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THERMOMECHANICAL THEORY OF MARTENSITIC PHASE TRANSFORMATIONS IN INELASTIC MATERIALS†

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Abstract—A general thermomechanical theory of martensitic phase transformations (PT) in inelastic materials is presented. The results are derived for small and large strains in the reference and actual configurations. PT is treated as a thermomechanical process of growth of transformation strain from the initial to the final value which is accompanied by a change in all material's properties. The theory is developed first of all for a homogeneously deformed material point (neighborhood) undergoing the PT which can belong to a new nucleus or a moving interface. It is shown that a standard thermodynamical approach cannot be directly applied. It can be applied after the averaging of thermodynamical parameters, related to PT, over a PT duration. PT criterion is derived which takes into account the plastic dissipation, temperature variation due to the PT and variation of internal variables. It is shown that the temperature gradient does not contribute to PT criterion. The twinning criterion is derived as a particular case of the PT criterion. 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. After the averaging of the PT criterion over the transforming volume the nucleation and interface propagation criteria, as well as conditions of nondissappearance of nucleus are derived. Using the postulate of realizability [Levitas, V.I. (1992a) Post-bifurcation behavior in finite elastoplasticity. Applications to strain localization and phase transitions, Universität Hannover. Institut für Baumechanik und Numerische Mechanik, IBNM-Bericht 92/5. (1995a) The postulate of realizability: formulation and applications to post-bifurcation behavior and phase transitions in elastoplastic materials. Part I and II. *International Journal of Engineering Science*, **33**, 921–971.], the extremum principle for the determination of all unknown parameters (e.g. position, shape and orientation of nuclei, transformation strain and so on) is derived. It is shown that for the PT in elastic materials the proposed approach gives alternative, but equivalent to the principle of minimum of Gibbs energy formulation. Some aspects of the formulation of boundary-value problem (BVP) are analyzed. Some possible ways of formulation of constitutive relations for inelastic deformations in the course of the PT are discussed. It is obtained that the dissipative threshold in the PT criterion is proportional to yield stress. The thermomechanical theory developed is extended to the case with displacement discontinuities across an interface (noncoherence and fracture). © 1997 Elsevier Science Ltd.

1. INTRODUCTION

Solid–solid phase transformations (PT) are phenomena that are very widespread in nature, physical experiments and modern technologies. Various sciences consider the PT from their own point of view, for instance materials science [Christian (1965); Hornbogen (1991); Olson and Cohen (1986)], solid state physics [Krumhansl, (1995)], thermodynamics [Wollants *et al.* (1993)], crystallography [Wayman (1964)], mathematics [Ball and James (1992); Kohn and Müller (1992)], theory of elasticity [Grinfeld (1991); Gurtin (1993a); Khachaturyan (1983); Roitburd (1993)], rational thermodynamics [Gurtin (1993b); Cermelli and Gurtin (1994a)]. We will consider here martensitic PT only, but nevertheless a lot of general results are applicable to diffusive PT and melting (crystallization). There are a lot of definitions of martensitic PT [see e.g. Clapp (1996)]. Here, the martensitic PT will be considered as a special type of deformation of a crystal lattice of parent phase (austenite) in a crystal lattice of product phase (martensite) without diffusion which is accompanied by a jump in all the thermomechanical properties. This deformation is called the transformation strain. Reverse PT transforms martensite into austenite. The transformation deformation gradient cannot be arbitrary (as elastic or plastic strain). For each PT the

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† Dedicated to my teacher, Professor Nickolay V. Novikov on the occasion of his 65th birthday.

right stretch transformation tensor is some fixed tensor to within symmetry operations. All intermediate values of the transformation right stretch tensor are unstable and cannot exist in an equilibrium. Due to the symmetry there is a finite number (e.g. 12 for the PT from a cubic to monoclinic lattice) of crystallographically equivalent variants of martensite with the same (to within symmetry operations) transformation right stretch tensor. The reason for the occurrence of PT is the loss of stability of the thermomechanical equilibrium of the parent crystal lattice for nondissipative materials or a thermomechanical deformation process without transformation strain for dissipative materials. Nondissipative materials transform into a new stable crystal lattice and dissipative materials undergo a stable deformation process with transformation strain. Typical values of components of transformation strain are the following: shear strain for shape memory alloys and steels reach $10 \sim 20\%$, volumetric strain is near zero for shape memory alloys, and varies from $1 \sim 4\%$ for steels to 50% for the PT graphite to diamond and rhomboedric boron nitride to cubic boron nitride. The appearance of such a large transformation strain in some regions of a body results in large stresses and accommodational inelastic strains in the transforming regions and surroundings. We will distinguish coherent PT when displacements are continuous across the interface and noncoherent PT in the opposite case. Practically all PT with volumetric transformation strain exceeding 0.5% are accompanied by plastic strains. PT in inelastic materials play a significant role in many advanced technical problems, e.g. for heat and thermomechanical treatment of metals, for transformation induced plasticity (TRIP), strain induced PT and for the activation of PT by large plastic shear straining in combination with high pressure. A knowledge of the influence of plastic strain, applied and local stress field on PT is very important for the understanding, simulation and improvement of the above processes, as well as for the development of new technologies and materials.

For the description of PT in an elastic solid the principle of a minimum of Gibbs free energy is usually used. For inelastic materials the corresponding principle was lacking and the theory of PT in inelastic solids is only in its early stages. We will limit ourselves to the thermodynamical description of PT and quasi-static processes. The first results were related to the solution of some simple model problems. Lifshitz and Gulida (1952) have considered the melting of a small spherical particle in an elastoplastic space. The appearance of the spherical nucleus in a sphere under applied external pressure was analyzed in a paper by Roitburd and Temkin (1986). Bar'yachtar *et al.* (1986) using the Landau-type theory examined the appearance of the spherical and the plate-like nucleus in an infinite space without external forces. The ellipsoidal nucleus in an infinite space without external forces was considered by Kaganova and Roitburd (1989). In both papers the deformation theory of plasticity was used, which is thermodynamically equivalent to nonlinear elasticity. In most of these papers the PT criterion and extremum principle for the definition of some unknown parameters are the same as for PT in elastic materials, i.e. Gibbs free energy of the whole system is minimized. It is known that, in contrast to elastic materials, for elastoplastic ones such an extremum principle could not be proved due to the necessity of considering of the plastic dissipation and path-dependency. Roitburd and Temkin (1986) and Kaganova and Roitburd (1987) studied the growth of the spherical nucleus. As the driving force of PT the variation of Gibbs energy plus the heat dissipated due to plastic straining in the whole body is adopted. This condition was not localized to the interface propagation condition and that is why it is difficult to estimate it validity. In the next paper by Kaganova and Roitburd (1989) another approach for the interface propagation is used which will be analyzed in Section 5.1. PT in viscoelastic materials are considered by Arutyunyan and Drosdov (1992).

Ganghoffer *et al.* (1991) and Marketz and Fischer (1995) maximize the transformation work using local stress in the place of nucleation before the PT. Such an assumption generalizes the Patel and Cohen (1953) extremum principle for the case of elastoplastic materials and presence of internal stresses. At the same time it leads to significant errors, because stresses change very significantly during the PT (growth of transformation strain) and even change a sign [see e.g. papers by Roitburd and Temkin (1986); Levitas (1996a); Levitas *et al.* (1996a, 1997a)]. Investigations of PT in elastoplastic materials by Fischer *et al.* (1994) and Marketz and Fischer (1994, 1995) are related to the comparison of Gibbs free energy before and after PT. Typical for all the above papers is that the PT conditions are not directly related to the second law of thermodynamics and dissipation due to the PT. That is why it is difficult to understand the physical sense of the proposed criteria and choose which one is correct and which is not. Consequently, all the above solutions have a preliminary character and should be checked based on more recent approaches.

In the paper by Kondaurov and Nikitin (1986) are obtained all the balance equation for the points of moving interface in viscoplastic material, including PT criterion, but the characteristic time of PT is assumed to be much smaller than the characteristic time of viscous relaxation and plastic strain increment is equal to zero in the course of PT. In this case, the PT conditions are the same as for elastic materials, which contradicts to very strong effect of plastic straining and plastic properties on PT.

An averaged description of PT in terms of the volume fraction of martensite is presented by Levitas (1990, 1992b, 1995b), Raniecki and Bruhns (1991) and Bhattacharya and Weng (1994) at small strain and in book by Levitas (1992b) at large strain. An averaging procedure for noncoherent PT at finite strain has been developed [Levitas (1996d)]. A numerical study of martensite formation and averaging is presented in Leblond *et al.* (1989), Ganghoffer *et al.* (1991), Marketz and Fischer (1994, 1995), Simonsson (1995) and Levitas *et al.* (1996a, 1997a). We will not analyze these results, because averaged description is not a topic of this paper. Current progress in the study of TRIP is presented in papers by Fischer *et al.* (1996) and Olson (1996).

In the paper a new general thermomechanical theory of PT in inelastic materials with arbitrary constitutive equations at small and large strains is developed. We will consider simple materials only, i.e. the material's response in the given point is independent of thermomechanical parameters in other points. In contrast to 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) we will start in Section 2 with a description of the PT as a thermomechanical process of growth of transformation strain from the initial to the final value (which is accompanied by a change in all the material's properties) in a *homogeneously deformed material point* (*infinitesimal volume*). The material point can belong to a new nucleus or a moving interface. We try to apply the standard thermomechanical methods of derivation of constitutive equations, as e.g. for a material point of elastoplastic materials, and get a contradiction. It is related to the fact that in experiments the thermodynamical equilibrium is possible for initial and final values of the transformation deformation gradient only. All other configurations (crystal structures) with intermediate values of transformation strain are unstable and thus impossible, but standard thermodynamics allows them. Consequently, a standard thermodynamical approach cannot be directly applied. It can be applied after *averaging* thermodynamical parameters, related to PT, over a PT duration.

Using the second law of thermodynamics we determine a dissipation increment during the PT X, related to the PT only (excluding plastic dissipation and dissipation due to other dissipative processes). For $X < 0$ PT is thermodynamically impossible, for $X = 0$ PT is possible, but without dissipation. Consequently, the criterion of PT without dissipation due to PT is obtained without any additional assumptions, using the second law of thermodynamics only. For PT with dissipation it is accepted that $X = k$, where k is an experimentally determined value of dissipation due to PT. The PT criterion derived takes into account the temperature variation due to the PT and variation of internal variables. It is shown that the temperature gradient does not contribute to the PT criterion. The twinning criterion is derived as a particular case of the PT criterion. Temperature variation in the course of PT is determined in Section 3 with the help of the entropy balance equation under the assumption that the process is adiabatic. In Sections 4 and 5, after the integration over the transforming volume the nucleation and interface propagation criteria, as well as conditions of nondissappearance of the nucleus, are derived. The PT criterion is only one scalar equation, which is not sufficient for the determination of all unknown parameters such as *position, shape and orientation of nuclei, transformation strain, transformation path* and so on. For these purposes the new thermomechanical postulate, named the *postulate of realizability*, was formulated [Levitas (1992a, 1995a)]. It was shown [Levitas (1992a, 1995a, 1995e, 1997)] that the postulate of realizability gives some known and some completely new results for various dissipative systems. Using it, the extremum principle for the determination of all unknown parameters is derived in Section 6. It is proved that for the PT in elastic materials our approach gives an alternative, but equivalent to the principle of minimum of Gibbs energy formulation. The modifications necessary for taking into account the dissipation due to the PT are found. The evaluation of the dissipative threshold k is given in Section 7. In Section 8 some aspects of the formulation of BVP are considered. Some possible ways of formulating constitutive relations for inelastic deformations in the course of the PT are discussed. The thermomechanical theory developed is extended in Section 9 to the case with displacement discontinuities across an interface (noncoherence and fracture). It is assumed that PT and fracture (or noncoherence) criteria are mutually independent and that these processes are coupled through the stress fields only. Growing transformation strain generates the stresses, which are necessary for fracture (sliding along the interface), and fracture (noncoherence) changes the stress variation in the transforming particle.

All derivations are made for three cases: small strains, finite strains in the reference configuration and finite strains in the actual configuration. Small strain formulation allows us to understand general ideas without unnecessary formal complications and to obtain simple analytical and numerical solutions. The equations for large strain in the reference configuration are simpler to derive than in the actual one, because the reference configuration is fixed and there are no problems related to the choice of objective derivative. At the same time some formulations are much more simple in the actual configuration, e.g. for noncoherent PT.

Some preliminary results were reported in [Levitas (1992a, 1995a, 1997)] and in short communications [Levitas (1995b, 1995c, 1995d, 1996a, 1996c)]. Direct tensor notations are used throughout this paper. Vectors and tensors are denoted in boldface type; $\mathbf{mn}$ is the dyadic product of vectors $\mathbf{m}$ and $\mathbf{n}$; $\mathbf{A}\cdot\mathbf{B}$ and $\mathbf{A}:\mathbf{B}$ are the contraction of tensors over one and two indices, in the formulas which are first performed $\cdot$ and then $:$ (e.g. $\mathbf{A}:\mathbf{B}\cdot\mathbf{K} = \mathbf{A}:(\mathbf{B}\cdot\mathbf{K})$). Let a superscript t and -1 denote transposition and inverse operation, subscript s symmetrization of the tensors, tr the trace operation, $[\mathbf{a}] = \mathbf{a}_2 - \mathbf{a}_1$ the jump of value $\mathbf{a}$ across the interface, $\Delta\mathbf{a} = \mathbf{a}_2 - \mathbf{a}_1$ the differences in $\mathbf{a}$, $\mathbf{I}$ the unit tensor second-order, dev $\mathbf{A}$ is a deviatoric part of $\mathbf{A}$, $|\mathbf{A}| := (\mathbf{A}:\mathbf{A})^{1/2}$ and $\mathbf{k} = \mathbf{A}/|\mathbf{A}|$ the modulus (amplitude) and the directing tensor of tensor $\mathbf{A}$, $\boldsymbol{\nabla}$ is the gradient operator, $:=$ means equals per definition.

2. THERMODYNAMICS OF MARTENSITIC PHASE TRANSITIONS IN A MATERIAL POINT

2.1. *Small strains*

Let us consider uniformly deformed material point (infinitesimal volume) in a process of martensitic PT. The point can belong to the new nucleus or interface. The martensitic PT will be considered as a growth of the transformation strain from the initial to final value without diffusion which is accompanied by a jump in all thermomechanical properties.

We will consider simple materials only, i.e. a material's response in the given point is independent of thermomechanical parameters in other points. In this section, we will neglect surface effects also, like surface energy or dissipation due to relative sliding on the noncoherent interface, but these effects will be taken into account in the following sections. 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 (order parameter) ξ $(0 \leqslant \xi \leqslant 1)$ 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 to $\boldsymbol{\varepsilon}_{t\max}$. During this process all the thermodynamic properties of phase 1 change into the properties of phase 2. It is possible to define

$$\xi := \frac{|\boldsymbol{\varepsilon}_t|}{|\boldsymbol{\varepsilon}_{t\max}|}, \quad \xi := \frac{\operatorname{tr}\boldsymbol{\varepsilon}_t}{\operatorname{tr}\boldsymbol{\varepsilon}_{t\max}} \quad \text{or} \quad \xi := \frac{|\mathbf{e}_t|}{|\mathbf{e}_{t\max}|}, \tag{2}$$

where $\mathbf{e}_t = \operatorname{dev}\boldsymbol{\varepsilon}_t$; a lot of other definitions are acceptable. An important point is, that all variable components of transformation strain tensor have to be included in the definition of ξ. In the opposite case, ξ can reach 1 before $\boldsymbol{\varepsilon}_t$ reaches $\boldsymbol{\varepsilon}_{t\max}$ and PT finishes. Consequently, definition $(2)_1$ is valid in the general case, eqn $(2)_2$ can be applied for purely dilatational PT and for dilatation free transformation strain definition $(2)_3$ is noncontradictory. The internal time, ξ, plays a similar role in 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 (per unit mass) Helmholtz free energy

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

where $\mathbf{g}$ is a set of internal variables, e.g. internal stress tensor (back stress), dislocations or point defect density. We admit the second law of thermodynamic in the form of the Clausius–Duhem inequality

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

Here, $\mathscr{D}$ is the rate of dissipation per unit mass, ρ the mass density, s the specific entropy, $\nabla\theta$ the temperature gradient, $\mathbf{h}$ the heat flux. In small strain approximation ρ = const. The substitution of the rate of free energy

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

with taking into account the additive decomposition of $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}_\theta = \boldsymbol{\varepsilon}_\theta(\theta, \xi)$ and

$$\dot{\boldsymbol{\varepsilon}}_\theta = \frac{\partial\boldsymbol{\varepsilon}_\theta}{\partial\theta}\dot{\theta} + \frac{\partial\boldsymbol{\varepsilon}_\theta}{\partial\xi}\dot{\xi} \tag{6}$$

in eqn (4) yields

$$\begin{aligned}\rho\mathscr{D} = {} & \left(\boldsymbol{\sigma} - \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_e}\right) : \dot{\boldsymbol{\varepsilon}}_e - \rho\left(s + \frac{\partial\psi}{\partial\theta} - \frac{\boldsymbol{\sigma}}{\rho} : \frac{\partial\boldsymbol{\varepsilon}_\theta}{\partial\theta}\right)\dot{\theta} + \left(\boldsymbol{\sigma} - \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p}\right) : \dot{\boldsymbol{\varepsilon}}_p \\ & - \rho\frac{\partial\psi}{\partial\mathbf{g}^t} : \dot{\mathbf{g}} - \frac{\nabla\theta}{\theta} \cdot \mathbf{h} + \left(\boldsymbol{\sigma} : \frac{\partial(\boldsymbol{\varepsilon}_t + \boldsymbol{\varepsilon}_\theta)}{\partial\xi} - \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_t} : \frac{\partial\boldsymbol{\varepsilon}_t}{\partial\xi} - \rho\frac{\partial\psi}{\partial\xi}\right)\dot{\xi} \geqslant 0.\end{aligned} \tag{7}$$

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:

$$\boldsymbol{\sigma} = \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_e}; \quad s = \frac{\boldsymbol{\sigma}}{\rho} : \frac{\partial\boldsymbol{\varepsilon}_\theta}{\partial\theta} - \frac{\partial\psi}{\partial\theta}; \tag{8}$$

$$\mathscr{D} = \mathbf{X}_p : \dot{\boldsymbol{\varepsilon}}_p + \mathbf{X}_g : \dot{\mathbf{g}} + \mathbf{X}_h \cdot \mathbf{h} + X_\xi\dot{\xi} \geqslant 0, \tag{9}$$

where

$$\mathbf{X}_{\mathrm{p}} = \frac{1}{\rho}\boldsymbol{\sigma} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_{\mathrm{p}}}; \quad \mathbf{X}_{\mathrm{g}} = -\frac{\partial \psi}{\partial \mathbf{g}^{\mathrm{t}}}; \quad \mathbf{X}_{\mathrm{h}} = -\frac{1}{\rho}\frac{\boldsymbol{\nabla}\theta}{\theta} \tag{10}$$

and

$$X_{\xi} = \frac{1}{\rho}\boldsymbol{\sigma} : \frac{\partial(\boldsymbol{\varepsilon}_{\mathrm{t}} + \boldsymbol{\varepsilon}_{\theta})}{\partial \xi} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_{\mathrm{t}}} : \frac{\partial \boldsymbol{\varepsilon}_{\mathrm{t}}}{\partial \xi} - \frac{\partial \psi}{\partial \xi} \tag{11}$$

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

$$\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} = \mathbf{f}_{\mathrm{p}}(\mathbf{X}_{\mathrm{p}}, \xi); \quad \dot{\mathbf{g}} = \mathbf{f}_{\mathrm{g}}(\mathbf{X}_{\mathrm{g}}, \xi); \quad \mathbf{h} = \mathbf{f}_{\mathrm{h}}(\mathbf{X}_{\mathrm{h}}, \xi); \quad \dot{\xi} = f_{\xi}(X_{\xi}, \xi). \tag{12}$$

Equation $(12)_1$ is the flow rule, eqn $(12)_2$ is the evolution equation for the internal variables, eqn $(12)_3$ is the generalized Fourier law and eqn $(12)_4$ is the kinetic equation for PT. All functions in eqn (12) can depend on temperature, plastic strain, internal variables and so on. The allowance for mutual influence of all thermomechanical processes can be made in a standard way. In fact, we will use independence of $\dot{\xi}$ from nonconjugate forces only.

It is necessary to explain why decomposition (6) is used for $\boldsymbol{\varepsilon}_{\theta}$ only. A similar decomposition is valid for $\boldsymbol{\varepsilon}_{\mathrm{e}}$, but it results in nothing new, due to the validity of eqn $(8)_1$. Equations $(12)_1$ and $(12)_2$ for $\boldsymbol{\varepsilon}_{\mathrm{p}}$ and $\mathbf{g}$ are rate-type; if we assume for $\boldsymbol{\varepsilon}_{\mathrm{p}}$ a decomposition similar to (6), then the term $(\partial \boldsymbol{\varepsilon}_{\mathrm{p}}/\partial \xi)\dot{\xi}$ is undefined (similarly for $\mathbf{g}$).

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

$$X_{\xi} = \frac{1}{\rho}\boldsymbol{\sigma} : \frac{\partial(\boldsymbol{\varepsilon}_{\mathrm{t}} + \boldsymbol{\varepsilon}_{\theta})}{\partial \xi} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_{\mathrm{t}}} : \frac{\partial \boldsymbol{\varepsilon}_{\mathrm{t}}}{\partial \xi} - \frac{\partial \psi}{\partial \xi} = 0. \tag{13}$$

Equation (13) is one scalar equation and it is always possible for each ξ and $\theta(\xi)$ to choose six components of stress tensor $\boldsymbol{\sigma}(\xi, \theta(\xi))$ to satisfy this equation. 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 $\xi = 1$ do we have the stable equilibrium. At $0 < \xi < 1$ a nonequilibrium process takes place, which requires energy and stress fluctuations.

We do not know any similar contradiction in the application of continuum thermodynamics. In this case a standard thermodynamic approach cannot be applied. It is necessary to average the thermodynamic 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 PT

$$\mathscr{D}_{\xi} := \frac{1}{t_{\mathrm{p}}}\int_0^{t_{\mathrm{p}}} X_{\xi}\dot{\xi}\,\mathrm{d}t = \frac{1}{t_{\mathrm{p}}}\int_0^1 X_{\xi}\,\mathrm{d}\xi = \frac{X}{t_{\mathrm{p}}} = X\dot{\chi}, \quad \text{where } X := \int_0^1 X_{\xi}\,\mathrm{d}\xi, \quad \dot{\chi} := \frac{1}{t_{\mathrm{p}}} \tag{14}$$

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 reverse PT the parameter ξ varies from 1 to 0 and

$$\mathscr{D}_{\xi} = \frac{1}{t_{\mathrm{p}}}\int_0^{t_{\mathrm{p}}} X_{\xi}\dot{\xi}\,\mathrm{d}t = \frac{1}{t_{\mathrm{p}}}\int_1^0 X_{\xi}\,\mathrm{d}\xi = -\frac{1}{t_{\mathrm{p}}}\int_0^1 X_{\xi}\,\mathrm{d}\xi = X\dot{\chi}, \tag{15}$$

where

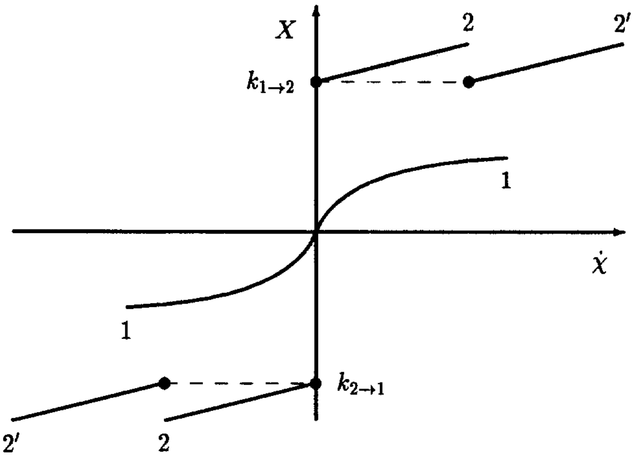

Fig. 1. Possible dependences between X and $\dot{\chi}$.

$$X := \int_0^1 X_\xi \, d\xi \leqslant 0, \quad \dot{\chi} = -\frac{1}{t_p} \leqslant 0.$$

For the macroscopically equilibrium direct or reverse PT the following equation is valid

$$X = \int_{\varepsilon_{t1}}^{\varepsilon_{t2}} \left(\frac{\sigma}{\rho} - \frac{\partial \psi}{\partial \varepsilon_t} \right) : d\varepsilon_t + \int_0^1 \left(\frac{\sigma}{\rho} : \frac{\partial \varepsilon_\theta}{\partial \xi} - \frac{\partial \psi}{\partial \xi} \right) d\xi = 0. \tag{16}$$

The indices 1 and 2 denote the values before and after PT. Equation (16) is the PT criterion for PT without dissipation.

Let $X \neq 0$ and $\dot{\chi} = f(X, \ldots)$. There are only two possibilities for the behavior of the function f at $\dot{\chi} \to 0$.

(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 $X = 0$ (Fig. 1, curve 1).

(2) Let (Fig. 1, curve 2)

$$\begin{aligned} &\text{at } \dot{\chi} = 0 \quad k_{2\to1} \leqslant X \leqslant k_{1\to2}, \\ &\textit{at } \dot{\chi} > 0 \quad X = k_{1\to2} > 0, \\ &\textit{at } \dot{\chi} < 0 \quad X = k_{2\to1} < 0, \end{aligned} \tag{17}$$

where $k_{1\to2}$ and $k_{2\to1}$ are the threshold values of X in the direct and the reverse PT, which can depend on θ, χ, ε_p, $\mathbf{g}, \ldots$. In this case there is a *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. Equation (17) means that the calculated value of the dissipation increment per unit mass due to PT reaches its experimentally determined value. When X reaches k the rate $\dot{\chi}$ has a jump till $10^6 \sim 10^{10}$ s^{-1} ($t_p = 10^{-6} \sim 10^{-10}$ s [Meyers (1979); Kaschenko (1993)] (see Fig. 1, curve 2′).

Remark. In the experiments the macroscopic parameters for the finite volume (not for a material point) are usually determined, e.g. force, averaged stress. For plastic materials, the hysteresis of this macroscopic parameter can occur at $k_{1\to2} = k_{2\to1} = 0$ as well, see an example in [Levitas (1995d)], and the above arguments for the existence of the dissipative threshold are invalid. For elastic materials the hysteresis of macroscopic parameters cannot be obtained theoretically at $k_{1\to 2} = k_{2\to 1} = 0$, but it practically always exists in the experiments. Consequently, the arguments leading to the existence of the dissipative threshold are noncontradictory.

