbol{\varepsilon}_{e\,1}}^{\boldsymbol{\varepsilon}_{e\,2}}\boldsymbol{\sigma}:d\boldsymbol{\varepsilon}_e \;&=\; \int\limits_{\boldsymbol{\varepsilon}_{e\,1}}^{\boldsymbol{\varepsilon}_{e\,2}}\boldsymbol{\varepsilon}_e:\boldsymbol{E}:d\boldsymbol{\varepsilon}_e \;=\; 0.5\int\limits_{\boldsymbol{\varepsilon}_{e\,1}}^{\boldsymbol{\varepsilon}_{e\,2}} d\,(\boldsymbol{\varepsilon}_e:\boldsymbol{E}:\boldsymbol{\varepsilon}_e) - 0.5\int\limits_0^1\boldsymbol{\varepsilon}_e:d\boldsymbol{E}\,(\xi)\,:\boldsymbol{\varepsilon}_e \;=\\ &=\; \rho\,(\psi_2^e - \psi_1^e) - 0.5\int\limits_0^1\boldsymbol{\varepsilon}_e:d\boldsymbol{E}\,(\xi)\,:\boldsymbol{\varepsilon}_e\;,\end{aligned} \tag{22}$$

it follows then from Eq.(18)

$$\begin{aligned} X \; &= \int\limits_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma} : d\,(\boldsymbol{\varepsilon}_\theta + \boldsymbol{\varepsilon}_t) \, - \, 0.5 \int\limits_{0}^{1} \boldsymbol{\varepsilon}_e : d\boldsymbol{E}\,(\xi) : \boldsymbol{\varepsilon}_e \, - \, \rho\left(\psi_2^\theta - \psi_1^\theta\right) - \int\limits_{\theta_1}^{\theta_2} \rho\, s\, d\theta \, + \\ &+ \int\limits_{\boldsymbol{g}_1}^{\boldsymbol{g}_2} \rho\, \frac{\partial\,\psi}{\partial\,\boldsymbol{g}^t} : d\boldsymbol{g} + \int\limits_{\boldsymbol{\varepsilon}_{p\,1}}^{\boldsymbol{\varepsilon}_{p\,2}} \rho\, \frac{\partial\,\psi}{\partial\,\boldsymbol{\varepsilon}_p} : d\boldsymbol{\varepsilon}_p \, = \, k\,. \end{aligned} \tag{23}$$

When $\boldsymbol{E}_1 \, = \, \boldsymbol{E}_1 \, = \, \boldsymbol{const}$ (e.g. independent of θ, $\boldsymbol{\varepsilon}_p\,, \ldots$), then the term with $d\boldsymbol{E}$ disappear. 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 will assume that for isothermal processes $\theta \, = \, \theta_o$ and we obtain $\boldsymbol{\varepsilon}_\theta \, = \, 0$. Consequently, for $\dfrac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p} \, = \, \dfrac{\partial\psi}{\partial\boldsymbol{g}} \, = \, 0$ and isothermal processes we have

$$X \, = \int_{\boldsymbol{\varepsilon}_{t\,1}}^{\boldsymbol{\varepsilon}_{t\,2}} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}_t \, - \, \rho\,\left(\psi_2^\theta - \psi_1^\theta\right)\,. \tag{24}$$

There is one *general* problem: for calculation of integrals in Eq. (19) it is necessary to determine the stress variation (as well as $\boldsymbol{\varepsilon}_p$, $\boldsymbol{g}$, θ) during PT (variation of $\boldsymbol{\varepsilon}_t$) by solving of a corresponding boundary–value problem.

Determination of temperature. For the determination of a temperature variation in the course of PT we can use an energy balance equation (the first law of thermodynamics) or an entropy balance equation

$$\rho\,\theta\,\dot{s} \, = \, \mathcal{D} + \operatorname{div}\boldsymbol{h} + \frac{\boldsymbol{\nabla}\,\theta}{\theta} \cdot \boldsymbol{h}\,. \tag{25}$$

Substitution of an expression (8) for the rate of dissipation $\mathcal{D}$ in Eq. (25) yields

$$\rho\,\theta\,\dot{s} \, = \, \operatorname{div}\boldsymbol{h} \, + \, \boldsymbol{X}_p : \dot{\boldsymbol{\varepsilon}}_p \, + \, \boldsymbol{X}_g : \dot{\boldsymbol{g}} \, + \, X_\xi\,\dot{\xi}\,. \tag{26}$$

According to Eq. $(7)_2$ $s \, = \, s\,(\theta\,, \, \boldsymbol{\sigma}\,, \, \boldsymbol{g}\,, \, \boldsymbol{\varepsilon}_p\,, \, \xi)$. Substitution of this expression and Eq. $(11)_3$ for the heat flux into Eq. (26) leads to the temperature evolution equation

$$\begin{aligned} \rho\,\nu\,\dot{\theta} \;\; &= \;\; \operatorname{div}\boldsymbol{f}_h\,\left(-\frac{\boldsymbol{\nabla}\,\theta}{\theta}\right) + \left(\boldsymbol{X}_p - \rho\,\frac{\partial\,s}{\partial\,\boldsymbol{\varepsilon}_p}\,\theta\right) : \dot{\boldsymbol{\varepsilon}}_p \, + \, \left(\boldsymbol{X}_g - \rho\,\frac{\partial\,s}{\partial\,\boldsymbol{g}}\,\theta\right) : \dot{\boldsymbol{g}} \, + \\ &+ \;\; \left(X_\xi - \rho\,\frac{\partial\,s}{\partial\,\xi}\,\theta\right)\,\dot{\xi} \, - \, \theta\,\frac{\partial\,s}{\partial\,\boldsymbol{\sigma}} : \dot{\boldsymbol{\sigma}}\,, \qquad \nu \, := \, \theta\,\frac{\partial\,s}{\partial\,\theta}\,, \end{aligned} \tag{27}$$

where ν is the specific heat. Due to the divergence term the temperature at the given point can be defined after formulation and solution of a boundary–value problem. Taking into account a very short duration of PT ($10^{-6} \, \div \, 10^{-11}$ s), the *adiabatic* process can be assumed (similar to the processes in shock waves). In this case $\operatorname{div}\boldsymbol{h} \, = \, 0$ and Eq. (27) 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 (19) and temperature evolution equation (27) is the following. All material properties, constitutive equations (11) and transformation strain $\boldsymbol{\varepsilon}_t\,(\xi)$ should be given as a function of ξ. Then assume that at some stress $\boldsymbol{\sigma}_s$ and temperature θ_s PT in the given point starts. Stress variation $\boldsymbol{\sigma}\,(\xi)$, as well as $\boldsymbol{\varepsilon}_p\,(\xi)$, $\boldsymbol{g}\,(\xi)$, 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. (27). 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 (15) allows us to determine (iteratively or explicitly) the temperature θ_s at the given

$\boldsymbol{\sigma}_s$ or one of the components of the stress tensor $\boldsymbol{\sigma}_s$ with the remaining five components of $\boldsymbol{\sigma}_s$ and the temperature θ_s given.

Let us consider some specifications and simplifications of Eq. (27). Assume the validity of Eq. (21) for the free energy with equal elastic properties of both phases and the following explicit expression for a thermal part of free energy [6]

$$\psi_1^\theta = \psi_{oi} - s_{oi}(\theta - \theta_o) - \nu_i\,\theta\,(\ln\theta/\theta_o - 1) - \nu_i\,\theta_o\,, \qquad i = 1,\ 2. \tag{28}$$

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. $(7)_2$ it follows

$$\rho\, s = \rho\, s_o(\xi) + \rho\,\nu(\xi)\ln\frac{\theta}{\theta_o} + \boldsymbol{\sigma}:\boldsymbol{\alpha}(\xi) \qquad \text{and} \qquad \theta\,\frac{\partial s}{\partial\theta} = \nu(\xi)\,, \tag{29}$$

i.e. the accepted Eq. $(27)_2$ 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. (28).

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

$$s_o = (1-\xi)\,s_{o1} + \xi\,s_{o2}\,, \qquad \nu = (1-\xi)\,\nu_1 + \xi\,\nu_2\,, \qquad \boldsymbol{\alpha}(\xi) = (1-\xi)\,\boldsymbol{\alpha}_1 + \xi\,\boldsymbol{\alpha}_2\,. \tag{30}$$