Let us consider the alternative expressions for X. From eqns (9) and (4) it follows

$$X_\xi \dot{\xi} = \mathscr{D} - \mathbf{X}_p : \dot{\boldsymbol{\varepsilon}}_p - \mathbf{X}_g : \dot{\mathbf{g}} - \mathbf{X}_h \cdot \mathbf{h} = \rho^{-1} \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{\psi} - s\dot{\theta} - \mathbf{X}_p : \dot{\boldsymbol{\varepsilon}}_p - \mathbf{X}_g : \dot{\mathbf{g}} ; \tag{18}$$

$$X = \frac{1}{\rho} \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon} - (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} s \, \mathrm{d}\theta - \int_0^{t_p} (\mathbf{X}_p : \dot{\boldsymbol{\varepsilon}}_p + \mathbf{X}_g : \dot{\mathbf{g}}) \, \mathrm{d}t = k. \tag{19}$$

Taking into account the decomposition (1) and eqn $(10)_1$ for $\mathbf{X}_p$ we obtain

$$X = \frac{1}{\rho} \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma} : d(\boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_\theta + \boldsymbol{\varepsilon}_t) - (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} s \, \mathrm{d}\theta + \int_{\mathbf{g}_1}^{\mathbf{g}_2} \frac{\partial \psi}{\partial \mathbf{g}^t} : \mathrm{d}\mathbf{g} + \int_{\boldsymbol{\varepsilon}_{p1}}^{\boldsymbol{\varepsilon}_{p2}} \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_p} : \mathrm{d}\boldsymbol{\varepsilon}_p = k. \tag{20}$$

The expressions (19) and (20) are sometimes more convenient for the analysis than eqn (16). At $\partial\psi/\partial\boldsymbol{\varepsilon}_p = 0$, eqn (20) is more suitable for application, because in this case the plastic strain $\boldsymbol{\varepsilon}_p$ disappears completely. Equation (19) shows that X is the total dissipation increment per unit mass minus plastic dissipation increment and the dissipation increment due to the internal variables. Equation (19) is more appropriate when the moving interface is considered and the Hadamard compatibility condition for $\boldsymbol{\varepsilon}_2 - \boldsymbol{\varepsilon}_1$ is taken into account (see Section 5).

Note that expressions $(10)_1$ and $(10)_2$ for $\mathbf{X}_p$ and $\mathbf{X}_g$ can be obtained using the standard thermomechanical approach for materials without PT. Then a very simple method of derivation of expression for X is evident [see eqn (19)]: *the dissipation increment due to PT only is the difference between the total dissipation increment and the dissipation increment due to other dissipative processes* (plastic flow, variation of internal variables and so on).

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

$$\int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon} = \rho(\psi_2 - \psi_1). \tag{21}$$

If PT proceeds at constant stress $\boldsymbol{\sigma}^0$, then $\boldsymbol{\sigma}^0 : (\boldsymbol{\varepsilon}_2 - \boldsymbol{\varepsilon}_1) = \rho(\psi_2 - \psi_1)$. This is the Maxwell rule. Geometrically speaking, it means that the areas (BCD) and (DEF) are the same, where OBCDEF is the shear stress τ-shear strain γ diagram (Fig. 2). Indeed, terms $\tau_0(\gamma_2 - \gamma_1)$ and

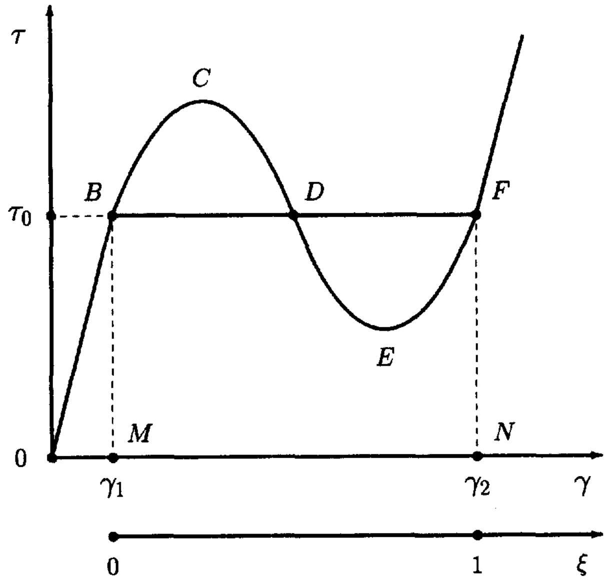

Fig. 2. Diagram of simple shearing for material with PT.

$\rho(\psi_2-\psi_1)$ correspond to areas (BFNM) and (BCDEFNM), respectively, and their equality results in the equality of areas (BCD) and (DEF). Consequently, eqn (17) is a generalization of the Maxwell rule for dissipative materials, nonisothermal processes and for variable stresses.

Figure 2 shows why it is impossible to apply the second law of thermodynamics for each ξ. To deform a material point in accordance with the curve BCDEF under the fixed stress τ_0, fluctuations are needed to overcome the energy barrier (BCD). The fluctuations can be thermoactivated or due to the local stress concentration on various defects (dislocations, grain boundaries). The material borrows energy (BCD) from the system and at the next instant returns the same energy (DEF) to it. The rate of dissipation formally calculated for each ξ in the interval $0<\xi<\xi_D$ is negative, because standard thermodynamics does not take into account the fluctuations.

Let

$$\rho\psi_i = 0.5\boldsymbol{\varepsilon}_{ei}:\mathbf{E}_i:\boldsymbol{\varepsilon}_{ei}+\rho\psi_i^\theta = \rho\psi_i^e+\rho\psi_i^\theta, \quad i=1,2, \tag{22}$$

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

$$\begin{aligned}\int_{\boldsymbol{\varepsilon}_{e1}}^{\boldsymbol{\varepsilon}_{e2}} \boldsymbol{\sigma}:\mathrm{d}\boldsymbol{\varepsilon}_e &= \int_{\boldsymbol{\varepsilon}_{e1}}^{\boldsymbol{\varepsilon}_{e2}} \boldsymbol{\varepsilon}_e:\mathbf{E}:\mathrm{d}\boldsymbol{\varepsilon}_e = \frac{1}{2}\int_{\boldsymbol{\varepsilon}_{e1}}^{\boldsymbol{\varepsilon}_{e2}} \mathrm{d}(\boldsymbol{\varepsilon}_e:\mathbf{E}:\boldsymbol{\varepsilon}_e)-\frac{1}{2}\int_0^1 \boldsymbol{\varepsilon}_e:\mathrm{d}\mathbf{E}(\xi):\boldsymbol{\varepsilon}_e \\ &= \rho(\psi_2^e-\psi_1^e)-0.5\int_0^1 \boldsymbol{\varepsilon}_e:\mathrm{d}\mathbf{E}(\xi):\boldsymbol{\varepsilon}_e,\end{aligned} \tag{23}$$

it follows then from eqn (20)

$$\begin{aligned}X = \frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma}:\mathrm{d}(\boldsymbol{\varepsilon}_\theta+\boldsymbol{\varepsilon}_t)-\frac{1}{2\rho}\int_0^1 \boldsymbol{\varepsilon}_e:\mathrm{d}\mathbf{E}(\xi):\boldsymbol{\varepsilon}_e-(\psi_2^\theta-\psi_1^\theta)-\int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta \\ +\int_{\mathbf{g}_1}^{\mathbf{g}_2} \frac{\partial\psi}{\partial\mathbf{g}^t}:\mathrm{d}\mathbf{g}+\int_{\boldsymbol{\varepsilon}_{p1}}^{\boldsymbol{\varepsilon}_{p2}} \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p}:\mathrm{d}\boldsymbol{\varepsilon}_p = k.\end{aligned} \tag{24}$$

When $\mathbf{E}_1=\mathbf{E}_2=$ const (e.g. independent of θ, $\boldsymbol{\varepsilon}_p,\ldots$), then the term with $\mathrm{d}\mathbf{E}$ disappear.

Since $\boldsymbol{\varepsilon}_\theta=\boldsymbol{\alpha}(\theta-\theta_0)$, where $\boldsymbol{\alpha}=\boldsymbol{\alpha}(\xi,\theta-\theta_0)$ is the thermal expansion tensor and θ_0 is the reference temperature, we will assume that for isothermal processes $\theta=\theta_0$ and we obtain $\boldsymbol{\varepsilon}_\theta=0$. Consequently, for $(\partial\psi/\partial\boldsymbol{\varepsilon}_p)=(\partial\psi/\partial\mathbf{g})=0$ and isothermal processes we have

$$X=\frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma}:\mathrm{d}\boldsymbol{\varepsilon}_t-(\psi_2^\theta--\psi_1^\theta)=k. \tag{25}$$

One of the physical mechanisms of plasticity, especially at low temperature, is twinning. For twinning $\psi_2^\theta=\psi_1^\theta$, $\boldsymbol{\varepsilon}_t=\gamma(\mathbf{mn})_s$ with γ for shear strain, $\mathbf{m}$ shear direction, $\mathbf{n}$ for normal to shear plane and eqn (24) gives

$$\begin{aligned}X=\frac{1}{\rho}\int_0^{\gamma_2}\tau\,\mathrm{d}\gamma+\frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_{1\theta}}^{\boldsymbol{\varepsilon}_{2\theta}} \boldsymbol{\sigma}:\mathrm{d}\boldsymbol{\varepsilon}_\theta-\frac{1}{2\rho}\int_0^1 \boldsymbol{\varepsilon}_e:\mathrm{d}\mathbf{E}(\xi):\boldsymbol{\varepsilon}_e-\int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta \\ +\int_{\mathbf{g}_1}^{\mathbf{g}_2} \frac{\partial\psi}{\partial\mathbf{g}^t}:\mathrm{d}\mathbf{g}+\int_{\boldsymbol{\varepsilon}_{p1}}^{\boldsymbol{\varepsilon}_{p2}} \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p}:\mathrm{d}\boldsymbol{\varepsilon}_p = k\end{aligned} \tag{26}$$

with $\tau=\mathbf{m}\cdot\boldsymbol{\sigma}\cdot\mathbf{n}$ the shear stress conjugated to γ. Variation of elastic moduli is related to reorientation of the crystal lattice during the twinning, i.e. elastic constants do not change and rotation of unit basis vectors $\mathbf{e}_i$, $i = 1, 2, 3$, is determined in terms of current value γ and orientation of $\mathbf{e}_i$ before twinning. For $(\partial\psi/\partial\boldsymbol{\varepsilon}_p) = (\partial\psi/\partial\mathbf{g}) = 0$ and isothermal processes we obtain

$$X = \frac{1}{\rho}\int_0^{\gamma_2} \tau\,\mathrm{d}\gamma = k. \tag{27}$$

A significant difference between the Schmid law $\tau = \tau_c$ (condition of plastic shear due to dislocation motion) and eqn (27) consists in the fact that shear stress τ varies significantly during the twinning (γ growth) and the variation depends on the solution of the corresponding BVP for the whole volume V.

The transformation from one martensitic variant with $\boldsymbol{\varepsilon}_{t1} = \gamma_1(\mathbf{mn})_s$ to another with $\boldsymbol{\varepsilon}_{t2} = \gamma_2(\mathbf{mn})_s$ at $\gamma_2 = -\gamma_1$ is a particular case of the reorientation process. In this case

$$X = \frac{1}{\rho}\int_{\gamma_1}^{\gamma_2} \tau\,\mathrm{d}\gamma = k. \tag{28}$$

Temperature variation and other dissipative contributions can be taken into account as in eqn (20).

2.2. *Finite strains description in the reference configuration*

Let the motion of the uniformly deformed infinitesimal neighborhood of a material point in a process of martensitic PT be described by the function $\mathbf{r} = \mathbf{r}(\mathbf{r}_\tau, t)$, where $\mathbf{r}$ and $\mathbf{r}_\tau$ are the positions of points in the actual V and reference V_τ configurations. We will use the variable reference configuration V_τ. In this section the reference configuration coincides with the plastic undeformable stress-free configuration of the first phase. We assume for the finite strains a multiplicative decomposition of a total deformation gradient $\mathbf{F}_\tau = \partial\mathbf{r}/\partial\mathbf{r}_\tau$ into elastic $\mathbf{F}_{e\tau}$, thermal $\mathbf{F}_{\theta\tau}$, transformational $\mathbf{F}_{t\tau}$ parts, a plastic deformation gradient in the phase 1 $\mathbf{F}_{p1\tau}$ (before PT), during PT $\mathbf{F}_{p\tau}(\xi)$ and after PT $\mathbf{F}_{p2\tau}$ (in phase 2), i.e.

$$\mathbf{F}_\tau = \mathbf{F}_{e\tau}\cdot\mathbf{F}_{\theta\tau}\cdot\mathbf{F}_{p2\tau}\cdot\mathbf{F}_{t\tau}\cdot\mathbf{F}_{p\tau}(\xi)\cdot\mathbf{F}_{p1\tau}. \tag{29}$$

Subscript τ means that the values relate to the configuration V_τ. Since the strain $\mathbf{F}_{p2\tau}$ after the PT does not affect the PT, assume without loss of generality $\mathbf{F}_{p2\tau} = \mathbf{I}$, i.e.

$$\mathbf{F}_\tau = \mathbf{F}_{e\tau}\cdot\mathbf{F}_{\theta\tau}\cdot\mathbf{F}_{t\tau}\cdot\mathbf{F}_{p\tau}(\xi)\cdot\mathbf{F}_{p1\tau}. \tag{30}$$

Plastic deformation after the PT can be described in a standard way. We can introduce the intermediate configurations related to each component of $\mathbf{F}_\tau$ in eqn (29), e.g. the configuration V_{p1}, formed by vectors $\mathbf{r}_{p1} = \mathbf{F}_{p1}\cdot\mathbf{r}_\tau$, or the configuration V_f, formed by vectors $\mathbf{r}_f = \mathbf{F}_{t\tau}\cdot\mathbf{F}_{p\tau}(\xi)\cdot\mathbf{F}_{p1\tau}\cdot\mathbf{r}_\tau$ and so on.

Decomposition eqn (29) is determined to within the rigid body rotations (RBR) related to each component of $\mathbf{F}_\tau$ in each intermediate configuration. As for a single crystal all the material's properties and functions are determined in the frame of reference connected with the crystal lattice, they are invariant under the RBR. For polycrystals we can use the method proposed [Levitas (1986, 1987, 1992b, 1992c, 1996b)].

It is possible to define the order parameter ξ e.g. as

$$\xi := \frac{|\mathbf{F}_{t\tau}|}{|\mathbf{F}_{t\tau\max}|} \tag{31}$$

in order to be sure that all variable components of transformation deformation gradient have participated in the definition of ξ. The specific Helmholtz free energy and the Clausius–Duhem inequality at finite strains:

$$\psi = \psi(\mathbf{F}_{e\tau}(\xi), \theta(\xi), \mathbf{F}_{p\tau}(\xi), \mathbf{g}_\tau(\xi), \mathbf{F}_{t\tau}(\xi), \xi), \tag{32}$$

$$\rho_\tau \mathscr{D} = \mathbf{P}^t : \dot{\mathbf{F}}_\tau - \rho_\tau \dot{\psi} - \rho_\tau s \dot{\theta} - \frac{\mathbf{\nabla}_\tau \theta}{\theta} \cdot \mathbf{h}_\tau \geqslant 0. \tag{33}$$

Here, **P** is the first Piola–Kirchhoff nonsymmetric stress tensor with respect to the reference configuration. Substitution of the rate of free energy ψ and allowance for the multiplicative decomposition (29) and

$$\dot{\mathbf{F}}_{\theta\tau} = \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \theta} \dot{\theta} + \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \xi} \dot{\xi}$$

in eqn (33) yield

$$\begin{aligned}
\rho_\tau \mathscr{D} = {} & \left(\mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{t\tau} \cdot \mathbf{F}_{p\tau} \cdot \mathbf{F}_{p1\tau} \cdot \mathbf{P}^t - \rho \frac{\partial \psi}{\partial \mathbf{F}^t_{e\tau}} \right) : \dot{\mathbf{F}}_{e\tau} \\
& + \left(\mathbf{P}^t : \mathbf{F}_{e\tau} \cdot \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \theta} \cdot \mathbf{F}_{t\tau} \cdot \mathbf{F}_{p\tau} \cdot \mathbf{F}_{p1\tau} - \rho_\tau \frac{\partial \psi}{\partial \theta} - \rho_\tau s \right) \dot{\theta} \\
& + \Bigg(\mathbf{P}^t : \mathbf{F}_{e\tau} \cdot \mathbf{F}_{\theta\tau} \cdot \frac{\partial \mathbf{F}_{t\tau}}{\partial \xi} \cdot \mathbf{F}_{p\tau} \cdot \mathbf{F}_{p1\tau} \\
& + \mathbf{P}^t : \mathbf{F}_{e\tau} \cdot \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \xi} \cdot \mathbf{F}_{t\tau} \cdot \mathbf{F}_{p\tau} \cdot \mathbf{F}_{p1\tau} - \rho_\tau \frac{\partial \psi}{\partial \mathbf{F}^t_{t\tau}} : \frac{\partial \mathbf{F}_{t\tau}}{\partial \xi} - \rho_\tau \frac{\partial \psi}{\partial \xi} \Bigg) \dot{\xi} \\
& + \left(\mathbf{F}_{p1\tau} \cdot \mathbf{P}^t \cdot \mathbf{F}_{e\tau} \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{t\tau} - \rho_\tau \frac{\partial \psi}{\partial \mathbf{F}^t_{p\tau}} \right) : \dot{\mathbf{F}}_{p\tau} - \frac{\mathbf{\nabla}_\tau \theta}{\theta} \cdot \mathbf{h}_\tau - \rho_\tau \frac{\partial \psi}{\partial \mathbf{g}^t_\tau} : \dot{\mathbf{g}}_\tau \geqslant 0.
\end{aligned} \tag{34}$$

The possibility of permutation of tensors in a scalar product is used, $\mathbf{P}^t : \dot{\mathbf{F}}_{e\tau} \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{t\tau} \cdot \mathbf{F}_{p\tau} \cdot \mathbf{F}_{p1\tau} = \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{t\tau} \cdot \mathbf{F}_{p\tau} \cdot \mathbf{F}_{p1\tau} \cdot \mathbf{P}^t : \dot{\mathbf{F}}_{e\tau} = \mathbf{F}_{e\tau}^{-1} \cdot \mathbf{F}_\tau \cdot \mathbf{P}^t : \dot{\mathbf{F}}_{e\tau}$ (decomposition (29) is taken into account). The assumption that the rate of dissipation is independent of $\dot{\mathbf{F}}_{e\tau}$ and $\dot{\theta}$ results in the hyperelasticity law and the expression for entropy, as well as in the reduced dissipative inequality:

$$\mathbf{F}_{e\tau}^{-1} \cdot \mathbf{F}_\tau \cdot \mathbf{P}^t = \rho_\tau \frac{\partial \psi}{\partial \mathbf{F}^t_{e\tau}}; \quad s = -\frac{\partial \psi}{\partial \theta} + \frac{1}{\rho_\tau} \mathbf{P}^t : \mathbf{F}_{e\tau} \cdot \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \theta} \cdot \mathbf{F}_{t\tau} \cdot \mathbf{F}_{p\tau} \cdot \mathbf{F}_{p1\tau}; \tag{35}$$

$$\mathscr{D} = \mathbf{X}_{p\tau} : \dot{\mathbf{F}}_{p\tau} + \mathbf{X}_{g\tau} : \dot{\mathbf{g}}_\tau + \mathbf{X}_{h\tau} \cdot \mathbf{h}_\tau + X_\xi \dot{\xi} \geqslant 0, \tag{36}$$

where

$$\mathbf{X}_{p\tau} = \frac{1}{\rho_\tau} \mathbf{F}_{p1\tau} \cdot \mathbf{P}^t \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{t\tau} - \frac{\partial \psi}{\partial \mathbf{F}^t_{p\tau}}; \quad \mathbf{X}_{g\tau} = -\frac{\partial \psi}{\partial \mathbf{g}^t_\tau}; \quad \mathbf{X}_{h\tau} = -\frac{1}{\rho_\tau} \frac{\mathbf{\nabla}_\tau \theta}{\theta} \tag{37}$$

and

$$X_\xi = \frac{1}{\rho_\tau} \mathbf{P}^t \cdot \mathbf{F}_{e\tau} : \left(\frac{\partial \mathbf{F}_{\theta\tau}}{\partial \xi} \cdot \mathbf{F}_{t\tau} + \mathbf{F}_{\theta\tau} \cdot \frac{\partial \mathbf{F}_{t\tau}}{\partial \xi} \right) \cdot \mathbf{F}_{p\tau} \cdot \mathbf{F}_{p1\tau} - \frac{\partial \psi}{\partial \mathbf{F}^t_{t\tau}} : \frac{\partial \mathbf{F}_{t\tau}}{\partial \xi} - \frac{\partial \psi}{\partial \xi} \tag{38}$$

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

$$\dot{\mathbf{F}}_{\mathrm{p}\tau} = \mathbf{f}_{\mathrm{p}\tau}(\mathbf{X}_{\mathrm{p}\tau}, \xi)\,; \quad \dot{\mathbf{g}}_{\tau} = \mathbf{f}_{\mathrm{g}\tau}(\mathbf{X}_{\mathrm{g}\tau}, \xi)\,; \quad \mathbf{h}_{\tau} = \mathbf{f}_{\mathrm{h}\tau}(\mathbf{X}_{\mathrm{h}\tau}, \xi)\,; \quad \dot{\xi} = f_{\xi}(X_{\xi}, \xi), \tag{39}$$

similar to eqn (12). Equation (17) and the definition of the driving force for PT X (14) are valid. Using eqn (38) for X_{ξ}, the following form of the PT criterion

$$X = \int_{\mathbf{F}_{\mathrm{t}1\tau}}^{\mathbf{F}_{\mathrm{t}2\tau}} \left(\frac{1}{\rho_\tau}\mathbf{F}_{\mathrm{p}\tau}\cdot\mathbf{F}_{\mathrm{pl}\tau}\cdot\mathbf{P}^{\mathrm{t}}\cdot\mathbf{F}_{\mathrm{e}\tau}\cdot\mathbf{F}_{\theta\tau} - \frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{t}}_{\mathrm{t}\tau}}\right) : \mathrm{d}\mathbf{F}_{\mathrm{t}\tau}$$
$$+ \int_0^1 \left(\frac{1}{\rho_\tau}\mathbf{F}_{\mathrm{t}\tau}\cdot\mathbf{F}_{\mathrm{p}\tau}\cdot\mathbf{F}_{\mathrm{pl}\tau}\cdot\mathbf{P}^{\mathrm{t}}\cdot\mathbf{F}_{\mathrm{e}\tau} : \frac{\partial\mathbf{F}_{\theta\tau}}{\partial\xi} - \frac{\partial\psi}{\partial\xi}\right)\mathrm{d}\xi = k \tag{40}$$

is obtained. The alternative expression for X follows from eqns (33) and (36)

$$X_{\xi}\dot{\xi} = \mathscr{D} - \mathbf{X}_{\mathrm{p}\tau} : \dot{\mathbf{F}}_{\mathrm{p}\tau} - \mathbf{X}_{\mathrm{g}\tau} : \dot{\mathbf{g}}_{\tau} - \mathbf{X}_{\mathrm{h}\tau}\cdot\mathbf{h}_{\tau} = \frac{1}{\rho_\tau}\mathbf{P}^{\mathrm{t}} : \dot{\mathbf{F}}_{\tau} - \dot{\psi} - s\dot{\theta} - \mathbf{X}_{\mathrm{p}\tau} : \dot{\mathbf{F}}_{\mathrm{p}\tau} - \mathbf{X}_{\mathrm{g}\tau} : \dot{\mathbf{g}}_{\tau}\,; \tag{41}$$

$$X = \int_{\mathbf{F}_{1\tau}}^{\mathbf{F}_{2\tau}} \frac{1}{\rho_\tau}\mathbf{P}^{\mathrm{t}} : \mathrm{d}\mathbf{F}_{\tau} - (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta - \int_0^{t_{\mathrm{p}}} (\mathbf{X}_{\mathrm{p}\tau} : \dot{\mathbf{F}}_{\mathrm{p}\tau} + \mathbf{X}_{\mathrm{g}\tau} : \dot{\mathbf{g}}_{\tau})\,\mathrm{d}t = k. \tag{42}$$

Taking into account the decomposition (29) and eqn $(37)_1$ for $\mathbf{X}_{\mathrm{p}\tau}$ we obtain

$$X = \int_{\mathbf{F}_{1\tau}}^{\mathbf{F}_{2\tau}} \frac{1}{\rho_\tau}\mathbf{P}^{\mathrm{t}} : (\mathrm{d}\mathbf{F}_{\mathrm{e}\tau}\cdot\mathbf{F}_{\theta\tau}\cdot\mathbf{F}_{\mathrm{t}\tau} + \mathbf{F}_{\mathrm{e}\tau}\cdot\mathrm{d}\mathbf{F}_{\theta\tau}\cdot\mathbf{F}_{\mathrm{t}\tau} + \mathbf{F}_{\mathrm{e}\tau}\cdot\mathbf{F}_{\theta\tau}\cdot\mathrm{d}\mathbf{F}_{\mathrm{t}\tau})\cdot\mathbf{F}_{\mathrm{p}\tau}\cdot\mathbf{F}_{\mathrm{pl}\tau}$$
$$- (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta + \int_{\mathbf{F}_{\mathrm{pl}\tau}}^{\mathbf{F}_{\mathrm{p}2\tau}} \frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{t}}_{\mathrm{p}\tau}} : \mathrm{d}\mathbf{F}_{\mathrm{p}\tau} + \int_{\mathbf{g}_{1\tau}}^{\mathbf{g}_{2\tau}} \frac{\partial\psi}{\partial\mathbf{g}^{\mathrm{t}}_{\tau}} : \mathrm{d}\mathbf{g}_{\tau} = k. \tag{43}$$

Assume that for the ith phase $\psi_i = \psi^{\mathrm{e}}_i(\mathbf{F}_{\mathrm{e}}, \mathbf{E}^{\mathrm{m}}_{i\tau}) + \psi^{\theta}_i(\theta, \mathbf{g}_{\tau}, \ldots)$, where $\mathbf{E}^{\mathrm{m}}_{i\tau}$ are the elasticity tensors of various orders. Then

$$\rho_\tau^{-1}\mathbf{P}^{\mathrm{t}} : \mathrm{d}\mathbf{F}_{\mathrm{e}\tau}\cdot\mathbf{F}_{\theta\tau}\cdot\mathbf{F}_{\mathrm{t}\tau}\cdot\mathbf{F}_{\mathrm{p}\tau}(\xi)\cdot\mathbf{F}_{\mathrm{pl}\tau} = \frac{\partial\psi^{\mathrm{e}}}{\partial\mathbf{F}^{\mathrm{t}}_{\mathrm{e}\tau}} : \mathrm{d}\mathbf{F}_{\mathrm{e}\tau} = \mathrm{d}\psi^{\mathrm{e}} - \frac{\partial\psi^{\mathrm{e}}}{\partial\mathbf{E}^{\mathrm{m}}_{\tau}} \ldots \mathrm{d}\mathbf{E}^{\mathrm{m}}_{\tau} \tag{44}$$

$$\int_{\mathbf{F}_{\mathrm{e}1\tau}}^{\mathbf{F}_{\mathrm{e}2\tau}} \frac{1}{\rho_\tau}\mathbf{P}^{\mathrm{t}} : \mathrm{d}\mathbf{F}_{\mathrm{e}\tau}\cdot\mathbf{F}_{\theta\tau}\cdot\mathbf{F}_{\mathrm{t}\tau}\cdot\mathbf{F}_{\mathrm{p}\tau}(\xi)\cdot\mathbf{F}_{\mathrm{pl}\tau} = \psi^{\mathrm{e}}(\mathbf{F}_{\mathrm{e}2\tau}) - \psi^{\mathrm{e}}(\mathbf{F}_{\mathrm{e}1\tau}) - \int_0^1 \frac{\partial\psi^{\mathrm{e}}}{\partial\mathbf{E}^{\mathrm{m}}_{\tau}} \ldots \mathrm{d}\mathbf{E}^{\mathrm{m}}_{\tau}(\xi) \tag{45}$$

and

$$X = \int_{\mathbf{F}_{1\tau}}^{\mathbf{F}_{2\tau}} \frac{1}{\rho_{\mathrm{s}}}(\mathbf{F}_{\mathrm{p}\tau}(\xi)\cdot\mathbf{F}_{\mathrm{pl}\tau}\cdot\mathbf{P}^{\mathrm{t}}\cdot\mathbf{F}_{\mathrm{e}\tau}) : (\mathrm{d}\mathbf{F}_{\theta\tau}\cdot\mathbf{F}_{\mathrm{t}\tau} + \mathbf{F}_{\theta\tau}\cdot\mathrm{d}\mathbf{F}_{\mathrm{t}\tau})$$
$$- \int_0^1 \frac{\partial\psi^{\mathrm{e}}}{\partial\mathbf{E}^{\mathrm{m}}_{\tau}} \ldots \mathrm{d}\mathbf{E}^{\mathrm{m}}_{\tau} - (\psi^{\theta}_2 - \psi^{\theta}_1) - \int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta + \int_{\mathbf{F}_{\mathrm{pl}\tau}}^{\mathbf{F}_{\mathrm{p}2\tau}} \frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{t}}_{\mathrm{p}\tau}} : \mathrm{d}\mathbf{F}_{\mathrm{p}\tau} + \int_{\mathbf{g}_{1\tau}}^{\mathbf{g}_{2\tau}} \frac{\partial\psi}{\partial\mathbf{g}^{\mathrm{t}}_{\tau}} : \mathrm{d}\mathbf{g}_{\tau} = k. \tag{46}$$

At small strains and rotation

$$\mathbf{F}_{\tau} = \mathbf{I} + \boldsymbol{\varepsilon}, \quad \mathbf{F}_{\mathrm{e}\tau} = \mathbf{I} + \boldsymbol{\varepsilon}_{\mathrm{e}}, \quad \mathbf{F}_{\theta\tau} = \mathbf{I} + \boldsymbol{\varepsilon}_{\theta}, \quad \mathbf{F}_{\mathrm{t}\tau} = \mathbf{I} - \boldsymbol{\varepsilon}_{\mathrm{t}},$$
$$\mathbf{F}_{\mathrm{p}\tau}(\xi) = \mathbf{I} + \boldsymbol{\varepsilon}_{\mathrm{p}}(\xi), \quad \boldsymbol{\varepsilon}_{\mathrm{pl}\tau} = \mathbf{I} + \boldsymbol{\varepsilon}_{\mathrm{pl}}, \quad \mathbf{F}_{\mathrm{p}\tau}\cdot\mathbf{F}_{\mathrm{pl}\tau} = \mathbf{I} + \boldsymbol{\varepsilon}_{\mathrm{p}}, \quad \boldsymbol{\varepsilon}_{\mathrm{p}} := \boldsymbol{\varepsilon}_{\mathrm{p}}(\xi) + \boldsymbol{\varepsilon}_{\mathrm{pl}}, \tag{47}$$

where $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}_{\mathrm{e}}$, ε_{θ}, $\boldsymbol{\varepsilon}_{\mathrm{t}}$, $\boldsymbol{\varepsilon}_{\mathrm{p}}(\xi)$, $\boldsymbol{\varepsilon}_{\mathrm{pl}}$, $\boldsymbol{\varepsilon}_{\mathrm{p}} \ll \mathbf{I}$, $\mathbf{P} = \boldsymbol{\sigma}$, $\mathbf{P}^{\mathrm{t}} : \dot{\mathbf{F}}_{\tau} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}$, reference and actual configurations coincide and eqns (29)–(46) coincide with the corresponding equations of Section 2.1.

2.3. *Finite strains description in the actual configuration*

All tensors in the actual configuration V are dependent on the RBR in V. To avoid the problems related to the choice of the objective time derivative we will use the method suggested [Levitas (1986, 1987, 1992b, 1992c, 1996b)]. We will derive all equations for the case of finite strains without rotations (i.e. in some rotating frame of reference) using the usual material time derivative, then going back to the fixed frame of reference we obtain equations in the actual configuration with some objective corotational rate. We assume that tensors $\mathbf{F}_{\theta\tau}$, $\mathbf{F}_{t\tau}$, $\mathbf{F}_{p\tau}(\xi)$ and $\mathbf{F}_{pl\tau}$ are defined for the finite strain without rotation in each intermediate configuration, i.e. they are invariant under the RBR in each intermediate configuration. To exclude the RBR in the actual configuration let us consider the motion of a homogeneously deformed particle in the rotating frame of reference δ in which $\mathbf{r}_\delta = \mathbf{R}_e^t \cdot \mathbf{r}$, where $\mathbf{R}_e^t$ is the orthogonal tensor defined by polar decomposition $\mathbf{F}_{e\tau} = \mathbf{R}_e \cdot \mathbf{U}_e$ with $\mathbf{U}_e$ for the elastic right stretch tensor. Expressions for the tensors in the system δ can be obtained in a simple way. If under the RBR $\mathbf{r}^* = \mathbf{Q} \cdot \mathbf{r}$ the tensors are transformed under some rule, i.e.

$$\mathbf{T}^* = \mathbf{Q} \cdot \mathbf{T} \cdot \mathbf{Q}^t; \quad \mathbf{d}^* = \mathbf{Q} \cdot \mathbf{d} \cdot \mathbf{Q}^t; \quad \mathbf{F}_\tau^* = \mathbf{Q} \cdot \mathbf{F}_\tau, \tag{48}$$

then to obtain the expressions for them in the system δ we should use $\mathbf{Q} = \mathbf{R}_e^t$:

$$\mathbf{T}_\delta = \mathbf{R}_e^t \cdot \mathbf{T} \cdot \mathbf{R}_e; \quad \mathbf{d}_\delta = \mathbf{R}_e^t \cdot \mathbf{d} \cdot \mathbf{R}_e; \quad \mathbf{F}_{\tau\delta} = \mathbf{R}_e^t \cdot \mathbf{F}_\tau. \tag{49}$$

Here $\mathbf{T}$ and $\mathbf{d} = (\dot{\mathbf{F}} \cdot \mathbf{F}^{-1})_s$ are the true Cauchy stress and the deformation rate tensors. The values without subscript τ ($\rho, \mathbf{T}, \mathbf{h}, \ldots$) relate to the actual configuration (exceptions are $\mathbf{R}_e$, $\mathbf{U}_e$ and $\mathbf{E}_e$). Kinematic decompositions in the system δ have the following form

$$\mathbf{F}_{\tau\delta} = \mathbf{R}_e^t \cdot \mathbf{F}_\tau = \mathbf{U}_e \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{t\tau} \cdot \mathbf{F}_{p\tau}(\xi) \cdot \mathbf{F}_{pl\tau}, \tag{50}$$

$$\begin{aligned} \mathbf{d}_\delta := (\dot{\mathbf{F}}_{\tau\delta} \cdot \mathbf{F}_{\tau\delta}^{-1})_s &= (\dot{\mathbf{U}}_e \cdot \mathbf{U}_e^{-1})_s + (\mathbf{U}_e \cdot \dot{\mathbf{F}}_{\theta\tau} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_e^{-1})_s \\ &+ (\mathbf{U}_e \cdot \mathbf{F}_{\theta\tau} \cdot \dot{\mathbf{F}}_{t\tau} \cdot \mathbf{F}_{t\tau}^{-1} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_e^{-1})_s + (\mathbf{U}_e \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{t\tau} \cdot \dot{\mathbf{F}}_{p\tau} \cdot \mathbf{F}_{p\tau}^{-1} \cdot \mathbf{F}_{t\tau}^{-1} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_e^{-1})_s. \end{aligned} \tag{51}$$

Since the temperature gradient plays no role in the PT criterion, then in the actual configuration instead of the Clausius–Duhem inequality

$$\rho\mathscr{D} = \mathbf{T} : \mathbf{d} - \rho\dot{\psi} - \rho s\dot{\theta} - \frac{\nabla\theta}{\theta} \cdot \mathbf{h} \geqslant 0 \tag{52}$$

we will use the Plank inequality. Then in the system δ

$$\rho\mathscr{D} = \mathbf{T}_\delta : \mathbf{d}_\delta - \rho\dot{\psi} - \rho s\dot{\theta} \geqslant 0. \tag{53}$$

The specific Helmholtz free energy in the rotated and fixed frames of reference is

$$\begin{aligned} \psi &= \psi(\mathbf{E}_e, \theta, \mathbf{F}_{p\tau}(\xi), \mathbf{g}_\tau(\xi), \mathbf{F}_{t\tau}, \mathbf{K}_\tau) \\ &= \psi(\mathbf{B}_e, \theta, \mathbf{F}_p(\xi), \mathbf{g}(\xi), \mathbf{F}_t, \mathbf{K}) \end{aligned} \tag{54}$$

where

$$\begin{aligned} &\mathbf{E}_e = 0.5(\mathbf{U}_e \cdot \mathbf{U}_e - \mathbf{I}), \quad \mathbf{B}_e = 0.5(\mathbf{V}_e \cdot \mathbf{V}_e - \mathbf{I}) = \mathbf{R}_e \cdot \mathbf{E}_e \cdot \mathbf{R}_e^t, \\ &\qquad \mathbf{V}_e = \mathbf{R}_e \cdot \mathbf{U}_e \cdot \mathbf{R}_e^t, \quad \mathbf{F}_t := \mathbf{R}_e \cdot \mathbf{F}_{t\tau} \cdot \mathbf{R}_e^t, \quad \mathbf{F}_p(\xi) := \mathbf{R}_e \cdot \mathbf{F}_{p\tau}(\xi) \cdot \mathbf{R}_e^t, \end{aligned} \tag{55}$$

and $\mathbf{K} = \mathbf{R}_e \cdot \mathbf{K}_\tau$ are the set of unit vectors describing the material's anisotropy. Vectors

$\mathbf{K}_\tau = \text{const}$ and they can be omitted in eqn (54), but vectors $\mathbf{K} \neq \text{const}$ and they should be the arguments of ψ in the actual configuration for the description of the initial anisotropy.

Substituting the rate of free energy $\dot{\psi}$ in eqn (53) and taking into account the relation $(\dot{\mathbf{U}}_\mathrm{e} \cdot \mathbf{U}_\mathrm{e}^{-1})_\mathrm{s} = \mathbf{U}_\mathrm{e}^{-1} \cdot \dot{\mathbf{E}}_\mathrm{e} \cdot \mathbf{U}_\mathrm{e}^{-1}$ we obtain

$$
\begin{aligned}
\rho \mathscr{D} = {} & \left(\mathbf{U}_\mathrm{e}^{-1} \cdot \mathbf{T}_\delta \cdot \mathbf{U}_\mathrm{e}^{-1} - \rho \frac{\partial \psi}{\partial \mathbf{E}_\mathrm{e}}\right) : \dot{\mathbf{E}}_\mathrm{e} \\
& + \left(\mathbf{T}_\delta : \left(\mathbf{U}_\mathrm{e} \cdot \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \theta} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1}\right)_\mathrm{s} - \rho \frac{\partial \psi}{\partial \theta} - \rho s\right) \dot{\theta} \\
& + \left(\mathbf{T}_\delta : \left(\mathbf{U}_\mathrm{e} \cdot \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \xi} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1}\right)_\mathrm{s} + \mathbf{T}_\delta : \left(\mathbf{U}_\mathrm{e} \cdot \mathbf{F}_{\theta\tau} \cdot \frac{\partial \mathbf{F}_{\mathrm{t}\tau}}{\partial \xi} \cdot \mathbf{F}_{\mathrm{t}\tau}^{-1} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1}\right)_\mathrm{s}\right. \\
& \left. - \rho \frac{\partial \psi}{\partial \mathbf{F}_{\mathrm{t}\tau}^\mathrm{t}} : \frac{\partial \mathbf{F}_{\mathrm{t}\tau}}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi}\right) \dot{\xi} \\
& + \left(\mathbf{F}_{\mathrm{p}\tau}^{-1} \cdot \mathbf{F}_{\mathrm{t}\tau}^{-1} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1} \cdot \mathbf{T}_\delta \cdot \mathbf{U}_\mathrm{e} \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{\mathrm{t}\tau} - \rho \frac{\partial \psi}{\partial \mathbf{F}_{\mathrm{p}\tau}^\mathrm{t}}\right) : \dot{\mathbf{F}}_{\mathrm{p}\tau} - \rho \frac{\partial \psi}{\partial \mathbf{g}_\tau^\mathrm{t}} : \dot{\mathbf{g}}_\tau \geqslant 0 ;
\end{aligned}
\tag{56}
$$

$$
\mathbf{T}_\delta = \rho \mathbf{U}_\mathrm{e} \cdot \frac{\partial \psi}{\partial \mathbf{E}_\mathrm{e}} \cdot \mathbf{U}_\mathrm{e}, \quad s = -\frac{\partial \psi}{\partial \theta} + \frac{1}{\rho} \mathbf{T}_\delta : \left(\mathbf{U}_\mathrm{e} \cdot \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \theta} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1}\right)_\mathrm{s} ;
\tag{57}
$$

$$
\mathscr{D} = X_\xi \dot{\xi} + \mathbf{X}_{\mathrm{p}\tau} : \dot{\mathbf{F}}_{\mathrm{p}\tau} + \mathbf{X}_{\mathrm{g}\tau} : \dot{\mathbf{g}}_\tau \geqslant 0,
\tag{58}
$$

$$
\begin{aligned}
X_\xi = {} & \frac{1}{\rho} \mathbf{T}_\delta : \left(\mathbf{U}_\mathrm{e} \cdot \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \xi} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1}\right)_\mathrm{s} + \frac{1}{\rho} \mathbf{T}_\delta : \left(\mathbf{U}_\mathrm{e} \cdot \mathbf{F}_{\theta\tau} \cdot \frac{\partial \mathbf{F}_{\mathrm{t}\tau}}{\partial \xi} \cdot \mathbf{F}_{\mathrm{t}\tau}^{-1} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1}\right)_\mathrm{s} \\
& - \frac{\partial \psi}{\partial \mathbf{F}_{\mathrm{t}\tau}^\mathrm{t}} : \frac{\partial \mathbf{F}_{\mathrm{t}\tau}}{\partial \xi} - \frac{\partial \psi}{\partial \xi} ;
\end{aligned}
\tag{59}
$$

$$
\mathbf{X}_{\mathrm{p}\delta} = \frac{1}{\rho} \mathbf{F}_{\mathrm{p}\tau}^{-1} \cdot \mathbf{F}_{\mathrm{t}\tau}^{-1} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1} \cdot \mathbf{T}_\delta \cdot \mathbf{U}_\mathrm{e} \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{\mathrm{t}\tau} - \frac{\partial \psi}{\partial \mathbf{F}_{\mathrm{p}\tau}^\mathrm{t}} ; \quad \mathbf{X}_{\mathrm{g}\tau} = -\frac{\partial \psi}{\partial \mathbf{g}_\tau^\mathrm{t}} .
\tag{60}
$$

Due to the equivalence of stress power $\rho_\tau^{-1} \mathbf{P}^\mathrm{t} : \dot{\mathbf{F}} \, \mathrm{d}t = \rho^{-1} \mathbf{T}_\delta : \mathbf{d}_\delta \, \mathrm{d}t$ we obtain from eqn (42)

$$
X = \int_0^{t_\mathrm{p}} \frac{1}{\rho} \mathbf{T}_\delta : \mathbf{d}_\delta \, \mathrm{d}t - (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} s \, \mathrm{d}\theta - \int_0^{t_\mathrm{p}} (\mathbf{X}_{\mathrm{p}\tau} : \dot{\mathbf{F}}_{\mathrm{p}\tau} + \mathbf{X}_{\mathrm{g}\tau} : \dot{\mathbf{g}}_\tau) \, \mathrm{d}t = k.
\tag{61}
$$

Using eqns (51) and $(60)_1$ we transform

$$
\begin{aligned}
X = {} & \int_0^{t_\mathrm{p}} \frac{1}{\rho} \mathbf{T}_\delta : ((\dot{\mathbf{U}}_\mathrm{e} \cdot \mathbf{U}_\mathrm{e}^{-1})_\mathrm{s} + (\mathbf{U}_\mathrm{e} \cdot \dot{\mathbf{F}}_{\theta\tau} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1})_\mathrm{s} + (\mathbf{U}_\mathrm{e} \cdot \mathbf{U}_{\theta\tau} \cdot \dot{\mathbf{F}}_{\mathrm{t}\tau} \cdot \mathbf{F}_{\mathrm{t}\tau}^{-1} \cdot \mathbf{F}_{\theta\tau}^{-1} \cdot \mathbf{U}_\mathrm{e}^{-1})_\mathrm{s}) \, \mathrm{d}t \\
& - (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} s \, \mathrm{d}\theta + \int_{\mathbf{F}_{\mathrm{p}1\tau}}^{\mathbf{F}_{\mathrm{p}2\tau}} \frac{\partial \psi}{\partial \mathbf{F}_{\mathrm{p}\tau}^\mathrm{t}} : \mathrm{d}\mathbf{F}_{\mathrm{p}\tau} + \int_{\mathbf{g}_{1\tau}}^{\mathbf{g}_{2\tau}} \frac{\partial \psi}{\partial \mathbf{g}_\tau^\mathrm{t}} : \mathrm{d}\mathbf{g}_\tau = k.
\end{aligned}
\tag{62}
$$

Now we transform all the equations to the fixed frame of reference, i.e. express them through the indifferent tensors. For the deformation gradient we have

$$
\begin{aligned}
\mathbf{F}_\tau & = \mathbf{V}_\mathrm{e} \cdot (\mathbf{R}_\mathrm{e} \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{R}_\mathrm{e}^\mathrm{t}) \cdot (\mathbf{R}_\mathrm{e} \cdot \mathbf{F}_{\mathrm{t}\tau} \cdot \mathbf{R}_\mathrm{e}^\mathrm{t}) \cdot (\mathbf{R}_\mathrm{e} \cdot \mathbf{F}_{\mathrm{p}\tau}(\xi) \cdot \mathbf{R}_\mathrm{e}^\mathrm{t}) \cdot (\mathbf{R}_\mathrm{e} \cdot \mathbf{F}_{\mathrm{p}1\tau} \cdot \mathbf{R}_\mathrm{e}^\mathrm{t}) \cdot \mathbf{R}_\mathrm{e} \\
& = \mathbf{V}_\mathrm{e} \cdot \mathbf{F}_\theta \cdot \mathbf{F}_\mathrm{t} \cdot \mathbf{F}_\mathrm{p}(\xi) \cdot \mathbf{F}_{\mathrm{p}1} \cdot \mathbf{R}_\mathrm{e},
\end{aligned}
\tag{63}
$$

with $\mathbf{F}_\theta := \mathbf{R}_e \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{R}_e^t$ and $\mathbf{F}_{p1} := \mathbf{R}_e \cdot \mathbf{F}_{p1\tau} \cdot \mathbf{R}_e^t$. Introducing $\mathbf{X}_p := \mathbf{R}_e \cdot \mathbf{X}_{p\tau} \cdot \mathbf{R}_e^t$ and using the transformations

$$\mathbf{X}_{p\tau} : \dot{\mathbf{F}}_{p\tau} = \mathbf{R}_e^t \cdot \mathbf{X}_p \cdot \mathbf{R}_e : \overline{(\mathbf{R}_e^t \cdot \mathbf{F}_p \cdot \mathbf{R}_e)}^{\boldsymbol{\cdot}} = \mathbf{X}_p : \mathbf{R}_e \cdot \overline{(\mathbf{R}_e^t \cdot \mathbf{F}_p \cdot \mathbf{R}_e)}^{\boldsymbol{\cdot}} \cdot \mathbf{R}_e^t = \mathbf{X}_p : \mathring{\mathbf{F}}_p, \tag{64}$$

where the corotational derivative

$$\mathring{\mathbf{F}}_p := \mathbf{R}_e \cdot \overline{(\mathbf{R}_e^t \cdot \mathbf{F}_p \cdot \mathbf{R}_e)}^{\boldsymbol{\cdot}} \cdot \mathbf{R}_e^t = \mathbf{R}_e \cdot (\dot{\mathbf{R}}_e^t \cdot \mathbf{F}_p \cdot \mathbf{R}_e + \mathbf{R}_e^t \cdot \dot{\mathbf{F}}_p \cdot \mathbf{R}_e + \mathbf{R}_e^t \cdot \mathbf{F}_p \cdot \dot{\mathbf{R}}_e) \cdot \mathbf{R}_e^t$$

$$= \dot{\mathbf{F}}_p + \mathbf{F}_p \cdot \mathbf{M} + \mathbf{M}^t \cdot \mathbf{F}_p, \tag{65}$$

is called the R-derivative [Levitas (1986, 1987, 1992, 1996b)], associated with the skew-symmetric spin tensor $\mathbf{M} = \dot{\mathbf{R}}_e \cdot \mathbf{R}_e^t = -\mathbf{M}^t = -\mathbf{R}_e \cdot \dot{\mathbf{R}}_e^t$. A similar objective derivative in finite elastoplasticity with the total rotation tensor was used for example in a paper by Green and Naghdi (1965). Direct calculations give

$$\mathscr{D} = X_\xi \dot{\xi} + \mathbf{X}_p : \mathring{\mathbf{F}}_p + \mathbf{X}_g : \mathring{\mathbf{g}}; \tag{66}$$

$$X_\xi = \frac{1}{\rho}\mathbf{T} : \left(\mathbf{V}_e \cdot \frac{\partial_R \mathbf{F}_\theta}{\partial \xi} \cdot \mathbf{F}_\theta^{-1} \cdot \mathbf{V}_e\right)_s + \frac{1}{\rho}\mathbf{T} : \left(\mathbf{V}_e \cdot \mathbf{F}_\theta \cdot \frac{\partial_R \mathbf{F}_t}{\partial \xi} \cdot \mathbf{F}_t^{-1} \cdot \mathbf{F}_\theta^{-1} \cdot \mathbf{V}_e^{-1}\right)_s$$

$$- \frac{\partial \psi}{\partial \mathbf{F}_t^t} : \frac{\partial_R \mathbf{F}_t}{\partial \xi} - \frac{\partial \psi}{\partial \xi}; \tag{67}$$

$$\mathbf{X}_p = \frac{1}{\rho}\mathbf{F}_p^{-1} \cdot \mathbf{F}_t^{-1} \cdot \mathbf{F}_\theta^{-1} \cdot \mathbf{V}_e^{-1} \cdot \mathbf{T} \cdot \mathbf{V}_e \cdot \mathbf{F}_\theta \cdot \mathbf{F}_t - \frac{\partial \psi}{\partial \mathbf{F}_p^t}; \tag{68}$$

$$\mathbf{X}_g := \mathbf{R}_e \cdot \mathbf{X}_{g\tau} \cdot \mathbf{R}_e^t = -\frac{\partial \psi}{\partial \mathbf{g}^t}; \tag{69}$$

$$\mathring{\mathbf{F}}_p = \mathbf{f}_p(\mathbf{X}_p); \quad \mathring{\mathbf{g}} = \mathbf{f}_g(\mathbf{X}_g); \tag{70}$$

$$\mathbf{T} = \rho \mathbf{V}_e \cdot \frac{\partial \psi}{\partial \mathbf{B}_e} \cdot \mathbf{V}_e, \quad s = -\frac{\partial \psi}{\partial \theta} + \frac{1}{\rho}\mathbf{T} : \left(\mathbf{V}_e \cdot \frac{\partial_R \mathbf{F}_\theta}{\partial \theta} \cdot \mathbf{F}_\theta^{-1} \cdot \mathbf{V}_e^{-1}\right)_s; \tag{71}$$

$$X = \int_0^1 \frac{1}{\rho}\left(\mathbf{T} : \left(\mathbf{V}_e \cdot \mathbf{F}_\theta \cdot \frac{\partial_R \mathbf{F}_t}{\partial \xi} \cdot \mathbf{F}_t^{-1} \cdot \mathbf{F}_\theta^{-1} \cdot \mathbf{V}_e^{-1}\right)_s + \mathbf{T} : \left(\mathbf{V}_e \cdot \frac{\partial_R \mathbf{F}_\theta}{\partial \xi} \cdot \mathbf{F}_\theta^{-1} \cdot \mathbf{V}_e^{-1}\right)_s\right.$$

$$\left. - \rho \frac{\partial \psi}{\partial \mathbf{F}_t^t} : \frac{\partial_R \mathbf{F}_t}{\partial \xi} - \rho \frac{\partial \psi}{\partial \xi}\right) \mathrm{d}\xi = k; \tag{72}$$

$$X = \int_0^{t_p} \frac{1}{\rho}\mathbf{T} : \mathbf{d}\,\mathrm{d}t - (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta - \int_0^{t_p} (\mathbf{X}_p : \mathring{\mathbf{F}}_p + \mathbf{X}_g : \mathring{\mathbf{g}})\,\mathrm{d}t = k; \tag{73}$$

$$X = \int_0^{t_p} \frac{1}{\rho}\mathbf{T} : ((\mathring{\mathbf{V}}_e \cdot \mathbf{V}_e^{-1})_s + (\mathbf{V}_e \cdot \mathring{\mathbf{F}}_\theta \cdot \mathbf{F}_\theta^{-1} \cdot \mathbf{V}_e^{-1})_s + (\mathbf{V}_e \cdot \mathbf{V}_\theta \cdot \mathring{\mathbf{F}}_t \cdot \mathbf{F}_t^{-1} \cdot \mathbf{V}_e^{-1})_s)\,\mathrm{d}t$$

$$- (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta + \int_0^{t_p} \frac{\partial \psi}{\partial \mathbf{F}_p^t} : \mathring{\mathbf{F}}_p\,\mathrm{d}t + \int_0^{t_p} \frac{\partial \psi}{\partial \mathbf{g}^t} : \mathring{\mathbf{g}}\,\mathrm{d}t = k; \tag{74}$$

with

$$\frac{\partial_{\mathrm{R}}\mathbf{F}_{\mathrm{t}}}{\partial\xi} := \mathbf{R}_{\mathrm{e}}\cdot\frac{\partial(\mathbf{R}_{\mathrm{e}}^{\mathrm{t}}\cdot\mathbf{F}_{\mathrm{t}}\cdot\mathbf{R}_{\mathrm{e}})}{\partial\xi}\cdot\mathbf{R}_{\mathrm{e}}^{\mathrm{t}} = \mathring{\mathbf{F}}_{\mathrm{t}}\frac{\mathrm{d}t}{\mathrm{d}\xi};\quad \frac{\partial_{\mathrm{R}}\mathbf{F}_{\theta}}{\partial\xi} = \mathring{\mathbf{F}}_{\theta|\theta=\mathrm{const}}\frac{\partial t}{\partial\xi};\quad \frac{\partial_{\mathrm{R}}\mathbf{F}_{\theta}}{\partial\theta} = \mathring{\mathbf{F}}_{\theta|\xi=\mathrm{const}}\frac{\partial t}{\partial\theta}. \tag{75}$$

We have used in calculations the known relation [see, e.g. Levitas (1996b)]

$$\mathbf{R}_{\mathrm{e}}\cdot\frac{\partial\psi(\mathbf{g}_{\tau},\ldots)}{\partial\mathbf{g}_{\tau}^{\mathrm{t}}}\cdot\mathbf{R}_{\mathrm{e}}^{\mathrm{t}} = \frac{\partial\psi(\mathbf{g},\ldots)}{\partial\mathbf{g}^{\mathrm{t}}} \tag{76}$$

and the same for $\mathbf{F}_{\mathrm{t}}$, $\mathbf{B}_{\mathrm{e}}$, $\mathbf{F}_{\mathrm{p}}$. The way to check eqns (66)–(76) is simple. If we consider them in the frame of reference δ they coincide with eqns (57)–(62).