Then Eq. (27) can be transformed into the form

$$\begin{aligned}\rho\,\nu(\xi)\,\dot{\theta} &= (X_\xi - \rho\,\theta\,\Delta s_o - \rho\,\Delta\nu\,\theta\ln\theta/\theta_o - \boldsymbol{\sigma}:\Delta\boldsymbol{\alpha}\,\theta)\,\dot{\xi} - \\ &- \dot{\boldsymbol{\sigma}}:\boldsymbol{\alpha}(\xi)\,\theta + \boldsymbol{X}_p:\dot{\boldsymbol{\varepsilon}}_p + \boldsymbol{X}_g:\dot{\boldsymbol{g}}\,,\end{aligned} \tag{31}$$

where $\Delta\boldsymbol{b} := \boldsymbol{b}_2 - \boldsymbol{b}_1$. If ψ_{oi} are independent of $\boldsymbol{g}$ and $\boldsymbol{\varepsilon}_p$, then $\boldsymbol{X}_g = 0$ and $\boldsymbol{X}_p = \boldsymbol{\sigma}$. In this case Eq. (14) is the most convenient form of X. PT criterion results in

$$\begin{aligned}\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma}:d\boldsymbol{\varepsilon}_t &+ \int_0^1 \boldsymbol{\sigma}:\Delta\boldsymbol{\alpha}\,(\theta-\theta_o)\,d\xi + \rho\,(\Delta s_o - \Delta\nu)\int_0^1 \theta\,d\xi + \\ &+ \rho\,\Delta\nu\int_0^1 \theta\ln\frac{\theta}{\theta_o}\,d\xi = k + \rho\,\Delta\psi_o + \rho\,(\Delta s_o - \Delta\nu)\,\theta_o\,.\end{aligned} \tag{32}$$

Eq. (32) shows that the thermal expansion tensors of each phase have no effect on the PT criterion, only their difference contributes to the driving force. For an isothermal process at $\theta = \theta_o$ Eq. (32) coincides with Eq. (24) at $\left(\psi_2^\theta - \psi_1^\theta\right) = \Delta\psi_o$.

For isotropic $\boldsymbol{\alpha} = \alpha\boldsymbol{I}$ we have $\boldsymbol{\sigma}:\Delta\boldsymbol{\alpha} = 3\,\sigma_o\,\Delta\alpha$, $\dot{\boldsymbol{\sigma}}:\boldsymbol{\alpha} = 3\,\dot{\sigma}_o\,\alpha$, where $\boldsymbol{I}$ is a unit tensor, σ_o is a mean pressure and for fixed σ_o, for elastic materials and constant $X_\xi = k$ Eq. (31) is independent of the stress variation

$$\rho\,((1-\xi)\,\nu_1 + \xi\,\nu_2)\,\dot{\theta} = (k - \rho\,\theta\,\Delta s_o - \rho\,\Delta\nu\,\theta\ln\theta/\theta_o - 3\,\sigma_o\,\Delta\alpha\,\theta)\,\dot{\xi}\,. \tag{33}$$

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 complicated for analysis. In the case $\Delta\nu = 0$ we have

$$d\theta = (A + B\,\theta)\,d\xi \qquad \text{or} \qquad \theta = \left(\frac{A}{B} + \theta_s\right)\exp(B\,\xi) - \frac{A}{B}\,, \tag{34}$$

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

$$\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma}:d\boldsymbol{\varepsilon}_t = \rho\,\nu\,B\int_0^1 \theta\,d\xi + k + U\,, \tag{35}$$

where $U = \rho\,(\Delta\,\psi_o + \Delta\,s_o\,\theta_o) + 3\,\sigma_o\,\Delta\,\alpha\,\theta_o$, or taking into account Eq. (34)

$$\int_{\boldsymbol{\varepsilon}_{t\,1}}^{\boldsymbol{\varepsilon}_{t\,2}} \boldsymbol{\sigma} \boldsymbol{:} d\boldsymbol{\varepsilon}_t = \rho\nu\left(\frac{A}{B} + \theta_s\right)(\exp\,B - 1) - \rho\nu A + k + U = \rho\nu\,(\theta_f - \theta_s) - \rho\nu A + k + U\,, \tag{36}$$

where $\theta_f = \theta\,(1)$ is a final temperature after the end of PT, determined by Eq. (34) at $\xi = 1$. At small B we have $\exp\,B\,\xi = 1 + B\,\xi$ and

$$\theta = \theta_s + (A + B\,\theta_s)\;\xi\,; \qquad\qquad \int_{\boldsymbol{\varepsilon}_{t\,1}}^{\boldsymbol{\varepsilon}_{t\,2}} \boldsymbol{\sigma} \boldsymbol{:} d\boldsymbol{\varepsilon}_t = \rho\nu B\theta_s + k + U\,. \tag{37}$$