Usually elastic and thermal strains are small, $\mathbf{V}_{\mathrm{e}} = \mathbf{I}+\boldsymbol{\varepsilon}_{\mathrm{e}}$, $\mathbf{V}_{\theta} = \mathbf{I}+\boldsymbol{\varepsilon}_{\theta}$, $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}_{\theta} \ll \mathbf{I}$. The we can simplify eqn (74)

$$X = \int_0^{t_{\mathrm{p}}}\frac{1}{\rho}\mathbf{T}:(\mathring{\boldsymbol{\varepsilon}}_{\mathrm{e}}+\mathring{\boldsymbol{\varepsilon}}_{\theta}+(\mathring{\mathbf{F}}_{\mathrm{t}}\cdot\mathbf{F}_{\mathrm{t}}^{-1})_{\mathrm{s}})\,\mathrm{d}t$$
$$-(\psi_2-\psi_1)-\int_{\theta_1}^{\theta_2}s\,\mathrm{d}\theta+\int_0^{t_{\mathrm{p}}}\frac{\partial\psi}{\partial\mathbf{F}_{\mathrm{p}}^{\mathrm{t}}}:\mathring{\mathbf{F}}_{\mathrm{p}}\,\mathrm{d}t+\int_0^{t_{\mathrm{p}}}\frac{\partial\psi}{\partial\mathbf{g}^{\mathrm{t}}}:\mathring{\mathbf{g}}\,\mathrm{d}t = k. \tag{77}$$

Let for ith phase $\psi_i = \psi_i(\mathbf{B}_{\mathrm{e}},\mathbf{E}_i^{\mathrm{m}})+\psi_i^{\theta}(\theta,\mathbf{g},\ldots)$ with $\mathbf{E}_i^{\mathrm{m}}$ for indifferent elasticity tensors of various orders. Then

$$\rho^{-1}\mathbf{T}:(\mathring{\mathbf{V}}_{\mathrm{e}}\cdot\mathbf{V}_{\mathrm{e}}^{-1})_{\mathrm{s}} = \rho^{-1}\mathbf{T}:\mathbf{V}_{\mathrm{e}}^{-1}\cdot(\mathring{\mathbf{V}}_{\mathrm{e}}\cdot\mathbf{V}_{\mathrm{e}})_{\mathrm{s}}\cdot\mathbf{V}_{\mathrm{e}}^{-1}$$
$$= \rho^{-1}\mathbf{V}_{\mathrm{e}}^{-1}\cdot\mathbf{T}\mathbf{V}_{\mathrm{e}}^{-1}:\mathring{\mathbf{B}}_{\mathrm{e}} = \frac{\partial\psi^{\mathrm{e}}}{\partial\mathbf{B}_{\mathrm{e}}}:\mathring{\mathbf{B}}_{\mathrm{e}} = \dot{\psi}-\frac{\partial\psi^{\mathrm{e}}}{\partial\mathbf{E}^{\mathrm{m}}}\ldots.\mathring{\mathbf{E}}^{\mathrm{m}}, \tag{78}$$

$$\int_0^{t_{\mathrm{p}}}\rho^{-1}\mathbf{T}:(\mathring{\mathbf{V}}_{\mathrm{e}}\mathbf{V}_{\mathrm{e}}^{-1})_{\mathrm{s}}\,\mathrm{d}t = \psi_2-\psi_1-\int_0^{t_{\mathrm{p}}}\frac{\partial\psi^{\mathrm{e}}}{\partial\mathbf{E}^{\mathrm{m}}}\ldots.\mathring{\mathbf{E}}^{\mathrm{m}}\,\mathrm{d}t \tag{79}$$

and eqn (74) can be concretized

$$X = \int_0^{t_{\mathrm{p}}}\frac{1}{\rho}\mathbf{T}:((\mathbf{V}_{\mathrm{e}}\cdot\mathring{\mathbf{F}}_{\theta}\cdot\mathbf{F}_{\theta}^{-1}\cdot\mathbf{V}_{\mathrm{e}}^{-1})_{\mathrm{s}}+(\mathbf{V}_{\mathrm{e}}\cdot\mathbf{V}_{\theta}\cdot\mathring{\mathbf{F}}_{\mathrm{t}}\cdot\mathbf{F}_{\mathrm{t}}^{-1}\cdot\mathbf{V}_{\mathrm{e}}^{-1})_{\mathrm{s}})\,\mathrm{d}t$$
$$-\int_0^{t_{\mathrm{p}}}\frac{\partial\psi^{\mathrm{e}}}{\partial\mathbf{E}^{\mathrm{m}}}\ldots.\mathring{\mathbf{E}}^{\mathrm{m}}\,\mathrm{d}t-(\psi_2^{\theta}-\psi_1^{\theta})-\int_{\theta_1}^{\theta_2}s\,\mathrm{d}\theta+\int_0^{t_{\mathrm{p}}}\frac{\partial\psi}{\partial\mathbf{F}_{\mathrm{p}}^{\mathrm{t}}}:\mathring{\mathbf{F}}_{\mathrm{p}}\,\mathrm{d}t+\int_0^{t_{\mathrm{p}}}\frac{\partial\psi}{\partial\mathbf{g}^{\mathrm{t}}}:\mathring{\mathbf{g}}\,\mathrm{d}t = k. \tag{80}$$

The transformations can be easily checked in the frame of reference δ.

3. DETERMINATION OF TEMPERATURE VARIATION

3.1. *Small strains*

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

$$\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}-\rho\dot{U}-\operatorname{div}\mathbf{h} = 0, \tag{81}$$

where U is the internal energy and div is the divergence operator; per definition $\psi = U-\theta s$. After substitution of this expression in eqn (4) we have

$$\rho\mathscr{D} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \rho\dot{U} + \rho\theta\dot{s} - \frac{\boldsymbol{\nabla}\theta}{\theta}\cdot\mathbf{h} \geqslant 0. \tag{82}$$

The combination of eqns (81) and (82) results in an entropy balance equation

$$\rho\theta\dot{s} = \rho\mathscr{D} - \operatorname{div}\mathbf{h} + \frac{\boldsymbol{\nabla}\theta}{\theta}\cdot\mathbf{h}. \tag{83}$$

Substitution of eqn (9) for the rate of dissipation $\mathscr{D}$ in eqn (83) yields

$$\rho\theta\dot{s} = -\operatorname{div}\mathbf{h} + \rho\mathbf{X}_{\mathrm{p}} : \dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} + \rho\mathbf{X}_{\mathrm{g}} : \dot{\mathbf{g}} + \rho X_{\xi}\dot{\xi}. \tag{84}$$

According to eqn $(8)_2$ $s = s(\theta, \boldsymbol{\sigma}, \mathbf{g}, \boldsymbol{\varepsilon}_{\mathrm{p}}, \xi)$. Substitution of this expression and eqn $(12)_3$ for the heat flux into eqn (84) leads to the temperature evolution equation

$$v\dot{\theta} = -\frac{1}{\rho}\operatorname{div}\mathbf{f}_{\mathrm{h}}\left(-\frac{\boldsymbol{\nabla}\theta}{\theta}\right) + \left(\mathbf{X}_{\mathrm{p}} - \frac{\partial s}{\partial \boldsymbol{\varepsilon}_{\mathrm{p}}}\theta\right) : \dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} + \left(\mathbf{X}_{\mathrm{g}} - \frac{\partial s}{\partial \mathbf{g}^{\mathrm{t}}}\theta\right) : \dot{\mathbf{g}}$$
$$+ \left(X_{\xi} - \frac{\partial s}{\partial \xi}\theta\right)\dot{\xi} - \theta\frac{\partial s}{\partial \boldsymbol{\sigma}} : \dot{\boldsymbol{\sigma}}, \quad v := \theta\frac{\partial s}{\partial \theta}, \tag{85}$$

where v is the specific heat.

For Fourier law $\mathbf{h} = -\lambda\boldsymbol{\nabla}\theta$ (i.e. $\mathbf{f}_{\mathrm{h}} = -\lambda\boldsymbol{\nabla}\theta$) is valid $-\operatorname{div}\mathbf{h} = \lambda\bar{\Delta}\theta$, where λ is the thermal conductivity and $\bar{\Delta}$ the Laplace operator.

Due to the divergence term the temperature in the given point can be defined after formulation and solution of a BVP. Taking into account a very short duration of the PT ($10^{-6} \sim 10^{-10}$ s), the *adiabatic* process can be assumed (similar to the processes in shock waves). In this case $\operatorname{div}\mathbf{h} = 0$ and eqn (85) determines the temperature evolution in each material point independently, i.e. without solution of a BVP.

A general scheme of application of the PT criterion (17) and temperature evolution equation (85) is as follows. All material properties, constitutive equations (12) and transformation strain $\boldsymbol{\varepsilon}_{\mathrm{t}}(\xi)$ should be given as a function of ξ. Then assume that at some stress $\boldsymbol{\sigma}_{\mathrm{s}}$ and temperature θ_{s} PT in the given point starts. Stress variation $\boldsymbol{\sigma}(\xi)$, as well as $\boldsymbol{\varepsilon}_{\mathrm{p}}(\xi)$, $\mathbf{g}(\xi)$, are determined by solution of a BVP or using some simplified models [e.g. Levitas (1995b)]. The temperature can be determined by solution of eqn (85). In the general case mechanical and thermal equations are *coupled* and should be considered together. After determination of all parameters for $0 \leqslant \xi \leqslant 1$ the criterion (17) allows us to determine (iteratively or explicitly) the temperature θ_{s} at the given $\boldsymbol{\sigma}_{\mathrm{s}}$ or one of the components of the stress tensor $\boldsymbol{\sigma}_{\mathrm{s}}$ with the remaining five components of $\boldsymbol{\sigma}_{\mathrm{s}}$ and the temperature θ_{s} given.

Let us consider some specifications and simplifications of eqn (85). Assume the validity of eqn (22) for the free energy with equal elastic properties of both phases and the following explicit expression for a thermal part of free energy [Fu *et al.* (1993)] for each phase

$$\psi_i^{\theta} = \psi_{0i} - s_{0i}(\theta - \theta_0) - v_i\theta(\ln\theta/\theta_0 - 1) - v_i\theta_0, \quad i = 1, 2. \tag{86}$$

Here $v_i > 0$ are the specific heats, s_{0i} and ψ_{0i} are the reference entropy and free energy at $\theta = \theta_0$. If the thermal expansion coefficient $\boldsymbol{\alpha}$ is independent of θ, then from eqn $(8)_2$ it follows

$$\rho s = \rho s_0(\xi) + \rho v(\xi)\ln\frac{\theta}{\theta_0} + \boldsymbol{\sigma} : \boldsymbol{\alpha}(\xi) \quad \text{and} \quad \theta\frac{\partial s}{\partial \theta} = v(\xi), \tag{87}$$

i.e. the accepted eqn $(85)_2$ 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 eqn (86).

Functions $s_0(\xi)$, $v(\xi)$ and $\boldsymbol{\alpha}(\xi)$ are usually unknown and we assume a linear approximation

$$s_0 = (1-\xi)s_{01}+\xi s_{02}, \quad v = (1-\xi)v_1+\xi v_2, \quad \boldsymbol{\alpha}(\xi) = (1-\xi)\boldsymbol{\alpha}_1+\xi\boldsymbol{\alpha}_2. \tag{88}$$

Then eqn (85) can be transformed into the form

$$v(\xi)\dot{\theta} = (X_\xi-\theta\,\Delta s_0-\Delta v\theta\ln\theta/\theta_0-\rho^{-1}\boldsymbol{\sigma}:\Delta\boldsymbol{\alpha}\theta)\dot{\xi}-\rho^{-1}\dot{\boldsymbol{\sigma}}:\boldsymbol{\alpha}(\xi)\theta+\mathbf{X}_{\mathrm{p}}:\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}}+\mathbf{X}_{\mathrm{g}}:\dot{\mathbf{g}}. \tag{89}$$

If ψ_i are independent of $\mathbf{g}$ and $\boldsymbol{\varepsilon}_{\mathrm{p}}$, the $\mathbf{X}_{\mathrm{g}} = 0$ and $\mathbf{X}_{\mathrm{p}} = \boldsymbol{\sigma}$. In this case eqn (16) is the most convenient form of X. The PT criterion results in

$$\frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_{\mathrm{t}1}}^{\boldsymbol{\varepsilon}_{\mathrm{t}2}}\boldsymbol{\sigma}:\mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{t}}+\frac{1}{\rho}\int_0^1\boldsymbol{\sigma}:\Delta\boldsymbol{\alpha}(\theta-\theta_0)\,\mathrm{d}\xi+(\Delta s_0-\Delta v)\int_0^1\theta\,\mathrm{d}\xi$$
$$+\Delta v\int_0^1\theta\ln\frac{\theta}{\theta_0}\mathrm{d}\xi = k+\Delta\psi_0+(\Delta s_0-\Delta v)\theta_0. \tag{90}$$

Equation (90) shows that the thermal expansion tensors of each phase do not affect the PT criterion, and only their difference contributes to the driving force. For an isothermal process at $\theta = \theta_0$ eqn (90) coincides with eqn (25) at $\psi_2^\theta-\psi_1^\theta = \Delta\psi_0$.

For isotropic $\boldsymbol{\alpha} = \alpha\mathbf{I}$ we have $\boldsymbol{\sigma}:\Delta\boldsymbol{\alpha} = 3\sigma_0\,\Delta\alpha$, $\dot{\boldsymbol{\sigma}}:\boldsymbol{\alpha} = 3\dot{\sigma}_0\alpha$, where σ_0 is a mean pressure and for fixed σ_0, for elastic materials and constant $X_\xi = k$ eqn (89) is independent of the stress variation

$$((1-\xi)v_1+\xi v_2)\dot{\theta} = (k-\theta\,\Delta s_0-\Delta v\theta\ln\theta/\theta_0-3\rho^{-1}\sigma_0\,\Delta\alpha\theta)\dot{\xi}. \tag{91}$$

Choosing a proper θ_0 we can meet the condition of smallness of (θ/θ_0-1) and, consequently, $\ln\theta/\theta_0 \simeq \theta/\theta_0-1$. In this case the temperature can be determined analytically, but the obtained equation is rather complicated for analysis. In the case $\Delta v = 0$ we have

$$\mathrm{d}\theta = (A+B\theta)\,\mathrm{d}\xi \quad \text{or}\ \theta = \left(\frac{A}{B}-\theta_{\mathrm{s}}\right)\exp(B\xi)-\frac{A}{B}, \tag{92}$$

where $A = k/v$, $B = -(1)/(\rho v)\ (\rho\,\Delta s_0+3\sigma_0\,\Delta\alpha)$. PT criterion at $\Delta v = 0$ reads as

$$\frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_{\mathrm{t}1}}^{\boldsymbol{\varepsilon}_{\mathrm{t}2}}\boldsymbol{\sigma}:\mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{t}} = vB\int_0^1\theta\,\mathrm{d}\xi+k+\Psi, \tag{93}$$

where $\Psi = (\Delta\psi_0+\Delta s_0\theta_0)+3\rho^{-1}\sigma_0\,\Delta\alpha\theta_0$, or taking into account eqn (92)

$$\frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_{\mathrm{t}1}}^{\boldsymbol{\varepsilon}_{\mathrm{t}2}}\boldsymbol{\sigma}:\mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{t}} = v\left(\frac{A}{B}+\theta_{\mathrm{s}}\right)(\exp B-1)-vA+k+\Psi = v(\theta_{\mathrm{f}}-\theta_{\mathrm{s}})-vA+k+\Psi, \tag{94}$$

where $\theta_{\mathrm{f}} = \theta(1)$ is a final temperature after the end of PT, determined by eqn (92) at $\xi = 1$.

For rigid-plastic materials, when a plastic power can be expressed in the form $\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} = \boldsymbol{\sigma}:\boldsymbol{\varepsilon}_{\mathrm{p}}\dot{\xi}$ with a constant value of specific plastic work $A_{\mathrm{p}} = \rho^{-1}\boldsymbol{\sigma}:\boldsymbol{\varepsilon}_{\mathrm{p}}$, then eqns (92)–(94) are valid at $A = (k+A_{\mathrm{p}})/v$. In eqn (94) $-vA+k = 0$ for elastic materials and $-vA+k = A_{\mathrm{p}}$ for rigid-plastic materials.

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

$$\theta = \theta_s + (A + B\theta_s)\xi; \quad \frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_t = vB\theta_s + k + \Psi. \tag{95}$$

Despite the temperature variation, the PT criterion $(95)_2$ has the same form as in the case of an isothermal process. The first contribution of the temperature variation to the PT criterion can be obtained at $\exp B \simeq 1 + B + 0.5B^2$; in this case we have

$$\frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_t = (vB\theta_s + k)(1 + 0.5B) + \Psi. \tag{96}$$

It is possible to choose the reference temperature from the condition $\Delta\psi^\theta(\theta_0) = 0$, from which $\Delta\psi_0 = 0$. Simple analytical results can also be obtained at variable pressure if we assume $\alpha_1 = \alpha_2 = 0$. In this case in eqns (90) and (91) $\Delta\alpha = 0$, and at $\Delta v = 0$ eqns (92)–(95) are valid at

$$A = \frac{k}{v}, \quad B = -\frac{\Delta s_0}{v}, \quad \frac{A}{B} = -\frac{k}{\Delta s_0}, \quad \Psi = \Delta s_0\theta_0, \tag{97}$$

i.e.

$$\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_t = \rho v\left(\theta_s - \frac{k}{\Delta s_0}\right)\left(\exp\left(-\frac{\Delta s_0}{v}\right) - 1\right) + \rho\,\Delta s_0\theta_0, \tag{98}$$

$$\theta = \left(\theta_s - \frac{k}{\Delta s_0}\right)\exp\left(-\frac{\Delta s_0}{v}\xi\right) + \frac{k}{\Delta s_0}. \tag{99}$$

For the isothermal case eqn (98) yields

$$\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_t = \rho k - \rho\,\Delta s_0(\theta_s - \theta_0). \tag{100}$$

Allowance for temperature variation in the first approximation (eqns (95) and (96)) results in

$$\theta = \theta_s + \frac{1}{v}(k - \Delta s_0\theta_s)\xi; \tag{101}$$

$$\frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_t = k - \Delta s_0(\theta_s - \theta_0) - 0.5\frac{\Delta s_0}{v}(k - \Delta s_0\theta_s). \tag{102}$$

When PT occurs at $\boldsymbol{\sigma} = \text{const}$, then the anisotropy of $\boldsymbol{\alpha}$ does not complicate the results. Equation (92) is valid at

$$A = \frac{k + A_p}{v}, \quad B = -\frac{1}{\rho v}(\rho\Delta s_0 + \boldsymbol{\sigma} : \Delta\boldsymbol{\alpha}) \quad \Psi = (\Delta\psi_0 + \Delta s_0\theta_0) + \rho^{-1}\boldsymbol{\sigma} : \Delta\boldsymbol{\alpha}\theta_0 \tag{103}$$

and PT criterion has the form

$$\boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t = \sigma_0\varepsilon_0 + \mathbf{S} : \mathbf{e}_t = \rho v(A/B + \theta_s)(\exp B - 1) - \rho A_p + \rho\Psi, \tag{104}$$

where $\mathbf{S} = \operatorname{dev}\boldsymbol{\sigma}$, $\varepsilon_0 = \mathbf{I} : \boldsymbol{\varepsilon}_t$ is the volumetric transformation strain.

3.2. *Large strains*

At finite strains in the reference configuration instead of eqns (85), (87)–(90) we obtain

$$\nu\dot{\theta} = \left(\mathbf{X}_{\mathrm{p}\tau} - \frac{\partial s}{\partial \mathbf{F}^{\mathrm{t}}_{\mathrm{p}\tau}}\theta\right) : \dot{\mathbf{F}}_{\mathrm{p}\tau} + \left(\mathbf{X}_{\mathrm{g}\tau} - \frac{\partial s}{\partial \mathbf{g}^{\mathrm{t}}_{\tau}}\theta\right) : \dot{\mathbf{g}}_{\tau} + \left(X_{\xi} - \frac{\partial s}{\partial \xi}\theta\right)\dot{\xi} - \theta\frac{\partial s}{\partial \mathbf{P}^{\mathrm{t}}} : \dot{\mathbf{P}}; \tag{105}$$

$$\rho s = \rho s_0(\xi) + \rho\nu(\xi)\ln\frac{\theta}{\theta_0} + \mathbf{P}^{\mathrm{t}} : \mathbf{F}_{\mathrm{e}\tau} \cdot \frac{\partial \mathbf{F}_{\theta\tau}}{\partial \theta} \cdot \mathbf{F}_{\mathrm{t}\tau} \cdot \mathbf{F}_{\mathrm{p}\tau} \cdot \mathbf{F}_{\mathrm{p}1\tau}; \tag{106}$$

$$\mathbf{F}_{\theta\tau} = \mathbf{I} + \boldsymbol{\alpha}_{\tau}(\theta - \theta_0); \quad \boldsymbol{\alpha}_{\tau} = (1-\xi)\boldsymbol{\alpha}_{1\tau} + \xi\boldsymbol{\alpha}_{2\tau}; \tag{107}$$

$$\begin{aligned} \nu(\xi)\dot{\theta} = {} & \left(X_{\xi} - \theta\,\Delta s_0 - \Delta\nu\theta\ln\frac{\theta}{\theta_0} - \rho_{\tau}^{-1}\mathbf{P}^{\mathrm{t}} : \mathbf{F}_{\mathrm{e}\tau} \cdot \Delta\boldsymbol{\alpha}_{\tau}\theta \cdot \mathbf{F}_{\mathrm{t}\tau} \cdot \mathbf{F}_{\mathrm{p}\tau} \cdot \mathbf{F}_{\mathrm{p}1\tau}\right)\dot{\xi} \\ & - \rho_{\tau}^{-1}\dot{\mathbf{P}}^{\mathrm{t}} : \mathbf{F}_{\mathrm{e}\tau} \cdot \boldsymbol{\alpha}_{\tau}(\xi)\theta \cdot \mathbf{F}_{\mathrm{t}\tau} \cdot \mathbf{F}_{\mathrm{p}\tau} \cdot \mathbf{F}_{\mathrm{p}1\tau} + \mathbf{X}_{\mathrm{p}\tau} : \dot{\mathbf{F}}_{\mathrm{p}\tau} + \mathbf{X}_{\mathrm{g}\tau} : \dot{\mathbf{g}}_{\tau}; \end{aligned} \tag{108}$$

$$\begin{aligned} & \int_{\mathbf{F}_{\mathrm{t}1\tau}}^{\mathbf{F}_{\mathrm{t}2\tau}} \frac{1}{\rho_{\tau}}\mathbf{F}_{\mathrm{p}\tau} \cdot \mathbf{F}_{\mathrm{p}1\tau} \cdot \mathbf{P}^{\mathrm{t}} \cdot \mathbf{F}_{\mathrm{e}\tau} \cdot (\mathbf{I} + \boldsymbol{\alpha}_{\tau}(\theta - \theta_0)) : \mathrm{d}\mathbf{F}_{\mathrm{t}\tau} \\ & + \int_0^1 \frac{1}{\rho_{\tau}}\mathbf{F}_{\mathrm{t}\tau} \cdot \mathbf{F}_{\mathrm{p}\tau} \cdot \mathbf{F}_{\mathrm{p}1\tau} \cdot \mathbf{P}^{\mathrm{t}} \cdot \mathbf{F}_{\mathrm{e}\tau} : \Delta\boldsymbol{\alpha}_{\tau}(\theta - \theta_0)\,\mathrm{d}\xi + (\Delta s_0 - \Delta\nu)\int_0^1 \theta\,\mathrm{d}\xi \\ & + \Delta\nu\int_0^1 \theta\ln\frac{\theta}{\theta_0}\mathrm{d}\xi = k + \Delta\psi_0 + (\Delta s_0 - \Delta\nu)\theta_0. \end{aligned} \tag{109}$$

All the remaining simplifications are the same as at small strains.

At finite strains in the actual configuration instead of eqns (85), (87)–(90) we have

$$\nu\dot{\theta} = \left(\mathbf{X}_{\mathrm{p}} - \frac{\partial s}{\partial \mathbf{F}^{\mathrm{t}}_{\mathrm{p}}}\theta\right) : \mathring{\mathbf{F}}_{\mathrm{p}} + \left(\mathbf{X}_{\mathrm{g}} - \frac{\partial s}{\partial \mathbf{g}^{\mathrm{t}}}\theta\right) : \mathring{\mathbf{g}} + \left(X_{\xi} - \frac{\partial s}{\partial \xi}\theta\right)\dot{\xi} - \theta\frac{\partial s}{\partial \mathbf{T}} : \mathring{\mathbf{T}}; \tag{110}$$

$$\rho s = \rho s_0(\xi) + \rho\nu(\xi)\ln\frac{\theta}{\theta_0} + \mathbf{T} : \left(\mathbf{V}_{\mathrm{e}} \cdot \frac{\partial_{\mathrm{R}}\mathbf{F}_{\theta}}{\partial \theta} \cdot \mathbf{F}_{\theta}^{-1} \cdot \mathbf{V}_{\mathrm{e}}^{-1}\right)_{\mathrm{s}}; \tag{111}$$

$$\mathbf{F}_{\theta} = \mathbf{I} + \boldsymbol{\alpha}(\theta - \theta_0); \quad \boldsymbol{\alpha} = (1-\xi)\boldsymbol{\alpha}_1 + \xi\boldsymbol{\alpha}_2; \quad \boldsymbol{\alpha}(\theta - \theta_0) \ll \mathbf{I}, \tag{112}$$

$$\begin{aligned} \nu(\xi)\dot{\theta} = {} & \left(X_{\xi} - \theta\,\Delta s_0 - \Delta\nu\theta\ln\frac{\theta}{\theta_0} - \rho^{-1}\mathbf{T} : (\mathbf{V}_{\mathrm{e}} \cdot \Delta\boldsymbol{\alpha}\theta \cdot \mathbf{V}_{\mathrm{e}}^{-1})_{\mathrm{s}}\right)\dot{\xi} \\ & - \rho^{-1}\mathring{\mathbf{T}} : (\mathbf{V}_{\mathrm{e}} \cdot \boldsymbol{\alpha}(\xi)\theta \cdot \mathbf{V}_{\mathrm{e}}^{-1})_{\mathrm{s}} + \mathbf{X}_{\mathrm{p}} : \mathring{\mathbf{F}}_{\mathrm{p}} + \mathbf{X}_{\mathrm{g}} : \mathring{\mathbf{g}}; \end{aligned} \tag{113}$$

$$\begin{aligned} & \int_0^1 \frac{1}{\rho}\mathbf{T} : \left(\left(\mathbf{V}_{\mathrm{e}} \cdot \frac{\partial_{\mathrm{R}}\mathbf{F}_{\mathrm{t}}}{\partial \xi} \cdot \mathbf{F}_{\mathrm{t}}^{-1} \cdot \mathbf{V}_{\mathrm{e}}^{-1}\right)_{\mathrm{s}} + (\mathbf{V}_{\mathrm{e}} \cdot \Delta\boldsymbol{\alpha}(\theta - \theta_0) \cdot \mathbf{V}_{\mathrm{e}}^{-1})_{\mathrm{s}}\right)\mathrm{d}\xi \\ & + (\Delta s_0 - \Delta\nu)\int_0^1 \theta\,\mathrm{d}\xi + \Delta\nu\int_0^1 \theta\ln\frac{\theta}{\theta_0}\mathrm{d}\xi = k + \Delta\psi_0 + (\Delta s_0 - \Delta\nu)\theta_0. \end{aligned} \tag{114}$$

In eqn (112) and later we consider small thermal strains, because in eqn (111) not only $\partial_{\mathrm{R}}\mathbf{F}_{\theta}/\partial\theta$, but also $\mathbf{F}_{\theta}^{-1}$ depends on ξ which makes the calculation of $\partial s/\partial\xi$ in eqn (113) more bulky.

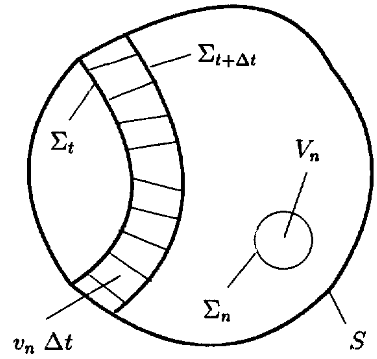

Fig. 3. Volume with PT.

4. NUCLEATION CRITERION

Consider a volume V of multiphase material with a boundary S. Let on one part of surface S_p the stress vector $\mathbf{p}$ be prescribed and on the other part S_u the displacement vector $\mathbf{u}$ be given, but mixed boundary conditions (BC) are also possible. Assume that in some volume V_n with the fixed relative the material's points boundary Σ_n, due to PT during the time Δt, the new nuclei appeared, i.e. some material mass m_n undergoes the PT (Fig. 3).

Assume that for each point of nuclei m_n PT criterion (19) is met. Integrating this criterion over the mass m_n we obtain the necessary condition of *nucleation*

$$\int_{m_n} X \mathrm{d}m_n = \int_{m_n} k \, \mathrm{d}m_n. \tag{115}$$

We take the integral over the mass and not over the volume of the nuclei, because the values X and k are defined per unit mass. If we take into account additionally a surface energy, the nucleation condition will look as follows

$$\int_{m_n} X \mathrm{d}m_n = \int_{\Sigma_n} E \, \mathrm{d}\Sigma_n + \int_{m_n} k \, \mathrm{d}m_n, \tag{116}$$

where Σ_n is the surface of nucleus after the finishing of PT and E is the surface energy per unit area after the PT. Energy per unit area is an idealization of energy per unit volume due to very nonhomogeneous strain distribution in a thin layer. In such an interpretation this energy can be in principle taken into account in the local form of PT condition (19), but this requires a usage of nonlocal gradient-type theory [e.g. Olson and Cohen (1986)], which we would like to avoid in the given paper. Due to surface energy nucleation should occur in a finite volume.

Let us consider one important question: is it really necessary to satisfy the local PT criterion (19) in each point of nucleus, or it is sufficient to fulfill the integral nucleation condition (116) only? Martensitic PT is a highly dynamical process, which requires energy and stress fluctuation and it is very sensitive to local heterogeneities. In such a situation, local values of k are distributed very nonhomogeneously and can depend on the transformation process in the neighboring points. To filter off these spatial fluctuations and to take into account approximately this nonlocality we should average X and k over the nucleus. Consequently, we assume *validity of nucleation condition* (116) *without fulfillment of local PT criterion* (19) *in each point of nucleus*. This implies, in particular, that at $k = 0$ the dissipation increment in some points is negative. Requirement of satisfaction of local PT criterion (19) in each point of nucleus can be too strong and results (at least in quasi-static formulation) in nonexistence of solution. As will be shown in Section 6.2, formulation based on nucleation condition (116) is consistent in limit case with classical description of PT in elastic materials.

Again, if we assume some constraints on the transformation strain distribution in the transforming region (e.g. the homogeneity of $\boldsymbol{\varepsilon}_t(\xi)$), then only the integral criterion should be valid.

For a small strain using eqn (19) we obtain

$$\int_{V_n}\int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2}\boldsymbol{\sigma}:\mathrm{d}\boldsymbol{\varepsilon}\,\mathrm{d}V_n=\int_t^{t+\Delta t}\int_{\Sigma_n}\mathbf{p}\cdot\mathbf{v}\,\mathrm{d}\Sigma_n\,\mathrm{d}t=\int_{V_n}\rho(\psi_2-\psi_1)\,\mathrm{d}V_n+\int_{V_n}\int_{\theta_1}^{\theta_2}\rho s\,\mathrm{d}\theta\,\mathrm{d}V_n$$
$$+\int_{V_n}\int_t^{t+\Delta t}\rho(\mathbf{X}_\mathrm{p}:\dot{\boldsymbol{\varepsilon}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\dot{\mathbf{g}})\,\mathrm{d}t\,\mathrm{d}V_n+\int_{V_n}\rho k\,\mathrm{d}V_n+\int_{\Sigma_n}E\,\mathrm{d}\Sigma_n, \quad (117)$$

where $\mathbf{v}$ is the velocity on Σ_n from the side of nucleus. Note that Gauss theorem was used. Equation (117) is a necessary condition for nucleation, because from the point of view of a stable post-bifurcation deformation process in the whole volume V, at the same BC increment another process (e.g. nucleation in another volume, interface propagation, deformation without PT and so on) can be more stable [Levitas (1992a, 1995a)].

Comparison of PT criterion (117) with the known approaches enumerated in Section 1 shows that they are completely different, because they did not consider the thermomechanical process and were not related to the consideration of the dissipation increment due to the PT. Consistent allowance for temperature and internal variable variation was absent as well.

Only in the paper by Roitburd and Temkin (1986) is an alternative description of the appearance of the spherical nucleus used. In our notation, after simple transformations, their criterion has the form as

$$\int_{V_n}\left(\int_{\varepsilon_{01}}^{\varepsilon_{02}}\sigma_0\,\mathrm{d}\varepsilon_0-\rho(\psi_2^\theta-\psi_1^\theta)-\frac{1}{2}\left(\frac{1}{K_2}-\frac{1}{K_1}\right)\sigma_{01}^2\right)\mathrm{d}V_n=0, \quad (118)$$

where V_n is the volume of a spherical nucleus, K_1 and K_2 are the compression moduli. At $K_1=K_2$ eqn (118) coincides with our simplified eqn (25) at $k=0$ and purely volumetric transformation strain; at $K_1\neq K_2$ the way of allowance for change of elastic moduli is different from eqn (24). The derivation of eqn (118) was not based on the second law of thermodynamics and plastic strain in the nucleus is absent. That is why it was not clear why this approach is better than others and how to extend it to general situations. Unfortunately, this approach did not receive any further development even by authors: the equilibrium of the ellipsoidal nucleus in paper by Kaganova and Roitburd (1989) is based on the principle of the minimum of Gibbs free energy.

At the finite strains in the reference configuration V_τ using eqn (42) we have

$$\int_{V_{n\tau}}\int_{\mathbf{F}_{1\tau}}^{\mathbf{F}_{2\tau}}\mathbf{P}^\mathrm{t}:\mathrm{d}\mathbf{F}_\tau\,\mathrm{d}V_{n\tau}=\int_t^{t+\Delta t}\int_{\Sigma_{n\tau}}\mathbf{p}_\tau\cdot\mathbf{v}\,\mathrm{d}\Sigma_{n\tau}\,\mathrm{d}t=\int_{V_{n\tau}}\rho_\tau(\psi_2-\psi_1)\,\mathrm{d}V_{n\tau}$$
$$+\int_{V_{n\tau}}\int_{\theta_1}^{\theta_2}\rho_\tau s\,\mathrm{d}\theta\,\mathrm{d}V_{n\tau}+\int_{V_{n\tau}}\int_t^{t+\Delta t}\rho_\tau(\mathbf{X}_{\mathrm{p}\tau}:\dot{\mathbf{F}}_{\mathrm{p}\tau}+\mathbf{X}_{\mathrm{g}\tau}:\dot{\mathbf{g}}_\tau)\,\mathrm{d}t\,\mathrm{d}V_{n\tau}$$
$$+\int_{V_{n\tau}}\rho_\tau k\,\mathrm{d}V_{n\tau}+\int_{\Sigma_{n\tau}}E_\tau\,\mathrm{d}\Sigma_{n\tau}. \quad (119)$$

In the actual configuration we can use it in two ways. It is possible to calculate X in eqn (73) and then integrate over the mass m_n, $\mathrm{d}m_n=\rho_2\,\mathrm{d}V_{n2}$, where ρ_2 and $\mathrm{d}V_{n2}$ are the mass density and infinitesimal volume after finishing the PT, then

$$\int_{V_{n2}} \left(\int_0^{t_p} \frac{1}{\rho} \mathbf{T} : \mathbf{d} \, \mathrm{d}t - (\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} s \, \mathrm{d}\theta - \int_0^{t_p} (\mathbf{X}_p : \mathring{\mathbf{F}}_p + \mathbf{X}_g : \mathring{\mathbf{g}}) \, \mathrm{d}t - k \right) \rho_2 \, \mathrm{d}V_{n2} + \int_{\Sigma_n} E \, \mathrm{d}\Sigma_n = 0. \quad (120)$$

In eqn (120) ρ_2 and $\mathrm{d}V_{n2}$ are time-independent and all other terms (including ρ) are variable. It is possible to use fixed ρ_0 and $\mathrm{d}V_{n0}$ in arbitrary time in eqn (120), $\mathrm{d}m_n = \rho_0 \, \mathrm{d}V_{n0}$. Another way is to use $\mathrm{d}m_n = \rho \, \mathrm{d}V_n$, where ρ and $\mathrm{d}V_n$ are the variable current mass density and infinitesimal volume during the PT. In this case we can transform the volume integral into the surface integral using the Gauss theorem

$$\int_{m_n} \int_0^{t_p} \frac{1}{\rho} \mathbf{T} : \mathbf{d} \, \mathrm{d}t \, \mathrm{d}m_n = \int_0^{t_p} \int_{m_n} \frac{1}{\rho} \mathbf{T} : \mathbf{d} \, \mathrm{d}m_n \, \mathrm{d}t = \int_0^{t_p} \int_{V_n} \mathbf{T} : \mathbf{d} \, \mathrm{d}V_n \, \mathrm{d}t = \int_0^{t_p} \int_{\Sigma_n} \mathbf{p} \cdot \mathbf{v} \, \mathrm{d}\Sigma_n \, \mathrm{d}t \quad (121)$$

and the nucleation criterion takes the form

$$\int_0^{t_p} \int_{V_n} \mathbf{T} : \mathbf{d} \, \mathrm{d}V_n \, \mathrm{d}t = \int_0^{t_p} \int_{\Sigma_n} \mathbf{p} \cdot \mathbf{v} \, \mathrm{d}\Sigma_n \, \mathrm{d}t = \int_{V_n} (\psi_2 - \psi_1) \rho \, \mathrm{d}V_n$$
$$+ \int_{\theta_1}^{\theta_2} \int_{V_n} s \, \mathrm{d}\theta \rho \, \mathrm{d}V_n + \int_0^{t_p} \int_{V_n} (\mathbf{X}_p : \mathring{\mathbf{F}}_p + \mathbf{X}_g : \mathring{\mathbf{g}}) \rho \, \mathrm{d}V_n \, \mathrm{d}t + \int_{V_n} k \rho \, \mathrm{d}V_n + \int_{\Sigma_n} E \, \mathrm{d}\Sigma_n. \quad (122)$$

It may be convenient to take some integrals in eqn (122) over the fixed volume, using the identity $\mathrm{d}m_n = \rho \, \mathrm{d}V_n = \rho_2 \, \mathrm{d}V_{n2}$.

5. INTERFACE PROPAGATION AND NUCLEUS NONDISAPPEARANCE CONDITIONS

5.1. *Large strains description in the reference configuration*

Assume that the volume $V_{n\tau}$ is obtained by the *interface* Σ_τ propagation with a normal velocity v_n in time Δt, i.e. it is bounded by surfaces $\Sigma_{\tau t}$ and $\Sigma_{\tau(t+\Delta t)}$ at time t and $t+\Delta t$, respectively, as well as by two lateral infinitesimal surfaces with the heights $v_n \Delta t$ (Fig. 3). Let us transform the stress work integral in eqn (119).

At the moving coherent interface, the position vector and the traction vector $\mathbf{p}_\tau$ are continuous, $\mathbf{p}_{2\tau} = \mathbf{p}_{1\tau}$, and due to Hadamard compatibility condition

$$[\mathbf{F}_\tau] = -[\mathbf{v}]\mathbf{n}_\tau / v_n, \quad \text{whence } [\mathbf{v}] = -[\mathbf{F}_\tau] \cdot \mathbf{n}_\tau v_n \quad \text{and} \quad [\mathbf{F}_\tau] = [\mathbf{F}_\tau] \cdot \mathbf{n}_\tau \mathbf{n}_\tau, \quad (123)$$

where $\mathbf{n}_\tau$ is the unit normal to the interface. Then neglecting all the terms of order Δt^2 we obtain

$$\int_t^{t+\Delta t} \int_{\Sigma_\tau} \mathbf{p}_\tau \cdot \mathbf{v} \, \mathrm{d}\Sigma_\tau \, \mathrm{d}t = \left(\int_{\Sigma_{\tau(t+\Delta t)}} \mathbf{p}_{1\tau} \cdot \mathbf{v}_1 \, \mathrm{d}\Sigma_{\tau(t+\Delta t)} - \int_{\Sigma_{\tau t}} \mathbf{p}_{2\tau} \cdot \mathbf{v}_2 \, \mathrm{d}\Sigma_{\tau(t)} \right) \Delta t$$
$$= -\int_{\Sigma_{\tau t}} [\mathbf{p}_\tau \cdot \mathbf{v}] \, \Delta t \, \mathrm{d}\Sigma_{\tau(t)},$$
$$-[\mathbf{p}_\tau \cdot \mathbf{v}] = -\mathbf{p}_\tau \cdot [\mathbf{v}] = \mathbf{n}_\tau \cdot \mathbf{P}^{\mathrm{t}} \cdot [\mathbf{F}_\tau] \cdot \mathbf{n}_\tau v_n = \mathbf{P}^{\mathrm{t}} : [\mathbf{F}_\tau] \cdot \mathbf{n}_\tau \mathbf{n}_\tau v_n$$
$$= \mathbf{P}^{\mathrm{t}} : [\mathbf{F}_\tau] v_n, \quad (124)$$

i.e. work-producing components of the stress tensor are fixed in the course of PT. Substitution of eqn (124) into eqn (119) with taking into account of $\mathrm{d}V_{n\tau} = v_n \Delta t\, \mathrm{d}\Sigma_{\tau(t)}$ and neglecting for simplicity of surface energy yields

$$\int_{V_{n\tau}} \mathbf{n}_\tau \cdot \mathbf{P}^{\mathrm{t}} \cdot [\mathbf{F}_\tau] \cdot \mathbf{n}_\tau \,\mathrm{d}V_{n\tau} = \int_{V_{n\tau}} \mathbf{P}^{\mathrm{t}} : [\mathbf{F}_\tau] \,\mathrm{d}V_{n\tau} = \int_{V_{n\tau}} \rho_\tau [\psi] \,\mathrm{d}V_{n\tau} + \int_{V_{n\tau}} \int_{\theta_1}^{\theta_2} \rho_\tau s \,\mathrm{d}\theta \,\mathrm{d}V_{n\tau}$$
$$+ \int_{V_{n\tau}} \int_{t}^{t+\Delta t} \rho_\tau (\mathbf{X}_{\mathrm{p}\tau} : \dot{\mathbf{F}}_{\mathrm{p}\tau} + \mathbf{X}_{\mathrm{g}\tau} : \dot{\mathbf{g}}_\tau) \,\mathrm{d}t \,\mathrm{d}V_n + \int_{V_{n\tau}} \rho_\tau k_\tau \,\mathrm{d}V_{n\tau} \qquad (125)$$

and

$$\rho_\tau^{-1} \mathbf{n}_\tau \cdot \mathbf{P}^{\mathrm{t}} \cdot [\mathbf{F}_\tau] \cdot \mathbf{n}_\tau = \rho_\tau^{-1} \mathbf{P}^{\mathrm{t}} : [\mathbf{F}_\tau] = [\psi] + \int_{\theta_1}^{\theta_2} s \,\mathrm{d}\theta + \int_{t}^{t+\Delta t} (\mathbf{X}_{\mathrm{p}\tau} : \dot{\mathbf{F}}_{\mathrm{p}\tau} + \mathbf{X}_{\mathrm{g}\tau} : \dot{\mathbf{g}}_\tau) \,\mathrm{d}t + k. \qquad (126)$$

The transition from an integral form (125) to a local one eqn (126) is based on the assumption that each point of an interface can move independently of another point and the volume $V_{n\tau}$ can be chosen arbitrarily. 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 (125) is valid.

Transformation of the term

$$\mathbf{n}_\tau \cdot \mathbf{P}^{\mathrm{t}} \cdot [\mathbf{F}_\tau] \cdot \mathbf{n}_\tau - \rho_\tau [\psi] = \mathbf{n}_\tau \cdot [\mathbf{P}^{\mathrm{t}} \cdot \mathbf{F}_\tau - \rho_\tau \psi \mathbf{I}] \cdot \mathbf{n}_\tau = \mathbf{n}_\tau \cdot [\mathbf{H}_\tau] \cdot \mathbf{n}_\tau ; \quad \mathbf{H}_\tau := \mathbf{P}^{\mathrm{t}} \cdot \mathbf{F}_\tau - \rho_\tau \psi \mathbf{I} \qquad (127)$$

allows us to use the chemical potential tensor $\mathbf{H}_\tau$ [Grinfeld (1991); Kondaurov and Nikitin (1986)] in the reference configuration. Equation (126) takes the form of

$$\mathbf{n}_\tau \cdot [\mathbf{H}_\tau] \cdot \mathbf{n}_\tau = \int_{\theta_1}^{\theta_2} \rho_\tau s \,\mathrm{d}\theta + \int_{t}^{t+\Delta t} \rho_\tau (\mathbf{X}_{\mathrm{p}\tau} : \dot{\mathbf{F}}_{\mathrm{p}\tau} + \mathbf{X}_{\mathrm{g}\tau} : \dot{\mathbf{g}}_\tau) \,\mathrm{d}t + \rho_\tau k. \qquad (128)$$

For elastic materials without dissipation and isothermal processes

$$\mathbf{n}_\tau \cdot [\mathbf{H}_\tau] \cdot \mathbf{n}_\tau = 0. \qquad (129)$$

A form of this kind or an equivalent form of phase equilibrium was presented in many publications [see Grinfeld (1991); Kaganova and Roitburd (1988) and references). The dissipative term k appears in the papers by Kondaurov and Nikitin (1986), Truskinovsky (1987), Abeyaratne and Knowles (1988). In a paper by Kondaurov and Nikitin (1986) the dissipative term was not concretized and it was mentioned that it is usually small. In a paper by Truskinovsky (1987) k is a linear function of the interface velocity, i.e. at $v_n \to 0$ we have $k \to 0$. Such behavior is typical of the PT in liquids, melting or diffusive PT, for martensitic PT k is rather large at $v_n \to 0$. The dependence $k(v_n)$ with the finite $k(0)$ was considered for one-dimensional interface propagation in a paper by Abeyaratne and Knowles (1988). In contrast to known relations eqn (128):

(1) considers not only a jump of parameters across the interface, but the whole thermomechanical process;
(2) takes into account the plastic flow and variation of internal variables in transforming points as well as temperature variation.

Some particular cases of eqn (126) were published earlier [Levitas (1992a, 1995a)]. The closest relation for plastic materials in the literature is obtained by Kaganova and Roitburd (1989) at small strain and it has the form

$$\boldsymbol{\sigma} : [\boldsymbol{\varepsilon}] = \rho[\psi] - \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_{p2} = 0. \tag{130}$$

The way of deriving eqn (130) is very tricky. The perfectly plastic material obeying the deformation theory of plasticity is considered. As it is thermodynamically equivalent to nonlinear elasticity theory, the principle of minimum of Gibbs energy is used and plastic work is included in the Gibbs energy. The use of the Gibbs energy in the interface equilibrium condition for elastic materials (e.g. eqn (129)) results in the appearance of a difference in plastic works in phase 2 and phase 1. Then since plastic work is not stored in the solid, but is dissipated, plastic work in phase 1 is excluded from the Gibbs potential and eqn (130) is obtained, but why is the plastic work in phase 2 not excluded? Nevertheless, under some assumptions ($k = \dot{\mathbf{g}}_\tau = \dot{\theta} = \boldsymbol{\varepsilon}_{p1} = 0$ and $\mathbf{X}_{p\tau} = \boldsymbol{\sigma} = \text{const}$) eqn (128) reduces to eqn (130).

In a review article by Fischer *et al.* (1994) the propagation condition equivalent to

$$\mathbf{n}_\tau \cdot [\mathbf{H}_\tau] \cdot \mathbf{n}_\tau = \rho_\tau k. \tag{131}$$

is considered. The remark that our propagation condition [Levitas (1992a)] is equivalent to eqn (131) is not correct, because in the paper [Levitas (1992a)] the plastic dissipation is excluded from the total dissipation in a similar way as here.

In a paper by Roitburd and Temkin (1986) it was mentioned that nucleation and interface propagation conditions in elastoplastic materials do not coincide. In this case the formulation of the problem of finding the equilibrium shape of new phase inclusion in a paper by Kaganova and Roitburd (1989) seems to us not to be correct. They look to see which shape of inclusion corresponds to minimum energy losses when it grows. As the new phase should appear first of all, the search for the shape of the new nucleus according to eqn (119) and the extremum principle formulated in Section 6 is more appropriate.

All simplifications from Section 2 as well as the temperature evolution equation are valid.

Note that for points of the interface it is possible to use the PT criterion in the form (42) without additional transformations. Equation (126) takes into account the peculiarity of the stress–strain variation typical for the interface points and allows us to avoid the integration over the deformation process in the left-hand side of eqn (126), but it is impossible to avoid such an integration in the remaining integral of eqn (126). That is why it is sometimes more convenient to use eqn (42) than (126). For example in finite element calculations, due to the possible irregular character of the interface and approximate fulfillment of the traction continuity and Hadamard compatibility conditions in a discrete formulation, eqn (42) can be more precise. From the computational point of view it is also simpler to use the same algorithm for the transformation of each finite element regardless of whether it belongs the interface or not [Levitas *et al.* (1997)].