For rigid–plastic materials, when a plastic power can be expressed in the form $\boldsymbol{\sigma} \boldsymbol{:} \dot{\boldsymbol{\varepsilon}}_p = \boldsymbol{\sigma} \boldsymbol{:} \boldsymbol{\varepsilon}_p\dot{\xi}$ with a constant value of plastic work $A_p = \boldsymbol{\sigma} \boldsymbol{:} \boldsymbol{\varepsilon}_p$, than Eq. (34)–(37) are valid at $A = (k + A_p)/(\rho\nu)$. In Eq. (36) − $\rho\nu A + k = 0$ for elastic materials and $-\rho\nu A + k = A_p$ for rigid–plastic materials.

3. Conditions of 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 $\boldsymbol{p}$ be prescribed and on the other part the velocity vector $\boldsymbol{v}$ be given, but mixed boundary conditions are also possible. Assume that at 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 (15) should be met. Integrating this criterion over the volume V_n we obtain the necessary condition of *nucleation*

$$\int_{V_n} X\;dV_n = \int_{V_n} k\;dV_n\,, \tag{38}$$

or taking into account Eq. (19) for X

$$\int\limits_{V_n}\int\limits_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma} \boldsymbol{:} d\boldsymbol{\varepsilon}\,dV_n = \int\limits_{t}^{t+\Delta\,t}\int\limits_{\Sigma_n} \boldsymbol{p} \boldsymbol{\cdot} \boldsymbol{v}\;d\Sigma_n\;dt = \int\limits_{V_n} \rho\;(\psi_2 - \psi_1)\;dV_n + \int\limits_{V_n}\int\limits_{\theta_1}^{\theta_2} \rho\,s\;d\theta\;dV_n +$$

$$+ \int\limits_{V_n}\int\limits_{t}^{t+\Delta\,t} (\boldsymbol{X}_p \boldsymbol{:} \dot{\boldsymbol{\varepsilon}}_p + \boldsymbol{X}_g \boldsymbol{:} \dot{\boldsymbol{g}})\;dt\;dV_n + \int\limits_{V_n} k\;dV_n\,, \tag{39}$$

where $\boldsymbol{v}$ is the velocity on Σ_n from the side of nucleus. Note that Gauss theorem was used.

Assume that the volume V_n is obtained by *interface* Σ propagation with a normal velocity v_n during time $\Delta\,t$, 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. (39).

On the moving coherent interface the position vector and the traction vector $\boldsymbol{p}$ are continuous, $\boldsymbol{p}_2 = \boldsymbol{p}_1$, and due to compatibility condition

$$[\boldsymbol{F}] = -\,[\boldsymbol{v}]\;\boldsymbol{n}/v_n\,, \qquad \text{whence} \qquad [\boldsymbol{v}] = -\,[\boldsymbol{F}]\,\boldsymbol{\cdot n}\,v_n \qquad \text{and} \qquad [\boldsymbol{F}] = [\boldsymbol{F}]\;\boldsymbol{\cdot n n}\,. \tag{40}$$

Here $\boldsymbol{n}$ is the unit normal to the interface, $\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{\varepsilon} + \boldsymbol{\omega}$, $\boldsymbol{\omega}$ the rotation tensor, $[\boldsymbol{a}] := \boldsymbol{a}_2 - \boldsymbol{a}_1$. Then neglecting all the terms of order $\Delta\,t^2$ we obtain

$$\int\limits_{t}^{t+\Delta\,t}\int\limits_{\Sigma} \boldsymbol{p} \boldsymbol{\cdot} \boldsymbol{v}\;d\Sigma\;dt = \left(\int\limits_{\Sigma_{t+\Delta\,t}} \boldsymbol{p}_1 \boldsymbol{\cdot} \boldsymbol{v}_1\;d\Sigma_{t+\Delta\,t} - \int\limits_{\Sigma_t} \boldsymbol{p}_2 \boldsymbol{\cdot} \boldsymbol{v}_2\;d\Sigma_t\right)\Delta\,t = -\int\limits_{\Sigma_t} [\boldsymbol{p} \boldsymbol{\cdot} \boldsymbol{v}]\;\Delta\,t\;d\Sigma_t\,,$$