Another aspect is related to the real physical mechanism of interface propagation. According to dislocation representations [Christian (1965); Boiko *et al.* (1991)], the interface does not move as a smooth surface, but first a small jog or transformation dislocation appears which then moves along the interface making the PT. The same is valid for the twin boundary and twinning dislocation. It is impossible to apply eqn (126) to this situation, because the PT progress occurs along the interface and not in the normal to the interface direction. As in the dissipative materials everything is history dependent, it makes sense to study such a mechanism of interface propagation in details on the macroscopic level. It can be simulated e.g. by FEM using eqn (42) for a transforming element rather than eqn (126). Nevertheless, there are enough problem formulations for which eqn (126) can be used.

For the interface propagation it is necessary that eqn (126) is met at time $t+\Delta t$ as well

$$\mathbf{P}^{t}_{\Delta} : [\mathbf{F}_{\tau\Delta}] = \rho_\tau[\psi_\Delta] + \int_{\theta_{1\Delta}}^{\theta_{2\Delta}} \rho_\tau s\,\mathrm{d}\theta + \int_{\mathbf{F}_{p1\tau\Delta}}^{\mathbf{F}_{p2\tau\Delta}} \rho_\tau \mathbf{X}_{p\tau} : \mathrm{d}\mathbf{F}_{p\tau} + \int_{\mathbf{g}_{1\tau\Delta}}^{\mathbf{g}_{2\tau\Delta}} \rho_\tau \mathbf{X}_{g\tau} : \mathrm{d}\mathbf{g}_\tau + \rho_\tau k_\Delta. \tag{132}$$

Equation (132) is a counterpart of the consistency condition in plasticity theory, where subscript Δ denotes that a parameter is determined at time $t+\Delta t$. For an infinitesimal Δt eqns (126) and (132) can be transformed into

$$
\begin{aligned}
(\dot{\mathbf{P}}^{\mathrm{t}}+\mathbf{n}_\tau\cdot\nabla_\tau\mathbf{P}^{\mathrm{t}}v_n):[\mathbf{F}_\tau]+\mathbf{P}^{\mathrm{t}}:([\dot{\mathbf{F}}_\tau]+\mathbf{n}_\tau\cdot[\nabla_\tau\mathbf{F}_\tau]v_n)-\rho_\tau([\dot{\psi}]+\mathbf{n}_\tau\cdot[\nabla_\tau\psi]v_n)\\
-\rho_\tau([s\dot{\theta}]+\mathbf{n}_\tau\cdot[s\nabla_\tau\theta]v_n)-\rho_\tau([\mathbf{X}_{\mathrm{p}\tau}:\dot{\mathbf{F}}_{\mathrm{p}\tau}]+[\mathbf{X}_{\mathrm{p}\tau}:(\mathbf{n}_\tau\cdot\nabla_\tau\mathbf{F}_{\mathrm{p}\tau})]v_n)\\
-\rho_\tau([\mathbf{X}_{\mathrm{g}\tau}:\dot{\mathbf{g}}_\tau]+[\mathbf{X}_{\mathrm{g}\tau}:(\mathbf{n}_\tau\cdot\nabla_\tau\mathbf{g}_\tau)]v_n)=\rho_\tau\frac{\partial k}{\partial u_n}v_n+\rho_\tau\frac{\partial k}{\partial\mathbf{y}_\tau^{\mathrm{t}}}:([\dot{\mathbf{y}}_\tau]+\mathbf{n}_\tau\cdot[\nabla_\tau\mathbf{y}_\tau]v_n),
\end{aligned}
\tag{133}
$$

where u_n is the interface displacement, $\dot{u}_n=v_n$, $\mathbf{y}_\tau=\{\theta,\mathbf{F}_{\mathrm{p}\tau},\mathbf{g}_\tau,\ldots\}$ is the set of arguments of k, $k=k(\mathbf{y}_\tau)$. We have taken into account

$$
\mathbf{a}_\Delta=\mathbf{a}+(\dot{\mathbf{a}}+\mathbf{n}_\tau\cdot\nabla_\tau\mathbf{a}v_n)\,\Delta t
\tag{134}
$$

for all parameters, equation

$$
\begin{aligned}
\int_{\mathbf{F}_{\mathrm{p}1\tau\Delta}}^{\mathbf{F}_{\mathrm{p}2\tau\Delta}}\mathbf{X}_{\mathrm{p}\tau}:\mathrm{d}\mathbf{F}_{\mathrm{p}\tau}&=\int_{\mathbf{F}_{\mathrm{p}1\tau}}^{\mathbf{F}_{\mathrm{p}2\tau}}\mathbf{X}_{\mathrm{p}\tau}:\mathrm{d}\mathbf{F}_{\mathrm{p}\tau}+\int_{\mathbf{F}_{\mathrm{p}2\tau}}^{\mathbf{F}_{\mathrm{p}2\tau\Delta}}\mathbf{X}_{\mathrm{p}\tau}:\mathrm{d}\mathbf{F}_{\mathrm{p}\tau}-\int_{\mathbf{F}_{\mathrm{p}1\tau}}^{\mathbf{F}_{\mathrm{p}1\tau\Delta}}\mathbf{X}_{\mathrm{p}\tau}:\mathrm{d}\mathbf{F}_{\mathrm{p}\tau}\\
&=\int_{\mathbf{F}_{\mathrm{p}1\tau}}^{\mathbf{F}_{\mathrm{p}2\tau}}\mathbf{X}_{\mathrm{p}\tau}:\mathrm{d}\mathbf{F}_{\mathrm{p}\tau}+\mathbf{X}_{\mathrm{p}2\tau}:(\dot{\mathbf{F}}_{\mathrm{p}2\tau}+\mathbf{n}_\tau\cdot\nabla_\tau\mathbf{F}_{\mathrm{p}2\tau}v_n)\,\Delta t-\mathbf{X}_{\mathrm{p}1\tau}:(\dot{\mathbf{F}}_{\mathrm{p}1\tau}+\mathbf{n}_\tau\cdot\nabla_\tau\mathbf{F}_{\mathrm{p}1\tau}v_n)\,\Delta t
\end{aligned}
\tag{135}
$$

and similar equations for all other parameters. Here the term $\nabla_\tau\mathbf{a}$ appears due to the fact that the tensor $\mathbf{a}_\Delta$ is determined on the $\Sigma_{\tau\Delta}$ surface, i.e. at point $\mathbf{r}_\tau+v_n\mathbf{n}_\tau\,\Delta t(\mathbf{r}_\tau\in\Sigma_\tau(t))$.

5.2. *Finite strain formulation in the actual configuration*

To derive the counterpart of eqn (126) in the actual configuration we will vary the reference configuration V_τ. We consider two cases, when the reference configuration coincides with the actual configuration of phase 1 V_1 (after straining with the deformation gradient $\mathbf{F}_{1\tau}$) and phase 2 V_2 (after deformation with $\mathbf{F}_{2\tau}$). Equation $(123)_1$ has the following form relative to the configurations V_1 and V_2, respectively,

$$
\mathbf{F}_{21}-\mathbf{I}=-\frac{[\mathbf{v}]}{v_{n1}}\cdot\mathbf{n}_1\quad\mathbf{I}-\mathbf{F}_{12}=-\frac{[\mathbf{v}]}{v_{n2}}\cdot\mathbf{n}_2,
\tag{136}
$$

where v_{n1} and v_{n2} is the interface velocity with respect to particles of phase 1 and 2, $\mathbf{n}_1=\mathbf{n}_2=\mathbf{n}$ is the unit normal to interface in V_1 and V_2, $\mathbf{F}_{21}$ (or $\mathbf{F}_{12}$) is the deformation gradient which transforms points from configuration V_1 (or V_2) to V_2 (or V_1), $\mathbf{F}_{11}=\mathbf{F}_{22}=\mathbf{I}$. As

$$
\mathbf{F}_{2\tau}=\frac{\partial\mathbf{r}_2}{\partial\mathbf{r}_\tau}=\frac{\partial\mathbf{r}_2}{\partial\mathbf{r}_1}\cdot\frac{\partial\mathbf{r}_1}{\partial\mathbf{r}_\tau}=\mathbf{F}_{21}\cdot\mathbf{F}_{1\tau},\quad\mathbf{F}_{12}=\frac{\partial\mathbf{r}_1}{\partial\mathbf{r}_2}=\mathbf{F}_{21}^{-1},
\tag{137}
$$

then

$$
\mathbf{F}_{21}=\mathbf{F}_{2\tau}\cdot\mathbf{F}_{1\tau}^{-1},\quad\mathbf{F}_{12}=\mathbf{F}_{1\tau}\cdot\mathbf{F}_{2\tau}^{-1}.
\tag{138}
$$

From eqn $(136)_1$ we have

$$
[\mathbf{v}]=-(\mathbf{F}_{21}-\mathbf{I})\cdot\mathbf{n}v_{n1},\quad(\mathbf{F}_{21}-\mathbf{I})=(\mathbf{F}_{21}-\mathbf{I})\cdot\mathbf{n}\mathbf{n}.
\tag{139}
$$

Decomposing $[\mathbf{v}]$ into components normal (along $\mathbf{n}$) and tangential (along $\mathbf{m}$) to the interface, we obtain from eqn $(136)_1$

$$\mathbf{F}_{21} = \mathbf{I}+\gamma\mathbf{mn}+\delta\mathbf{nn}, \quad \gamma := -\frac{[\mathbf{v}]}{v_{n1}}\cdot\mathbf{m} \quad \delta := -\frac{[\mathbf{v}]}{v_{n1}}\cdot\mathbf{n}$$

$$\mathbf{F}_{12} = \mathbf{F}_{21}^{-1} = \mathbf{I}-\frac{\gamma}{1+\delta}\mathbf{mn}-\frac{\delta}{1+\delta}\mathbf{nn}, \tag{140}$$

where γ and δ are the shear and normal components of $\mathbf{F}_{21}$. Tensor $\mathbf{F}_{21}$ describes simple shear along the interface and tension (compression) along the normal $\mathbf{n}$; the interface is nondeformable. The transformation deformation gradient $\mathbf{F}_t$ has the same structure in the crystallographic theory of PT at transformation with an invariant (nondeformable) plane in a stress-free case [Christian (1965)]. Equation (140) is valid at arbitrary $\mathbf{F}_t$ and stress, but γ and δ are not the transformation strain. By definition $(\rho_1/\rho_2) = \det\mathbf{F}_{21} = 1+\delta$. Using the mass conservation $\rho_1 v_{n1} = \rho_2 v_{n2}$ and eqn (136) we derive the identity

$$\rho_2(\mathbf{F}_{21}-\mathbf{I}) = \rho_1(\mathbf{I}-\mathbf{F}_{21}^{-1}). \tag{141}$$

Let us transform eqn (136), considering V_2 as the reference configuration; then $\rho_\tau = \rho_2$, $\mathbf{P}_\tau = \mathbf{T}_2$. As all the terms in eqn (126) are scalars referring to unit mass, they are independent of a change of reference configuration. In particular

$$\rho_\tau^{-1}\mathbf{n}_\tau\cdot\mathbf{P}_\tau\cdot[\mathbf{F}_\tau]\cdot\mathbf{n}_\tau = \rho_2^{-1}\mathbf{n}\cdot\mathbf{T}_2\cdot(\mathbf{I}-\mathbf{F}_{21})\cdot\mathbf{n} = \rho_2^{-1}\mathbf{T}_2:(\mathbf{I}-\mathbf{F}_{21})\cdot\mathbf{nn} = \rho_2^{-1}\mathbf{T}:(\mathbf{I}-\mathbf{F}_{21}) \tag{142}$$

and

$$\rho_2^{-1}\mathbf{n}\cdot\mathbf{T}_2\cdot(\mathbf{I}-\mathbf{F}_{12})\cdot\mathbf{n} = \rho_2^{-1}\mathbf{T}_2:(\mathbf{I}-\mathbf{F}_{12}) = [\psi]+\int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta+\int_t^{t+\Delta t}(\mathbf{X}_\mathrm{p}:\mathring{\mathbf{F}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\mathring{\mathbf{g}})\,\mathrm{d}t+k, \tag{143}$$

see also eqn (122). Using $\mathbf{n}\cdot\mathbf{T}_2 = \mathbf{n}\cdot\mathbf{T}_1 = \mathbf{n}\cdot\mathbf{T}$ and eqn (141) we obtain

$$\rho_1^{-1}\mathbf{n}\cdot\mathbf{T}\cdot(\mathbf{F}_{21}-\mathbf{I})\cdot\mathbf{n} = \rho_1^{-1}\mathbf{T}:(\mathbf{F}_{21}-\mathbf{I}) = [\psi]+\int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta+\int_t^{t+\Delta t}(\mathbf{X}_\mathrm{p}:\mathring{\mathbf{F}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\mathring{\mathbf{g}})\,\mathrm{d}t+k \tag{144}$$

or with account for eqn (138)

$$\begin{aligned}\rho_1^{-1}\mathbf{n}\cdot\mathbf{T}\cdot(\mathbf{F}_{2\tau}-\mathbf{F}_{1\tau})\cdot\mathbf{F}_{1\tau}^{-1}\cdot\mathbf{n} &= \rho_1^{-1}\mathbf{T}:(\mathbf{F}_{2\tau}-\mathbf{F}_{1\tau})\cdot\mathbf{F}_{1\tau}^{-1}\\ &= [\psi]+\int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta+\int_t^{t+\Delta t}(\mathbf{X}_\mathrm{p}:\mathring{\mathbf{F}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\mathring{\mathbf{g}})\,\mathrm{d}t+k.\end{aligned} \tag{145}$$

Note that the stress work in eqn (144) as well as eqn $(136)_1$ are the same as in the paper by Raniecki and Tanaka (1994). The left-hand side of eqn (144) can be transformed into

$$0.5\rho_1^{-1}\mathbf{n}\cdot(\mathbf{T}_1+\mathbf{T}_2)\cdot(\mathbf{F}_{21}-\mathbf{I})\cdot\mathbf{n} = 0.5\rho_1^{-1}(\mathbf{T}_1+\mathbf{T}_2):(\mathbf{F}_{21}-\mathbf{I}). \tag{146}$$

Using eqn (140) we have

$$\rho_2^{-1}\mathbf{T}_2:(\mathbf{F}_{21}-\mathbf{I}) = \rho_2^{-1}(\tau\gamma+\sigma\delta), \tag{147}$$

where $\tau = \mathbf{n}\cdot\mathbf{T}\cdot\mathbf{m}$ and $\sigma = \mathbf{n}\cdot\mathbf{T}\cdot\mathbf{n}$ are shear and normal stresses on the interface. Another transformation using eqn (138) leads to

$$\begin{aligned}
&\rho_1^{-1}\mathbf{n}\cdot\mathbf{T}\cdot(\mathbf{F}_{21}-\mathbf{I})\cdot n-[\psi] \\
&\quad=\mathbf{n}\cdot(\rho_1^{-1}\mathbf{T}\cdot\mathbf{F}_{21}-\rho_1^{-1}\mathbf{T}\cdot\mathbf{F}_{11}-[\psi]\mathbf{I})\cdot\mathbf{n}=\mathbf{n}\cdot[\rho_1^{-1}\mathbf{T}\cdot\mathbf{F}_1-\psi\mathbf{I}]\cdot\mathbf{n} \\
&\quad=\mathbf{n}\cdot(\rho_2^{-1}\mathbf{T}\cdot\mathbf{F}_{22}-\rho_2^{-1}\mathbf{T}\cdot\mathbf{F}_{12}-[\psi]\mathbf{I})\cdot\mathbf{n}=\mathbf{n}\cdot[\rho_2^{-1}\mathbf{T}\cdot\mathbf{F}_2-\psi\mathbf{I}]\cdot\mathbf{n}=\mathbf{n}\cdot[\mathbf{H}]\cdot\mathbf{n},
\end{aligned} \tag{148}$$

$$\mathbf{H}:=\rho_1^{-1}\mathbf{T}\cdot\mathbf{F}_1-\psi\mathbf{I}=\rho_2^{-1}\mathbf{T}\cdot\mathbf{F}_2-\psi\mathbf{I}=\rho_1^{-1}\mathbf{T}\cdot\mathbf{F}_\tau\cdot\mathbf{F}_{1\tau}^{-1}-\psi\mathbf{I}=\rho_2^{-1}\mathbf{T}\cdot\mathbf{F}_\tau\cdot\mathbf{F}_{2\tau}^{-1}-\psi\mathbf{I}, \tag{149}$$

where $\mathbf{F}_1$ and $\mathbf{F}_2$ is the deformation gradient with respect to configuration V_1 and V_2, respectively, $\mathbf{F}_1=\mathbf{F}_\tau\cdot\mathbf{F}_{1\tau}^{-1}$, $\mathbf{F}_2=\mathbf{F}_\tau\cdot\mathbf{F}_{2\tau}^{-1}$. By analogy with the known publications [Bowen (1967); Kondaurov and Nikitin (1986)] tensor $\mathbf{H}$ can be called the chemical potential tensor in the actual configuration. To get the chemical potential tensor in the reference configuration is not a problem, but in the actual configuration such a tensor does not look natural [Kondaurov and Nikitin (1986); Mukhamediev (1990)]. It seems to us that the expression (149) does not look worse than in the reference configuration.

Equation (144) at the time $t+\Delta t$ in the frame of reference δ is

$$\rho_{1\Delta}^{-1}\mathbf{T}_{\delta\Delta}:(\mathbf{F}_{2\Delta}-\mathbf{I})=[\psi_\Delta]+\int_{\theta_{1\Delta}}^{\theta_{2\Delta}}s\,\mathrm{d}\theta+\int_{\mathbf{F}_{\mathrm{p}1\tau\Delta}}^{\mathbf{F}_{\mathrm{p}2\tau\Delta}}\mathbf{X}_{\mathrm{p}\tau}:\mathrm{d}\mathbf{F}_{\mathrm{p}\tau}+\int_{\mathbf{g}_{1\tau\Delta}}^{\mathbf{g}_{2\tau\Delta}}\mathbf{X}_{\mathrm{g}\tau}:\mathrm{d}\mathbf{g}_\tau+k_\Delta. \tag{150}$$

For an infinitesimal Δt using expression

$$\mathbf{a}_\Delta=\mathbf{a}+(\dot{\mathbf{a}}+\mathbf{n}\cdot\nabla\mathbf{a}v_{n1})\,\Delta t, \tag{151}$$

and eqn (144) in frame of reference δ, eqn (150) can be transformed into

$$\begin{aligned}
&\rho_1^{-1}(\dot{\mathbf{T}}_\delta+\mathbf{n}\cdot\nabla\mathbf{T}_\delta v_{n1}):(\mathbf{F}_{21\delta}-\mathbf{I})+\rho_1^{-1}\mathbf{T}_\delta:(\dot{\mathbf{F}}_{21\delta}+\mathbf{n}\cdot\nabla\mathbf{F}_{21\delta}v_{n1}) \\
&\qquad+(\dot{\rho}_1^{-1}+\mathbf{n}\cdot\nabla\rho_1^{-1}v_{n1})\mathbf{T}_\delta:(\mathbf{F}_{21\delta}-\mathbf{I})-([\dot{\psi}]+\mathbf{n}\cdot[\nabla\psi]v_{n1}) \\
&\qquad-([s\dot{\theta}]+\mathbf{n}\cdot[s\nabla\theta]v_{n1})-([\mathbf{X}_{\mathrm{p}\tau}:\dot{\mathbf{F}}_{\mathrm{p}\tau}]+[\mathbf{X}_{\mathrm{p}\tau}:(\mathbf{n}\cdot\nabla\mathbf{F}_{\mathrm{p}\tau})]v_{n1}) \\
&\qquad-([\mathbf{X}_{\mathrm{g}\tau}:\dot{\mathbf{g}}_\tau]+[\mathbf{X}_{\mathrm{g}\tau}:(\mathbf{n}\cdot\nabla\mathbf{g}_\tau)]v_{n1})=\frac{\partial k}{\partial u_{n1}}v_{n1}+\frac{\partial k}{\partial\mathbf{y}_\delta^{\mathrm{t}}}:([\dot{\mathbf{y}}_\delta]+\mathbf{n}\cdot[\nabla\mathbf{y}_\delta]v_{n1}),
\end{aligned} \tag{152}$$

where $\mathbf{F}_{21\delta}=\mathbf{R}_{\mathrm{e}}^{\mathrm{t}}\cdot\mathbf{F}_{21}\cdot\mathbf{R}_{\mathrm{e}}$, $\mathbf{y}_\delta=\mathbf{R}_{\mathrm{e}}^{\mathrm{t}}\cdot\mathbf{y}\cdot\mathbf{R}_{\mathrm{e}}$. Passing to fixed frame of reference (i.e. substituting $\mathbf{T}_\delta=\mathbf{R}_{\mathrm{e}}^{\mathrm{t}}\cdot\mathbf{T}\cdot\mathbf{R}_{\mathrm{e}}$, $\mathbf{y}_\delta=\mathbf{R}_{\mathrm{e}}^{\mathrm{t}}\cdot\mathbf{y}\cdot\mathbf{R}_{\mathrm{e}}$ and so on) and introducing corotational normal to interface component of gradient operator

$$\mathbf{n}\cdot\mathring{\nabla}\mathbf{a}:=\mathbf{R}_{\mathrm{e}}\cdot(\mathbf{n}\cdot\nabla\cdot(\mathbf{R}_{\mathrm{e}}^{\mathrm{t}}\cdot\mathbf{a}\cdot\mathbf{R}_{\mathrm{e}}))\cdot\mathbf{R}_{\mathrm{e}}^{\mathrm{t}} \tag{153}$$

we obtain

$$\begin{aligned}
&\rho_1^{-1}(\mathring{\mathbf{T}}+\mathbf{n}\cdot\mathring{\nabla}\mathbf{T}v_{n1}):(\mathbf{F}_{21}-\mathbf{I})+\rho^{-1}\mathbf{T}:(\mathring{\mathbf{F}}_{21}+\mathbf{n}\cdot\mathring{\nabla}\mathbf{F}_{21}v_{n1}) \\
&\qquad+(\dot{\rho}_1^{-1}+\mathbf{n}\cdot\nabla\rho_1^{-1}v_{n1})\mathbf{T}:(\mathbf{F}_{21}-\mathbf{I})-([\dot{\psi}]+\mathbf{n}\cdot[\nabla\psi]v_{n1}) \\
&\qquad-([s\dot{\theta}]+\mathbf{n}\cdot[s\nabla\theta]v_{n1})-([\mathbf{X}_{\mathrm{p}}:\mathring{\mathbf{F}}_{\mathrm{p}}]+[\mathbf{X}_{\mathrm{p}}:(\mathbf{n}\cdot\mathring{\nabla}\mathbf{F}_{\mathrm{p}})]v_{n1}) \\
&\qquad-([X_{\mathrm{g}}:\mathring{\mathbf{g}}_\tau]+[\mathbf{X}_{\mathrm{g}}:(\mathbf{n}\cdot\mathring{\nabla}\mathbf{g})]v_{n1})=\frac{\partial k}{\partial u_{n1}}v_{n1}+\frac{\partial k}{\partial\mathbf{y}^{\mathrm{t}}}:([\mathring{\mathbf{y}}]+\mathbf{n}\cdot[\mathring{\nabla}\mathbf{y}]v_{n1}).
\end{aligned} \tag{154}$$

5.3. *Small strain*

At small strains $\mathbf{F}_\tau = \mathbf{I}+\boldsymbol{\varepsilon}+\boldsymbol{\omega} = \mathbf{F}$, $\boldsymbol{\omega} \ll \mathbf{I}$ is the skew-symmetric small rotational tensor, $\mathbf{n}_\tau \cdot \mathbf{P}^t \cdot [\mathbf{F}_\tau] \cdot \mathbf{n}_\tau = \mathbf{n} \cdot \boldsymbol{\sigma} \cdot [\boldsymbol{\varepsilon}+\boldsymbol{\omega}] \cdot \mathbf{n}$, $\mathbf{P}^t : [\mathbf{F}_\tau] = \boldsymbol{\sigma} : [\boldsymbol{\varepsilon}]$ (as $\boldsymbol{\sigma} : \boldsymbol{\omega} \equiv 0$) and eqn (126) looks as

$$\rho^{-1}\mathbf{n} \cdot \boldsymbol{\sigma} \cdot [\mathbf{F}] \cdot \mathbf{n} = \rho^{-1}\boldsymbol{\sigma} : [\boldsymbol{\varepsilon}] = [\psi] + \int_{\theta_1}^{\theta_2} s \, \mathrm{d}\theta + \int_t^{t+\Delta t} (\mathbf{X}_\mathrm{p} : \dot{\boldsymbol{\varepsilon}}_\mathrm{p} + \mathbf{X}_\mathrm{g} : \dot{\mathbf{g}}) \, \mathrm{d}t + k. \tag{155}$$

The same condition at the time $t+\Delta t$ reads

$$\rho_\Delta^{-1}\boldsymbol{\sigma}_\Delta : [\boldsymbol{\varepsilon}_\Delta] = [\psi_\Delta] + \int_{\theta_{1\Delta}}^{\theta_{2\Delta}} s \, \mathrm{d}\theta + \int_{\boldsymbol{\varepsilon}_{\mathrm{p}1\Delta}}^{\boldsymbol{\varepsilon}_{\mathrm{p}2\Delta}} \mathbf{X}_\mathrm{p} : \mathrm{d}\boldsymbol{\varepsilon}_\mathrm{p} + \int_{\mathbf{g}_{1\Delta}}^{\mathbf{g}_{2\Delta}} \mathbf{X}_\mathrm{g} : \mathrm{d}\mathbf{g} + k_\Delta. \tag{156}$$

For infinitesimal Δt

$$\begin{aligned}\rho^{-1}(\dot{\boldsymbol{\sigma}} + \mathbf{n} \cdot \nabla\boldsymbol{\sigma} v_n) : [\boldsymbol{\varepsilon}] + \rho^{-1}\boldsymbol{\sigma} : ([\dot{\boldsymbol{\varepsilon}}] + \mathbf{n} \cdot [\nabla\boldsymbol{\varepsilon}]v_n) - ([\dot{\psi}] + \mathbf{n} \cdot [\nabla\psi]v_n) \\ - ([s\dot{\theta}] + \mathbf{n} \cdot [s\nabla\theta]v_n) - ([\mathbf{X}_\mathrm{p} : \dot{\boldsymbol{\varepsilon}}_\mathrm{p}] + [\mathbf{X}_\mathrm{p} : (\mathbf{n} \cdot \nabla\boldsymbol{\varepsilon}_\mathrm{p})]v_n) \\ - ([\mathbf{X}_\mathrm{g} : \dot{\mathbf{g}}] + [\mathbf{X}_\mathrm{g} : (\mathbf{n} \cdot \nabla\mathbf{g})]v_n) = \frac{\partial k}{\partial u_n} v_n + \frac{\partial k}{\partial \mathbf{y}} \cdot ([\dot{\mathbf{y}}] + \mathbf{n} \cdot [\nabla\mathbf{y}]v_n).\end{aligned} \tag{157}$$