$$-\,[\boldsymbol{p} \boldsymbol{\cdot} \boldsymbol{v}] = -\boldsymbol{p} \boldsymbol{\cdot}\;[\boldsymbol{v}] = \boldsymbol{n} \boldsymbol{\cdot} \boldsymbol{\sigma} \boldsymbol{\cdot}\;[\boldsymbol{F}]\;\boldsymbol{\cdot n}\,v_n = \boldsymbol{\sigma} \boldsymbol{:}\;[\boldsymbol{F}]\;\boldsymbol{\cdot n n}\,v_n = \boldsymbol{\sigma} \boldsymbol{:}\;[\boldsymbol{\varepsilon}]\;v_n\,, \tag{41}$$

i.e. work–producing components of stress tensor are fixed in the course of PT. Substitution of Eq. (41) into Eq. (39) with account for $dV_n = v_n \Delta t \, d\Sigma_t$ results in

$$\boldsymbol{n} \cdot \boldsymbol{\sigma} \cdot [\boldsymbol{F}] \cdot \boldsymbol{n} = \boldsymbol{\sigma} : [\boldsymbol{\varepsilon}] = \rho [\psi] + \int_{\theta_1}^{\theta_2} \rho \, s \, d\theta + \int_{t}^{t+\Delta t} (\boldsymbol{X}_p : \dot{\boldsymbol{\varepsilon}}_p + \boldsymbol{X}_g : \dot{\boldsymbol{g}}) \, dt + k \, . \tag{42}$$

Eqs. (39) and (42) 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. (42) is valid at time $t + \Delta t$ as well [2, 3, 7]. 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-hand side of Eqs. (39) and (42). Eq. (42) is valid for *noncoherent* PT with small jump of displacement as well, since we can assume that in Eq. (41) $[\boldsymbol{v}]$ is a part of a jump of velocities, which meet the compatibility condition, for the second part of $[\boldsymbol{v}]$, related to a relative sliding along the interface, an equation can be derived independently [2, 3, 7].

To determine all unknown parameters in the PT criterion (38), e.g. position and geometry of nucleus, transformation strain and so on, the extremum principle can be derived based on the postulate of realizability [2, 3, 7].

4. Model problem

Let us consider the following plane strain problem for perfectly rigid–plastic material: an infinite half–space with prescribed normal stress σ_n and horizontal displacement u on the whole surface (Fig. 1). Assume that a coherent PT occurs in the layer along the whole surface and the solution does not depend on the x coordinate. The same solution is valid, if PT occurs in the parallel to the external surface layer inside of the half–space. The material outside of the layer is rigid. Let $\alpha = 0$, $\boldsymbol{\varepsilon}_t = (1/2\varepsilon_o \boldsymbol{i} + \gamma_t (\boldsymbol{t}\boldsymbol{n})_s) \, \xi$, where ε_o and γ_t are the volumetric and shear transformation strains, $\boldsymbol{i}$ the two dimensional unit tensor, subscript s means symmetrization. The von Mises yield condition results in $(\sigma_n - \sigma_t)^2 + 4\tau^2 = \sigma_y^2$, where σ_t and τ are the tangential and shear stresses, σ_y the yield limit of phase 2. Assume that stresses are fixed in the course of PT.

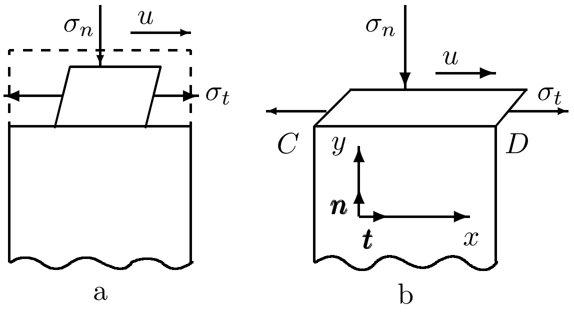

FIG. 1. Coherent PT in thin layer

In Fig. 1a a transformed particle is shown after transformation strain, but to satisfy displacement continuity across the interface CD and independence of solution of x, the plastic strain is needed (Fig. 1b). This problem was solved in [3] at constant temperature and a number of experimental effects were described. Here we will show that temperature variation plays a fundamental role. The work integral in Eq. (39) reads $W = 1/2 \, (\sigma_n + \sigma_t) \, \varepsilon_o + \tau \gamma_t$. From the yield condition we have $\sigma_t = \sigma_n - \sqrt{\sigma_y^2 - 4\tau^2}$. To determine τ we will use the associated flow rule

$$\dot{\varepsilon}_p = h \, (\sigma_n - \sigma_t) \qquad \dot{\gamma}_p = 4 \, h \, \tau \, , \qquad \dot{\gamma}_p / \dot{\varepsilon}_p = 4 \, \tau / \, (\sigma_n - \sigma_t) \, , \tag{43}$$

where $\boldsymbol{\varepsilon}_p = (\varepsilon_p \, (\boldsymbol{n}\boldsymbol{n} - \boldsymbol{t}\boldsymbol{t}) + \gamma_p \, (\boldsymbol{t}\boldsymbol{n})_s) \, \xi$, ε_p and γ_p are the normal and the shear plastic strain, h is a scalar. From the condition $\boldsymbol{t} \cdot \boldsymbol{\varepsilon} \cdot \boldsymbol{t} = 0$ (Fig. 1) it follows $\varepsilon_p = 1/2 \, \varepsilon_o$. Then from Eq. (43)

$$\gamma_p = \varepsilon_o \frac{a}{\sqrt{1 - a^2}} \, , \qquad a = \frac{2\tau}{\sigma_y} \, , \qquad \sqrt{\sigma_y^2 - 4\,\tau^2} = \sigma_y \, \frac{\varepsilon_o}{\sqrt{\varepsilon_o^2 + \gamma_p^2}} \, , \qquad \tau = \frac{\sigma_y}{2} \, \frac{\gamma_p}{\sqrt{\varepsilon_o^2 + \gamma_p^2}} \, . \tag{44}$$

In Eqs. (34)—(36) we should take into account plastic dissipation $\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}_p \, = \, \boldsymbol{\sigma} : \boldsymbol{\varepsilon}^p \, \dot{\xi}$,

$$A_p \, := \, \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_p \, = \, 0.5 \, \varepsilon_o \, (\sigma_n - \sigma_t) + \tau \, \gamma_p \, = \, 0.5 \, \sigma_y \sqrt{\varepsilon_o^2 + \gamma_p^2} \; . \qquad (45)$$

Eq. (36) at $-\rho \, \nu \, A + k \, = \, A_p$ results in

$$\sigma_n \varepsilon_o + \frac{\sigma_y}{2} \frac{(\gamma_p \gamma_t - \varepsilon_o^2)}{\sqrt{\varepsilon_0^2 + \gamma_p^2}} - \left(k + \frac{\sigma_y}{2} \sqrt{\varepsilon_o^2 + \gamma_p^2} + \rho \nu \theta_s B \right) \frac{(\exp B - 1)}{B} + \frac{\sigma_y}{2} \sqrt{\varepsilon_o^2 + \gamma_p^2} - U = 0 \, . \quad (46)$$

The value $\gamma_p \, = \, u/b - \gamma_t$, where b is the width of transformed layer, is undetermined. According to the postulate of realizability [2, 3, 7] the real value of γ_p maximizes the left side of Eq. (46), whence

$$\varepsilon_p^2 \frac{(\gamma_t + \gamma_p)}{\left(\varepsilon_o^2 + \gamma_p^2\right)} - \left[\frac{(\exp B - 1)}{B} - 1 \right] \gamma_p \, = \, 0 \, . \qquad (47)$$

When we neglect the thermal effect the second term in Eq. (47) is zero and $\gamma_p \to \infty$, $b \to 0$, i.e. PT occurs in infinitesimal narrow layer [3]. Heating due to plastic dissipation results in finite γ_p and b . At $\gamma_p >> \gamma_t$, $\gamma_p >> \varepsilon_o$ Eq. (47) leads to

$$\gamma_p = \varepsilon_o \sqrt{B / \left(\exp B - B - 1\right)} \qquad \text{and at} \qquad \exp B \simeq 1 + B + B^2/2 \qquad \text{to} \qquad \gamma_p = \varepsilon_o \sqrt{2/B} \, .$$

5. Concluding remarks

A developed theory of PT in the material point of inelastic continuum allows a consistent derivation of nucleation and interface propagation conditions for quite general situation. The PT criterion is derived using the second law of thermodynamics and value of dissipation increment due to PT only. It is valid for an arbitrary dissipative material, because the material's constitutive equations are not used in the derivation. It is easy to extend the approach to new situations, using the second law of thermodynamics, for example to take into account the electromagnetic field: it is necessary to calculate the dissipation increment due to PT itself. Generalization for the dynamic case is also trivial, because the expressions for dissipation increment used are the same as in the quasi–static case.

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