It follows from eqn (140)

$$[\mathbf{F}] = [F_{11}]\mathbf{nn} + [F_{12}]\mathbf{mn} = [\varepsilon_{11}]\mathbf{nn} + [\varepsilon_{12} + \omega_{12}]\mathbf{mn}, \tag{158}$$

where the terms not in bold with the double subscripts are the tensor components. From the condition

$$[F_{21}] = 0 = [\varepsilon_{21} + \omega_{21}] = [\varepsilon_{12} - \omega_{12}], \tag{159}$$

we obtain

$$[\omega_{12}] = [\varepsilon_{12}] \quad \text{and} \quad [\mathbf{F}] = [\varepsilon_{11}]\mathbf{nn} + 2[\varepsilon_{12}]\mathbf{nn}. \tag{160}$$

Let us transform eqn (155), assuming that $(\partial\psi/\partial\boldsymbol{\varepsilon}_\mathrm{p}) = 0$ and $\mathbf{X}_\mathrm{p} = \rho^{-1}\boldsymbol{\sigma}$. As

$$\mathbf{n} \cdot \boldsymbol{\sigma}_1 = \mathbf{n} \cdot \boldsymbol{\sigma}_2 = 0.5\mathbf{n} \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) = \mathbf{n} \cdot \langle\boldsymbol{\sigma}\rangle \quad \text{with } \langle\boldsymbol{\sigma}\rangle := 0.5(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2), \tag{161}$$

then

$$\mathbf{n} \cdot \boldsymbol{\sigma}[\mathbf{F}] \cdot \mathbf{n} = \mathbf{n} \cdot \langle\boldsymbol{\sigma}\rangle \cdot [\mathbf{F}] \cdot \mathbf{n} = \langle\boldsymbol{\sigma}\rangle : [\varepsilon]. \tag{162}$$

When eqn (22) is valid, then

$$\begin{aligned}0.5(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)(\boldsymbol{\varepsilon}_{\mathrm{e}2} - \boldsymbol{\varepsilon}_{\mathrm{e}1}) &= 0.5(\boldsymbol{\varepsilon}_{\mathrm{e}2} : \mathbf{E}_2 : \boldsymbol{\varepsilon}_{\mathrm{e}2} - \boldsymbol{\varepsilon}_{\mathrm{e}1} : \mathbf{E}_1 : \boldsymbol{\varepsilon}_{\mathrm{e}1} - (\boldsymbol{\varepsilon}_{\mathrm{e}1} : (\mathbf{E}_2 - \mathbf{E}_1) : \boldsymbol{\varepsilon}_{\mathrm{e}2})) \\ &= \rho(\psi_2^\mathrm{e} - \psi_1^\mathrm{e}) - 0.5\boldsymbol{\varepsilon}_{\mathrm{e}1} : \Delta\mathbf{E} : \boldsymbol{\varepsilon}_{\mathrm{e}2}.\end{aligned} \tag{163}$$

Consequently, eqn (155) results in

$$\rho^{-1}\langle\boldsymbol{\sigma}\rangle:[\boldsymbol{\varepsilon}_{\rm p}+\boldsymbol{\varepsilon}_\theta+\boldsymbol{\varepsilon}_{\rm t}]-[\psi^\theta]+0.5\rho^{-1}\boldsymbol{\varepsilon}_{\rm e1}:\Delta\mathbf{E}:\boldsymbol{\varepsilon}_{\rm e2}=\int_{\theta_1}^{\theta_2}s\,{\rm d}\theta+\int_t^{t+\Delta t}(\rho^{-1}\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}_{\rm p}+\mathbf{X}_{\rm g}:\dot{\mathbf{g}})\,{\rm d}t+k. \tag{164}$$

At $\Delta\mathbf{E}=0$ the third in the left-hand side of eqn (164) disappears. Let us decompose $\boldsymbol{\sigma}=\boldsymbol{\sigma}_n+\boldsymbol{\sigma}_{\rm a}$, where

$$\boldsymbol{\sigma}_n:=\begin{pmatrix}\sigma_{11}&\sigma_{12}&\sigma_{13}\\ \sigma_{21}&0&0\\ \sigma_{31}&0&0\end{pmatrix},\quad \boldsymbol{\sigma}_a:=\begin{pmatrix}0&0&0\\ 0&\sigma_{22}&\sigma_{23}\\ 0&\sigma_{32}&\sigma_{33}\end{pmatrix} \tag{165}$$

in the orthogonal coordinate system with axis 1 directed along the normal $\mathbf{n}$ (similar decomposition will be used for other tensors as well). Assume that vector $\boldsymbol{\sigma}_1\cdot\mathbf{n}$ is given and fixed during the PT. Then tensor $\boldsymbol{\sigma}_n$ is also fixed and due to condition $\boldsymbol{\sigma}_1\cdot\mathbf{n}=\boldsymbol{\sigma}_2\cdot\mathbf{n}$, tensor $\langle\boldsymbol{\sigma}_n\rangle=\boldsymbol{\sigma}_n$ is constant independent of ξ. In this case

$$\int_{\boldsymbol{\varepsilon}_{\rm p1}}^{\boldsymbol{\varepsilon}_{\rm p2}}\boldsymbol{\sigma}:{\rm d}\boldsymbol{\varepsilon}_{\rm p}=\int_{\boldsymbol{\varepsilon}_{\rm p1}}^{\boldsymbol{\varepsilon}_{\rm p2}}(\boldsymbol{\sigma}_n+\boldsymbol{\sigma}_{\rm a}):{\rm d}\boldsymbol{\varepsilon}_{\rm p}=\boldsymbol{\sigma}_n:[\boldsymbol{\varepsilon}_{\rm p}]+\int_{\boldsymbol{\varepsilon}_{\rm p1}}^{\boldsymbol{\varepsilon}_{\rm p2}}\boldsymbol{\sigma}_{\rm a}:{\rm d}\boldsymbol{\varepsilon}_{\rm pa}, \tag{166}$$

eqn (164) gives

$$\langle\boldsymbol{\sigma}\rangle:[\boldsymbol{\varepsilon}_\theta+\boldsymbol{\varepsilon}_{\rm t}]-\rho[\psi^\theta]=\rho\int_{\theta_1}^{\theta_2}s\,{\rm d}\theta+\left(\int_{\boldsymbol{\varepsilon}_{\rm p1}}^{\boldsymbol{\varepsilon}_{\rm p2}}\boldsymbol{\sigma}_{\rm a}:{\rm d}\boldsymbol{\varepsilon}_{\rm pa}-\langle\boldsymbol{\sigma}_{\rm a}\rangle:[\boldsymbol{\varepsilon}_{\rm pa}]\right)+\rho\int_{\mathbf{g}_1}^{\mathbf{g}_2}\mathbf{X}_{\rm g}:{\rm d}\mathbf{g}+\rho k. \tag{167}$$

The terms in the bracket in eqn (167) are equal to $(\boldsymbol{\sigma}_{\rm a}^0-\langle\boldsymbol{\sigma}_{\rm a}\rangle):[\boldsymbol{\varepsilon}_{\rm pa}]$ with $\boldsymbol{\sigma}_{\rm a}^0$ for some intermediate value of $\boldsymbol{\sigma}_{\rm a}$ in the interval between $\boldsymbol{\varepsilon}_{\rm p1a}$ and $\boldsymbol{\varepsilon}_{\rm p2a}$. If tensor $\boldsymbol{\sigma}_{\rm a}$ is independent of ξ, then $\boldsymbol{\sigma}_{\rm a}^0=\boldsymbol{\sigma}_{\rm a}=\langle\boldsymbol{\sigma}_{\rm a}\rangle$ and the bracket with the plastic strain disappears. When the tensor $\boldsymbol{\varepsilon}_{\rm ta}$ exceeds $\boldsymbol{\varepsilon}_{\rm ea}+\boldsymbol{\varepsilon}_{\theta{\rm a}}$ significantly, then from the condition $\boldsymbol{\varepsilon}_{\rm a}=0$ (see eqn (160)) we obtain

$$\boldsymbol{\varepsilon}_{\rm pa}(\xi)=-\boldsymbol{\varepsilon}_{\rm ta}(\xi). \tag{168}$$

Let us determine the stress–strain state for the points of moving interface. Assume that $\boldsymbol{\varepsilon}_{\rm t1}=0$, $\boldsymbol{\varepsilon}_{\rm t}(\xi)=\boldsymbol{\varepsilon}_{\rm t}(1)\xi=\boldsymbol{\varepsilon}_{\rm t2}\xi$ and, consequently $\dot{\boldsymbol{\varepsilon}}_{\rm t}=\boldsymbol{\varepsilon}_{\rm t2}\dot{\xi}$. Equation (168) gives $\boldsymbol{\varepsilon}_{\rm pa}(\xi)=-\boldsymbol{\varepsilon}_{\rm t2a}\xi$, $\dot{\boldsymbol{\varepsilon}}_{\rm pa}=-\boldsymbol{\varepsilon}_{\rm t2a}\dot{\xi}$. Assume that the constitutive equations have the form $\boldsymbol{\sigma}=\boldsymbol{\Sigma}(\dot{\boldsymbol{\varepsilon}}_{\rm p},\boldsymbol{\varepsilon}_{\rm p})$. By definition, for time-independent plastic materials $\boldsymbol{\Sigma}(\dot{\boldsymbol{\varepsilon}}_{\rm p},\boldsymbol{\varepsilon}_{\rm p})$ is a homogeneous function of degree zero in $\dot{\boldsymbol{\varepsilon}}_{\rm p}$, so $\boldsymbol{\Sigma}(\dot{\boldsymbol{\varepsilon}}_{\rm p}\boldsymbol{\varepsilon}_{\rm p})=\boldsymbol{\Sigma}(\mathbf{k},\boldsymbol{\varepsilon}_{\rm p})$, where $\mathbf{k}=\dot{\boldsymbol{\varepsilon}}_{\rm p}/|\dot{\boldsymbol{\varepsilon}}_{\rm p}|$ is the directing tensor (unit vector in R^6) and $|\dot{\boldsymbol{\varepsilon}}_{\rm p}|=(\dot{\boldsymbol{\varepsilon}}_{\rm p}:\boldsymbol{\varepsilon}_{\rm p})^{1/2}$ is the modulus of $\dot{\boldsymbol{\varepsilon}}_{\rm p}$. When varying all possible vectors $\mathbf{k}\in R^6$ at fixed $\boldsymbol{\varepsilon}_{\rm p}$, the ends of vectors $\boldsymbol{\sigma}=\boldsymbol{\Sigma}(\mathbf{k},\boldsymbol{\varepsilon}_{\rm p})$ corresponding to them, describe the yield surface $\varphi(\boldsymbol{\sigma},\boldsymbol{\varepsilon}_{\rm p})=0$ in the stress space. Inverting the function $\boldsymbol{\sigma}=\boldsymbol{\Sigma}(\mathbf{k},\boldsymbol{\varepsilon}_{\rm p})$ at $\boldsymbol{\varepsilon}_{\rm p}=\text{const}$ in the form $\mathbf{k}=\mathbf{f}(\boldsymbol{\sigma},\boldsymbol{\varepsilon}_{\rm p})$ we obtain the flow rule $\dot{\boldsymbol{\varepsilon}}_{\rm p}=|\dot{\boldsymbol{\varepsilon}}_{\rm p}|\mathbf{k}=|\dot{\boldsymbol{\varepsilon}}_{\rm p}|\mathbf{f}(\boldsymbol{\sigma},\boldsymbol{\varepsilon}_{\rm p})$, where $|\dot{\boldsymbol{\varepsilon}}_{\rm p}|$ can be determined from the compatibility condition $\dot{\varphi}=0$. For perfectly plastic materials $\boldsymbol{\Sigma}(\dot{\boldsymbol{\varepsilon}}_{\rm p})$ and $\varphi(\boldsymbol{\sigma})=0$ are independent of $\boldsymbol{\varepsilon}_{\rm p}$ and the modulus $|\dot{\boldsymbol{\varepsilon}}_{\rm p}|$ is undetermined.

For the points of the interface

$$\begin{pmatrix}\underline{\sigma_{11}}&\underline{\sigma_{12}}&\underline{0}\\ \underline{\sigma_{21}}&\sigma_{22}&\sigma_{23}\\ \underline{0}&\sigma_{32}&\sigma_{33}\end{pmatrix}=\boldsymbol{\Sigma}\left[\begin{pmatrix}\dot{\varepsilon}_{\rm p11}&\dot{\varepsilon}_{\rm p12}&\dot{\varepsilon}_{\rm p13}\\ \dot{\varepsilon}_{\rm p21}&\underline{-\varepsilon_{\rm t22}(1)\dot{\xi}}&\underline{-\varepsilon_{\rm t23}(1)\dot{\xi}}\\ \dot{\varepsilon}_{\rm p31}&\underline{-\varepsilon_{\rm t32}(1)\dot{\xi}}&\underline{-\varepsilon_{\rm t33}(1)\dot{\xi}}\end{pmatrix},\varepsilon_{\rm p}\right] \tag{169}$$

where for the convenience axis 2 coincides with the direction of shear stress on the interface (i.e. $\sigma_{32}=0$) and the known components of $\boldsymbol{\sigma}$ and $\dot{\boldsymbol{\varepsilon}}_{\rm p}$ are underlined (vector $\boldsymbol{\sigma}_1\cdot\mathbf{n}$ is given, or more precisely, one of the components, σ_{11} or σ_{12}, should be given and another is considered as a parameter determined by the PT criterion (167)). Assume, for example, that σ_{12} is prescribed. As the number of known components (including σ_{11}) is equal to six, then all the components of stress and plastic strain tensor can be determined using six scalar eqn (169) as a function of σ_{11}, all integrals in PT criterion (167) can be calculated and the value σ_{11} is determined by the PT criterion. For a plastic incompressible material

$$\varepsilon_{\mathrm{p}11}(\xi) = -(\varepsilon_{\mathrm{p}22}(\xi)+\varepsilon_{\mathrm{p}33}(\xi)) = \varepsilon_{\mathrm{t}22}(\xi)+\varepsilon_{\mathrm{t}33}(\xi) = (\varepsilon_{\mathrm{t}22}(1)+\varepsilon_{\mathrm{t}33}(1))\xi = \varepsilon_{\mathrm{p}11}(1)\xi,$$
$$\dot{\varepsilon}_{\mathrm{p}11} = \varepsilon_{\mathrm{p}11}(1)\dot{\xi}, \tag{170}$$

the hydrostatic pressure is undetermined and the tensor $\boldsymbol{\sigma}$ should be replaced by the stress deviator **S**

$$\begin{pmatrix} S_{11} & \underline{\sigma_{12}} & \underline{0} \\ \underline{\sigma_{21}} & S_{22} & \sigma_{23} \\ \underline{0} & \sigma_{32} & S_{33} \end{pmatrix} = \boldsymbol{\Sigma}\left[\begin{pmatrix} \underline{\varepsilon_{\mathrm{p}11}\dot{\xi}} & \dot{\varepsilon}_{\mathrm{p}12} & \dot{\varepsilon}_{\mathrm{p}13} \\ \dot{\varepsilon}_{\mathrm{p}21} & \underline{-\varepsilon_{\mathrm{t}22}(1)\dot{\xi}} & \underline{-\varepsilon_{\mathrm{t}23}(1)\dot{\xi}} \\ \dot{\varepsilon}_{\mathrm{p}31} & \underline{-\varepsilon_{\mathrm{t}32}(1)\dot{\xi}} & \underline{-\varepsilon_{\mathrm{t}33}(1)\dot{\xi}} \end{pmatrix}, \boldsymbol{\varepsilon}_{\mathrm{p}}\right]. \tag{171}$$

Equation (171) determines all the components of $\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}}$ and **S**, and the hydrostatic pressure is determined by the PT criterion.

For perfectly plastic materials the assumption that the stress tensor $\boldsymbol{\sigma}$ (or **S**) is independent of ξ is noncontradictory. As the stress tensor is constant during the PT, then $\mathbf{k} = \mathrm{const}$ and

$$\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} = |\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}}|\mathbf{k} = \left|\frac{\partial \boldsymbol{\varepsilon}_{\mathrm{p}}}{\partial \xi}\right|\dot{\xi}\mathbf{k} = \left|\frac{\partial \boldsymbol{\varepsilon}_{\mathrm{p}}}{\partial \xi}\right|\frac{\boldsymbol{\varepsilon}_{\mathrm{p}}}{|\boldsymbol{\varepsilon}_{\mathrm{p}}|}\dot{\xi} \quad \text{with } \boldsymbol{\varepsilon}_{\mathrm{p}} := \boldsymbol{\varepsilon}_{\mathrm{p}}(1)-\boldsymbol{\varepsilon}_{\mathrm{p}}(0), \tag{172}$$

i.e. the components $\dot{\varepsilon}_{\mathrm{p}1i}$, $i = 1, 2, 3$, are proportional to $\dot{\xi}$ as well. In this case $\boldsymbol{\sigma} = \boldsymbol{\Sigma}(\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}}) = \boldsymbol{\Sigma}(\boldsymbol{\varepsilon}_{\mathrm{p}})$, because $\boldsymbol{\Sigma}$ is homogeneous function of degree zero and validity of eqn (172).

For hardening materials the only components σ_{1i} can be prescribed and fixed; the others vary to satisfy the variable yield condition. The direction of the stress tensor $\boldsymbol{\sigma}/|\boldsymbol{\sigma}|$ in stress space and, consequently, **k** cannot be constant, and $\dot{\varepsilon}_{\mathrm{p}1i} \neq \varepsilon_{\mathrm{p}1i}(\xi)\dot{\xi}$ ($i = 2, 3$ for incompressible materials and $i = 1, 2, 3$ in the general case).

Let us consider a perfectly plastic material with the von Mises yield condition $|\mathbf{S}| = \sqrt{2/3}\sigma_{\mathrm{y}}$ where σ_{y} is the yield stress during the PT. Associated flow rule reads

$$\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} = |\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}}|\sqrt{\frac{3}{2}}\frac{\mathbf{S}}{\sigma_{\mathrm{y}}} \quad \text{or } \mathbf{S} = \sqrt{\frac{2}{3}}\sigma_{\mathrm{y}}\frac{\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}}}{|\dot{\boldsymbol{\varepsilon}}_{\mathrm{p}}|} = \sqrt{\frac{2}{3}}\sigma_{\mathrm{y}}\frac{\boldsymbol{\varepsilon}_{\mathrm{p}}}{|\boldsymbol{\varepsilon}_{\mathrm{p}}|}, \quad \varepsilon_{\mathrm{p}13} = 0, \quad |\boldsymbol{\varepsilon}_{\mathrm{p}}| := \sqrt{a^2+2\varepsilon_{\mathrm{p}12}^2}, \tag{173}$$

$$a^2 := \varepsilon_{\mathrm{p}11}^2+\varepsilon_{\mathrm{p}22}^2+\varepsilon_{\mathrm{p}33}^2+2\varepsilon_{\mathrm{p}32}^2 = 2(\varepsilon_{\mathrm{t}22}^2+\varepsilon_{\mathrm{t}33}^2+\varepsilon_{\mathrm{t}22}\varepsilon_{\mathrm{t}33}+\varepsilon_{\mathrm{t}32}^2). \tag{174}$$

The component $\varepsilon_{\mathrm{p}12}$ is separated because it is unknown. According to eqn (173)

$$\varepsilon_{\mathrm{p}12} = \varepsilon_{\mathrm{p}22}\frac{S_{12}}{S_{22}} \quad \text{and} \quad |\boldsymbol{\varepsilon}_{\mathrm{p}}| = \frac{\sqrt{a^2 S_{22}^2+2\varepsilon_{\mathrm{p}22}^2 S_{12}^2}}{S_{22}}. \tag{175}$$

Since

$$S_{22} = \sqrt{\frac{2}{3}}\sigma_{\mathrm{y}}\frac{\varepsilon_{\mathrm{p}22}}{|\boldsymbol{\varepsilon}_{\mathrm{p}}|} = \sqrt{\frac{2}{3}}\sigma_{\mathrm{y}}\frac{\varepsilon_{\mathrm{p}22}S_{22}}{\sqrt{a^2 S_{22}^2+2\varepsilon_{\mathrm{p}22}^2 S_{12}^2}}, \tag{176}$$

then

$$S_{22} = \sqrt{\frac{2}{3}}\sigma_y\frac{\varepsilon_{p22}}{a}\sqrt{1-\frac{3S_{12}^2}{\sigma_y^2}}, \quad |\boldsymbol{\varepsilon}_p| = a\left(1-\frac{3S_{12}^2}{\sigma_y^2}\right)^{-1/2},$$

and using eqn (168) and (173) we have

$$\mathbf{S}_a = -\sqrt{\frac{2}{3}}\sigma_y\frac{\boldsymbol{\varepsilon}_{ta}}{a}\sqrt{1-\frac{3S_{12}^2}{\sigma_y^2}}, \quad \varepsilon_{p12} = aS_{12}\left(\sqrt{\frac{2}{3}}\sigma_y\sqrt{1-\frac{3S_{12}^2}{\sigma_y^2}}\right)^{-1}, \tag{177}$$

$$S_{11} = -(S_{22}+S_{33}) = \sqrt{\frac{2}{3}}\frac{\sigma_y}{a}\sqrt{1-\frac{3S_{12}^2}{\sigma_y^2}}(\varepsilon_{t22}+\varepsilon_{t33}). \tag{178}$$

Equations (176)–(178) explicitly determine the tensors $\mathbf{S}$ and $\boldsymbol{\varepsilon}_p$. Now we can calculate

$$\mathbf{S}:\mathbf{e}_t = \mathbf{S}_n:\mathbf{e}_{tn}+\mathbf{S}_a:\mathbf{e}_{ta} = \sqrt{\frac{2}{3}}\frac{\sigma_y}{a}\sqrt{1-\frac{3S_{12}^2}{\sigma_y^2}}((\varepsilon_{t22}+\varepsilon_{t33})e_{t11}-\boldsymbol{\varepsilon}_{ta}:\mathbf{e}_{ta})+S_{12}e_{t12}, \tag{179}$$

$$\rho A_p = \mathbf{S}:\boldsymbol{\varepsilon}_p = |\mathbf{S}|\,|\boldsymbol{\varepsilon}_p| = \sqrt{\frac{2}{3}}\sigma_y a\left(1-\frac{3S_{12}^2}{\sigma_y^2}\right)^{-1/2}. \tag{180}$$

As $\langle\boldsymbol{\sigma}\rangle:[\varepsilon_t] = \sigma_0\varepsilon_{t0}+\mathbf{S}:\mathbf{e}_t$, then after substitution of eqn (179) in eqn (167) and neglecting for compactness $[\varepsilon_\theta]$, the temperature and **g** variation, we obtain the explicit equation for PT pressure σ_0 (or $\sigma_{11} = \sigma_0+\mathrm{S}_{11}$)

$$\sigma_0\varepsilon_0+\sqrt{\frac{2}{3}}\frac{\sigma_y}{a}\sqrt{-\frac{3S_{12}^2}{\sigma_y^2}}((\varepsilon_{t22}+\varepsilon_{t33})e_{t11}-\boldsymbol{\varepsilon}_{ta}:\mathbf{e}_{ta})+S_{12}e_{t12} = \rho[\psi^\theta]+\rho k. \tag{181}$$

To obtain the PT pressure while taking into account the adiabatic heating we will use the same assumption as in Section 3.1 and eqn (104), because at $\boldsymbol{\sigma} = \mathbf{const}$ eqns (104) and (167) should coincide. Using for temperature θ eqns (92) and (103) we obtain from eqn (104)

$$\boldsymbol{\sigma}:\boldsymbol{\varepsilon}_t = \sigma_0\varepsilon_0+\mathbf{S}:\mathbf{e}_t = \rho v(A/B+\theta_s)(\exp B-1)-\rho A_p+\rho\Psi \tag{182}$$

with eqns (179) and (180) for $\mathbf{S}:\mathbf{e}_t$ and A_p the explicit expression for PT pressure σ_0.

Note that in papers by Levitas (1995d, 1996c) the plane strain problem of PT in a thin horizontal layer in a rigid-plastic half-space under the action of applied pressure and shear stresses is solved. Since the stress tensor is constant in the layer during the PT, the above solution is valid not only for interface propagation, but or nucleation as well. Consequently, eqn (182) determines the pressure σ_{11} necessary for PT in the horizontal layer in a half-space in the three-dimensional case with allowance for adiabatic heating. It is easy to generalize the solution for the case of arbitrary inclined layers, as was done in [Levitas (1995c)] for the plane-strain problem.

5.4. *Condition of nucleus nondissappearance*

It is not necessary that after nucleation eqns (126) and (132) be valid for the points of the interface Σ_n, because after nucleation the interface Σ_n can be fixed. However, we should be sure that under the same BC the interface Σ_n does not move back and the nucleus does not disappear. The condition of nondisappearance of a nucleus is a violation of the propagation condition, when $v_n < 0$ and PT 2 → 1 occurs, i.e.

$$X \geqslant k_{2\rightarrow 1} < 0; \quad X_{\Delta} > k_{2\rightarrow 1\Delta}. \tag{183}$$

As the second nondisappearance condition we should exclude the possibility of appearance and growth under the same BC of the parent phase inside the nucleus of the product phase, i.e. eqn (105) for the reverse PT should be violated.

6. THE POSTULATE OF REALIZABILITY

6.1. *General case*

The PT criterion (115) (or its explicit forms (117), (125) and (126)) is only one scalar equation which is not sufficient for the determination of all unknown parameters. To determine all unknown parameters **b**, e.g. position, shape and orientation of nucleus, jump of **F**, transformation $\mathbf{F}_t$ and plastic deformation $\mathbf{F}_p$ gradients, related to $\mathbf{F}_p$ 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 [Levitas (1992a, 1995a)].

Let for the given BC

$$\int_{m_n^*} X(\mathbf{b}^*)\,\mathrm{d}m_n - \int_{m_n^*} k_{1\rightarrow 2}(\mathbf{b}^*)\,\mathrm{d}m_n - \int_{\Sigma_n^*} E^*\,\mathrm{d}\Sigma_n < 0 \tag{184}$$

for all possible PT parameters **b***, i.e. PT does not occur. If in the course of continuous variation of BC and for each BC continuous variation of all admissible parameters **b*** the condition (116) is fulfilled the *first* time for some of parameters **b**, then PT will occur with these **b** (if condition (116) is not violated in the course of PT, e.g. interface propagation).

If, in the course of continuous variation of BC and for each BC continuous variation of all admissible parameters **b*** the equality (116) is met the first time for one or several **b**, then for arbitrary other **b*** inequality (184) should be held, as in the opposite case for this **b*** condition (116) had to be met before it was satisfied for **b**. Consequently, we obtain the extremum principle

$$\begin{aligned}
&\int_{m_n} X(\mathbf{b})\,\mathrm{d}m_n - \int_{m_n} k_{1\rightarrow 2}(\mathbf{b})\,\mathrm{d}m_n - \int_{\Sigma_n} E\,\mathrm{d}\Sigma_n = 0 \\
&\qquad > \int_{m_n^*} X(\mathbf{b}^*)\,\mathrm{d}m_n - \int_{m_n^*} k_{1\rightarrow 2}(\mathbf{b}^*)\,\mathrm{d}m_n - \int_{\Sigma_n^*} E^*\,\mathrm{d}\Sigma_n,
\end{aligned} \tag{185}$$

for determination of all unknown parameters **b**. The explicit form of principle (185) for small strain regimes has the form of

$$\begin{aligned}
&\int_{V_n}\int_{\varepsilon_1}^{\varepsilon_2} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}\,\mathrm{d}V_n - \int_{V_n} \rho(\psi_2 - \psi_1)\,\mathrm{d}V_n - \int_{V_n}\int_{\theta_1}^{\theta_2} \rho s\,\mathrm{d}\theta\,\mathrm{d}V_n \\
&\quad - \int_{V_n}\int_{t}^{t+\Delta t} \rho(\mathbf{X}_p : \dot{\boldsymbol{\varepsilon}}_p + \mathbf{X}_g : \dot{\mathbf{g}})\,\mathrm{d}t\,\mathrm{d}V_n - \int_{V_n} \rho k_{1\rightarrow 2}\,\mathrm{d}V_n - \int_{\Sigma_n} E\,\mathrm{d}\Sigma_n = 0 \\
&\quad > \int_{V_n^*}\int_{\varepsilon_1^*}^{\varepsilon_2^*} \boldsymbol{\sigma}^* : \mathrm{d}\boldsymbol{\varepsilon}^*\,\mathrm{d}V_n - \int_{V_n^*} \rho(\psi_2^* - \psi_1^*)\,\mathrm{d}V_n - \int_{V_n^*}\int_{\theta_1^*}^{\theta_2^*} \rho s^*\,\mathrm{d}\theta^*\,\mathrm{d}V_n \\
&\quad - \int_{V_n^*}\int_{t}^{t+\Delta t} \rho(\mathbf{X}_p^* : \dot{\boldsymbol{\varepsilon}}_p^* + \mathbf{X}_g^* : \dot{\mathbf{g}}^*)\,\mathrm{d}t\,\mathrm{d}V_n - \int_{V_n^*} \rho k_{1\rightarrow 2}^*\,\mathrm{d}V_n - \int_{\Sigma_n^*} E^*\,\mathrm{d}\Sigma_n
\end{aligned} \tag{186}$$

for the nucleation and the form of

$$\begin{aligned}
&\rho^{-1}\boldsymbol{\sigma}:[\boldsymbol{\varepsilon}]-[\psi]-\int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta-\int_t^{t+\Delta t}(\mathbf{X}_\mathrm{p}:\dot{\boldsymbol{\varepsilon}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\dot{\mathbf{g}})\,\mathrm{d}t-k_{1\to 2}=0\\
&\qquad > \rho^{-1}\boldsymbol{\sigma}^*:[\boldsymbol{\varepsilon}^*]-[\psi^*]-\int_{\theta_1^*}^{\theta_2^*} s^*\,\mathrm{d}\theta^*-\int_t^{t+\Delta t}(\mathbf{X}_\mathrm{p}^*:\dot{\boldsymbol{\varepsilon}}_\mathrm{p}^*+\mathbf{X}_\mathrm{g}^*:\dot{\mathbf{g}}^*)\,\mathrm{d}t-k_{1\to 2}^* \qquad (187)
\end{aligned}$$

for interface propagation. In the particular case of nondissipative materials, isothermal processes and equal elastic moduli, when PT occurs at constant stresses, the inequality (186) is equivalent to the Patel and Cohen (1953) condition $\boldsymbol{\sigma}:\boldsymbol{\varepsilon}_\mathrm{t} > \boldsymbol{\sigma}:\boldsymbol{\varepsilon}_\mathrm{t}^*$. The extremum principles obtained play a similar role in the description of PT in dissipative materials, as does the principle of the minimum of Gibbs energy for nondissipative materials.

For finite strains in the reference configuration principle (185) can be written for nucleation

$$\begin{aligned}
&\int_{V_{n\tau}}\int_{\mathbf{F}_{1\tau}}^{\mathbf{F}_{2\tau}}\mathbf{P}^\mathrm{t}:\mathrm{d}\mathbf{F}_\tau\,\mathrm{d}V_{n\tau}-\int_{V_{n\tau}}\rho_\tau(\psi_2-\psi_1)\,\mathrm{d}V_{n\tau}-\int_{V_{n\tau}}\int_{\theta_1}^{\theta_2}\rho_\tau s\,\mathrm{d}\theta\,\mathrm{d}V_{n\tau}\\
&\quad-\int_{V_{n\tau}}\int_t^{t+\Delta t}\rho_\tau(\mathbf{X}_{\mathrm{p}\tau}:\dot{\mathbf{F}}_{\mathrm{p}\tau}+\mathbf{X}_{\mathrm{g}\tau}:\dot{\mathbf{g}}_\tau)\,\mathrm{d}t\,\mathrm{d}V_{n\tau}-\int_{V_{n\tau}}\rho_\tau k_{1\to 2}\,\mathrm{d}V_{n\tau}-\int_{\Sigma_{n\tau}}E_\tau\,\mathrm{d}\Sigma_{n\tau}=0\\
&\quad>\int_{V_{n\tau}^*}\int_{\mathbf{F}_{1\tau}^*}^{\mathbf{F}_{2\tau}^*}\mathbf{P}^{\mathrm{t}*}:\mathrm{d}\mathbf{F}_\tau^*\mathrm{d}V_{n\tau}-\int_{V_{n\tau}^*}\rho_\tau(\psi_2^*-\psi_1^*)\,\mathrm{d}V_{n\tau}-\int_{V_{n\tau}^*}\int_{\theta_1^*}^{\theta_2^*}\rho_\tau s^*\,\mathrm{d}\theta^*\,\mathrm{d}V_{n\tau}\\
&\quad-\int_{V_{n\tau}^*}\int_t^{t+\Delta t}\rho_\tau(\mathbf{X}_{\mathrm{p}\tau}^*:\dot{\mathbf{F}}_{\mathrm{p}\tau}^*+\mathbf{X}_{\mathrm{g}\tau}^*:\dot{\mathbf{g}}_\tau^*)\,\mathrm{d}t\,\mathrm{d}V_{n\tau}-\int_{V_{n\tau}^*}\rho_\tau k_{1\to 2}^*\,\mathrm{d}V_{n\tau}-\int_{\Sigma_{n\tau}^*}E^*\,\mathrm{d}\Sigma_{n\tau} \qquad (188)
\end{aligned}$$

and for interface propagation

$$\begin{aligned}
&\rho_\tau^{-1}\mathbf{P}^\mathrm{t}:[\mathbf{F}_\tau]-[\psi]-\int_{\theta_1}^{\theta_2}s\,\mathrm{d}\theta-\int_t^{t+\Delta t}(\mathbf{X}_{\mathrm{p}\tau}:\dot{\mathbf{F}}_{\mathrm{p}\tau}+\mathbf{X}_{\mathrm{g}\tau}:\dot{\mathbf{g}}_\tau)\,\mathrm{d}t-k_{1\to 2}=0\\
&\qquad>\rho_\tau^{-1}\mathbf{P}^{\mathrm{t}*}:[\mathbf{F}_\tau^*]-[\psi^*]-\int_{\theta_1^*}^{\theta_2^*}s^*\,\mathrm{d}\theta^*-\int_t^{t+\Delta t}(\mathbf{X}_{\mathrm{p}\tau}^*:\dot{\mathbf{F}}_{\mathrm{p}\tau}^*+\mathbf{X}_{\mathrm{g}\tau}^*:\dot{\mathbf{g}}_\tau^*)\,\mathrm{d}t-k_{1\to 2}^*. \qquad (189)
\end{aligned}$$

Similar expressions are valid in the actual configuration

$$\begin{aligned}
&\int_{V_n}\int_t^{t+\Delta t}\mathbf{T}:\mathbf{d}\,\mathrm{d}t\,\mathrm{d}V_n-\int_{V_n}\rho(\psi_2-\psi_1)\,\mathrm{d}V_n-\int_{V_n}\int_{\theta_1}^{\theta_2}\rho s\,\mathrm{d}\theta\,\mathrm{d}V_n\\
&\quad-\int_{V_n}\int_t^{t+\Delta t}\rho(\mathbf{X}_\mathrm{p}:\mathring{\mathbf{F}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\mathring{\mathbf{g}})\,\mathrm{d}t\,\mathrm{d}V_n-\int_{V_n}\rho k_{1\to 2}\,\mathrm{d}V_n-\int_{\Sigma_n}E\,\mathrm{d}\Sigma_n=0\\
&\quad>\int_{V_n^*}\int_t^{t+\Delta t}\mathbf{T}^*:\mathbf{d}^*\,\mathrm{d}t\,\mathrm{d}V_n-\int_{V_n^*}\rho^*(\psi_2^*-\psi_1^*)\,\mathrm{d}V_n-\int_{V_n^*}\int_{\theta_1^*}^{\theta_2^*}\rho^* s^*\,\mathrm{d}\theta^*\,\mathrm{d}V_n\\
&\quad-\int_{V_n^*}\int_t^{t+\Delta t}\rho^*(\mathbf{X}_\mathrm{p}^*:\mathring{\mathbf{F}}_\mathrm{p}^*+\mathbf{X}_\mathrm{g}^*:\mathring{\mathbf{g}}^*)\,\mathrm{d}t\,\mathrm{d}V_n-\int_{V_n^*}\rho^* k_{1\to 2}^*\,\mathrm{d}V_n-\int_{\Sigma_n^*}E^*\,\mathrm{d}\Sigma_n \qquad (190)
\end{aligned}$$

for nucleation and for interface propagation

$$\rho_1^{-1}\mathbf{T}:(\mathbf{F}_{21}-\mathbf{I})-[\psi]-\int_{\theta_1}^{\theta_2} s\,\mathrm{d}\theta-\int_t^{t+\Delta t}(\mathbf{X}_\mathrm{p}:\mathring{\mathbf{F}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\mathring{\mathbf{g}})\,\mathrm{d}t-k_{1\to 2}=0$$

$$>\rho_1^{-1*}\mathbf{T}^*:(\mathbf{F}_{21}^*-\mathbf{I})-[\psi^*]-\int_{\theta_1^*}^{\theta_2^*} s^*\,\mathrm{d}\theta^*-\int_t^{t+\Delta t}(\mathbf{X}_\mathrm{p}^*:\mathring{\mathbf{F}}_\mathrm{p}^*+\mathbf{X}_\mathrm{g}^*:\mathring{\mathbf{g}}^*)\,\mathrm{d}t-k_{1\to 2}^*. \qquad (191)$$

For the reverse PT similar reasoning lead to the following extremum principle

$$\int_{m_n} X(\mathbf{b})\,\mathrm{d}m_n-\int_{m_n} k_{2\to 1}(\mathbf{b})\,\mathrm{d}m_n-\int_{\Sigma_n} E\,\mathrm{d}\Sigma_n=0$$

$$<\int_{m_n^*} X(\mathbf{b}^*)\,\mathrm{d}m_n-\int_{m_n^*} k_{2\to 1}(\mathbf{b}^*)\,\mathrm{d}m_n-\int_{\Sigma_n^*} E^*\,\mathrm{d}\Sigma_n, \qquad (192)$$

and its explicit forms.

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. A number of applications of the postulate [Levitas (1992a, 1995a, 1995e, 1997)] give the impression that such an essence is a property of dissipative systems.

6.2. *PT in elastic materials*

Extremum principle (188) for elastic materials at $\theta=$ const and neglected surface energy has the form

$$\int_{V_{n\tau}}\int_{\mathbf{F}_{1\tau}}^{\mathbf{F}_{2\tau}}\mathbf{P}^\mathrm{t}:\mathrm{d}\mathbf{F}_\tau\,\mathrm{d}V_{n\tau}-\int_{V_{n\tau}}\rho_\tau(\psi_2-\psi_1)\,\mathrm{d}V_{n\tau}-\int_{V_{n\tau}}\rho_\tau k\,\mathrm{d}V_{n\tau}=0$$

$$>\int_{V_{n\tau}^*}\int_{\mathbf{F}_{1\tau}^*}^{\mathbf{F}_{2\tau}^*}\mathbf{P}_\tau^{\mathrm{t}*}:\mathrm{d}\mathbf{F}_\tau^*\mathrm{d}V_{n\tau}-\int_{V_{n\tau}^*}\rho_\tau(\psi_2^*-\psi_1^*)\,\mathrm{d}V_{n\tau}-\int_{V_{n\tau}^*}\rho_\tau k^*\,\mathrm{d}V_{n\tau}. \qquad (193)$$

There are some questions concerning PT in elastic materials:

(a) Do the PT conditions depend on the variation of elastic properties during the PT, i.e. $\mathbf{E}(\xi)$, and history $\mathbf{F}_{\mathrm{t}\tau}(\xi)$, if $\mathbf{F}_{\mathrm{t}1\tau}$, $\mathbf{F}_{\mathrm{t}2\tau}$, $\mathbf{E}_1$ and $\mathbf{E}_2$ are fixed ($k\neq 0$)?

(b) Will the interface equilibrium conditions (eqn (129) at $k=0$) be satisfied after the appearance of the nucleus according to the PT criterion and extremum principle (193)?

(c) Do the nucleation condition and extremum principle (193) coincide at $k=0$ with the principle of the minimum of Gibbs energy?

The last question is the most important. A negative answer would mean that our theory is contradictory, because it cannot describe the simplest known situation.

As the interface $\Sigma_{n\tau}$ is considered as the fixed one, then

$$\int_{S_\tau}\int_{\mathbf{u}_1}^{\mathbf{u}_2}\mathbf{p}_\tau\cdot\mathrm{d}\mathbf{u}\,\mathrm{d}S_\tau=\int_{V_{n\tau}}\int_{\mathbf{F}_{1\tau}}^{\mathbf{F}_{2\tau}}\mathbf{P}^\mathrm{t}:\mathrm{d}\mathbf{F}_\tau\,\mathrm{d}V_{n\tau}+\int_{V_\tau}-V_{n\tau}\int_{\mathbf{F}_{1\tau}}^{\mathbf{F}_{2\tau}}\mathbf{P}^\mathrm{t}:\mathrm{d}\mathbf{F}_\tau\,\mathrm{d}V_{n\tau}=\int_{S_{\mathrm{p}\tau}}\mathbf{p}_\tau\cdot\Delta\mathbf{u}\,\mathrm{d}S_\tau, \qquad (194)$$

because the vector $\mathbf{p}_\tau$ is fixed on the $S_{\mathrm{p}\tau}$ and vector $\mathbf{u}$ is fixed on $S_{\mathrm{u}\tau}$ during the PT. In the volume $V_\tau-V_{n\tau}$ $\mathbf{F}_\tau=\mathbf{F}_{\mathrm{e}\tau}\cdot\mathbf{F}_{\mathrm{t}\tau}$, when the PT took part before current time t, or $\mathbf{F}_\tau=\mathbf{F}_{\mathrm{e}\tau}$ ($\mathbf{F}_{\mathrm{t}\tau}=\mathbf{I}$) in the opposite case, and $\mathrm{d}\mathbf{F}_\tau=\mathrm{d}\mathbf{F}_{\mathrm{e}\tau}\cdot\mathbf{F}_{\mathrm{t}\tau}$ (as $\mathbf{F}_{\mathrm{t}\tau}$ does not change in the volume $V_\tau-V_{n\tau}$). Since $\psi=\psi(\mathbf{F}_{\mathrm{e}\tau},\ldots)$ with dots for nonvariable arguments,

$\mathbf{P}^t : \mathrm{d}\mathbf{F}_{e\tau} \cdot \mathbf{F}_{t\tau} = \mathbf{F}_{t\tau} \cdot \mathbf{P}^t : \mathrm{d}\mathbf{F}_{e\tau} = \rho_\tau (\partial\psi/\partial F^t_{e\tau}) : \mathrm{d}\mathbf{F}_{e\tau} = \rho_\tau\, \mathrm{d}\psi$ (elasticity law $(35)_1$ is used), then in $V_\tau - V_{n\tau}$

$$\int_{\mathbf{F}_{1\tau}}^{\mathbf{F}_{2\tau}} \mathbf{P}^t : \mathrm{d}\mathbf{F}_\tau = \psi(\mathbf{F}_{e2\tau}) - \psi(\mathbf{F}_{e1\tau}) = \psi_2 - \psi_1. \tag{195}$$

Substitution of the work integral over the $V_{n\tau}$ from eqn (194) into eqn (193) with the allowance for eqn (195) gives

$$\int_{S_{p\tau}} \mathbf{p}_\tau \cdot \Delta\mathbf{u}\, \mathrm{d}S_\tau - \int_{V_\tau} \rho_\tau \Delta\psi\, \mathrm{d}V_\tau - \int_{V_{n\tau}} \rho_\tau k\, \mathrm{d}V_{n\tau} = 0$$

$$> \int_{S_{p\tau}} \mathbf{p}_\tau \cdot \Delta\mathbf{u}^*\, \mathrm{d}S_\tau - \int_{V_\tau} \rho_\tau \Delta\psi^*\, \mathrm{d}V_\tau - \int_{V_{n\tau}} \rho_\tau k^*\, \mathrm{d}V_{n\tau}. \tag{196}$$

Using the Gibbs energy

$$G(\mathbf{F}_e, \mathbf{F}_{t\tau}, \mathbf{p}_\tau, \mathbf{u}) := \int_{V_\tau} \rho_\tau \psi\, \mathrm{d}V_\tau - \int_{S_{p\tau}} \mathbf{p}_\tau \cdot \mathbf{u}\, \mathrm{d}S_\tau, \tag{197}$$

we obtain

$$\Delta G(\mathbf{F}_e, \mathbf{F}_{t\tau}, \mathbf{p}_\tau, \mathbf{u}) + \int_{V_\tau} \rho_\tau k\, \mathrm{d}V_\tau = 0 < \Delta G(\mathbf{F}_e^*, \mathbf{F}_{t\tau}^*, \mathbf{p}_\tau, \mathbf{u}^*) + \int_{V_\tau} \rho_\tau k^*\, \mathrm{d}V_\tau, \tag{198}$$

where $k^* = k = 0$ in $V_\tau - V_{n\tau}$. Now we can answer the above questions. All the values in eqn (198) depend on the stress–strain state before and after PT and not on the intermediate state. The initial state is given, the final state in an elastic solid is determined by BC and distributions of $\mathbf{F}_{t2\tau}(\mathbf{r}_\tau)$ and $\mathbf{E}_2(\mathbf{r}_\tau)$ after the PT. Consequently, the PT conditions in elastic solids are independent of $\mathbf{F}_{t\tau}(\xi)$ and $\mathbf{E}(\xi)$. In elastoplastic materials the work integrals in eqn (188) and the stress–strain state are history dependent, so they depend on the history of $\mathbf{F}_{t\tau}$ and variations in elastoplastic properties.

Equation (198) at $k = 0$ exhibits known results for the phase equilibrium in elastic materials: the total Gibbs free energy of a system G before and after PT is the same and all unknown parameters are determined from the minimum of Gibbs energy. To derive this result we assumed *validity of nucleation condition* (116) *without fulfillment of local PT criterion* (19) *in each point of nucleus*, i.e. such an assumption is noncontradictory. In this case it is not necessary to use an incremental formulation. At the same time the interface equilibrium equation (129) can also be derived [Grinfeld (1991)] from the condition $\delta G = 0$. If eqn (129) corresponds not only to a stationary value of G, but also to the minimum of G, then both the nucleation condition (193) and the interface equilibrium condition (129) follow from the principle of the minimum of Gibbs energy, i.e. they are equivalent. If for the given interface S_n and stress–strain state eqn (129) corresponds to $\delta G = 0$ only, but not to the minimum of G, then the phase equilibrium is unstable and such nucleus and stress–strain fields cannot be obtained from the nucleation condition (193) or (198). If there is no stable interface under the given BC, then the single phase state is stable.

Consequently, eqn (193) at $k = 0$ is an alternative expression of the principle of the minimum of Gibbs energy, which can be more convenient for analytical and numerical study. Usually $V_{n\tau} \ll V_\tau$ and numerical integration over $V_{n\tau}$ is more economical than over V_τ. When the nucleation place is approximately known, the refined (adapted) finite element mesh is used in this region and all fields in the region are defined more precisely than in the remaining volume. Calculation of the integral over the interface is more economical than over the volume $V_{n\tau}$, but due to the possible irregular character of the interface and approximate fulfillment of conditions $[\mathbf{n}_\tau \cdot \mathbf{P}^t] = 0$, $[\mathbf{F}_\tau] = [\mathbf{F}_\tau] \cdot \mathbf{n}_\tau \mathbf{n}_\tau$ and

$\mathbf{n}_\tau \cdot [\mathbf{P}^t \cdot \mathbf{F}_\tau] \cdot \mathbf{n}_\tau = \mathbf{P}^t : [\mathbf{F}_\tau]$ in a discrete formulation the accuracy can be lower. Consideration of the transforming volume (and not the whole system) allows us to distinguish various types of stress variation in the transforming region in an analytically averaged description of PT in elastic [Levitas and Stein (1995, 1997b)] and elastoplastic [Levitas (1995b)] materials.

At $k \neq 0$ only the incremental solution is possible. For each external load increment the same methods as for PT in elastic materials at $k = 0$ can be used, if we formally use $\bar{\psi}_2 = \psi_2 + k$ instead of ψ_2 in the transforming region. At constant k we can use ψ_2. As the PT criterion (198) is independent of history $\boldsymbol{\varepsilon}_t(\xi)$ and $\mathbf{E}(\xi)$, we can simplify calculation of the integrals in eqn (24). We can first vary $\mathbf{E}(\xi)$ at $\boldsymbol{\varepsilon}_t = \boldsymbol{\varepsilon}_t(0)$ and calculate the integral $\int_{\mathbf{E}_1}^{\mathbf{E}_2} \boldsymbol{\varepsilon}_e(\mathbf{E}) : d\mathbf{E} : \boldsymbol{\varepsilon}_e(\mathbf{E})$ and then at fixed $\mathbf{E} = \mathbf{E}_2$ calculate the integral $\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}_t$ (or first to vary $\boldsymbol{\varepsilon}_t(\xi)$ at $\mathbf{E} = \mathbf{E}_1$ and then $\mathbf{E}(\xi)$ at $\boldsymbol{\varepsilon}_t = \boldsymbol{\varepsilon}_{t2}$). A similar simplification is valid at finite strains.

7. EVALUATION OF THE DISSIPATIVE THRESHOLD k

There are a lot of possible sources of dissipation k due to PT: interaction of transformation strain with the various defects (point defects, dislocations, grain and subgrain boundary), emission of acoustic waves, the necessity to overcome the energy barrier BCD (Fig. 2), interface friction and so on. For the evaluation of the dissipative threshold k let us use the experimental regularity presented in [Estrin (1993)]. The linear dependence between microhardness of materials and pressure hysteresis during the PT was obtained for a number of materials. The microhardness has measured after different types of plastic straining (hydroextrusion, PT) or at various temperatures. Pressure hysteresis was determined as the difference between points of the beginning of direct and reverse PT at compression in the cylinder–piston chamber [Fig. 4(a)]. The conclusion was drawn that due to linear dependence between the hysteresis and hardness (yield stress), hysteresis is completely caused by resistance to plastic deformation and at the zero yield limit the hysteresis would be absent. The additional dissipative threshold k is not considered in Estrin (1993). The above experiments allow us to relate k and yield stress.

The relation between the yield stress and the hardness $\sigma_y = 0.383 H_\mu$ follows from the solution of the axisymmetric problem of the indentation of rigid punch in a perfectly plastic half-space [Ishlinsky (1944)]. This relation is in good agreement with experiments for perfectly plastic materials [Del (1978), Levitas (1987, 1996b)], for hardening materials $\sigma_y = (0.32 \sim 0.37) H_\mu$ depending on the hardening modulus [Del (1978)]. Using the coefficient 0.383 we present schematically experimental results from Estrin (1993) in the coordinates hysteresis H—yield stress σ_y [Fig. 4(b)].

For the interpretation of these results we assume that PT in the piston–cylinder chamber can be described by the axisymmetric problem of coherent PT in a horizontal layer under prescribed pressure σ_n in a chamber [Fig. 4(a)]. We neglect the elastic strain and assume that material outside of the layer is rigid and $\boldsymbol{\varepsilon}_t = 1/3 \varepsilon_0 \mathbf{I} \xi$. We assume that transformation and plastic strains are homogeneous in a layer and stress field is homogeneous and time independent during the PT. We adopt the validity of the von Mises yield condition with equal yield stress of both phases and the equality of value k for the direct and reverse PT. Due to the displacement continuity (coherent PT) and condition $\sigma = \text{const}$ we can apply the same eqns (173)–(181) as for the points of coherent interface in rigid-plastic materials. As $\mathbf{e}_t = 0$, then eqn (181) take a simple form

$$\rho X = \sigma_0 \varepsilon_0 - \rho \Delta \psi^\theta = \rho k. \tag{199}$$

Since $\sigma_n = \sigma_{zz} = \sigma_0 + S_{11}$, $a = \sqrt{2/3} \varepsilon_0$ (eqn (174)), $S_{11} = \sqrt{2/3} \sigma_y$ (eqn (178)), the nucleation criterion (199) gives

$$\rho X = (\sigma_n - 2/3 \sigma_y) \varepsilon_0 - \rho \Delta \psi^\theta = \rho k; \tag{200}$$

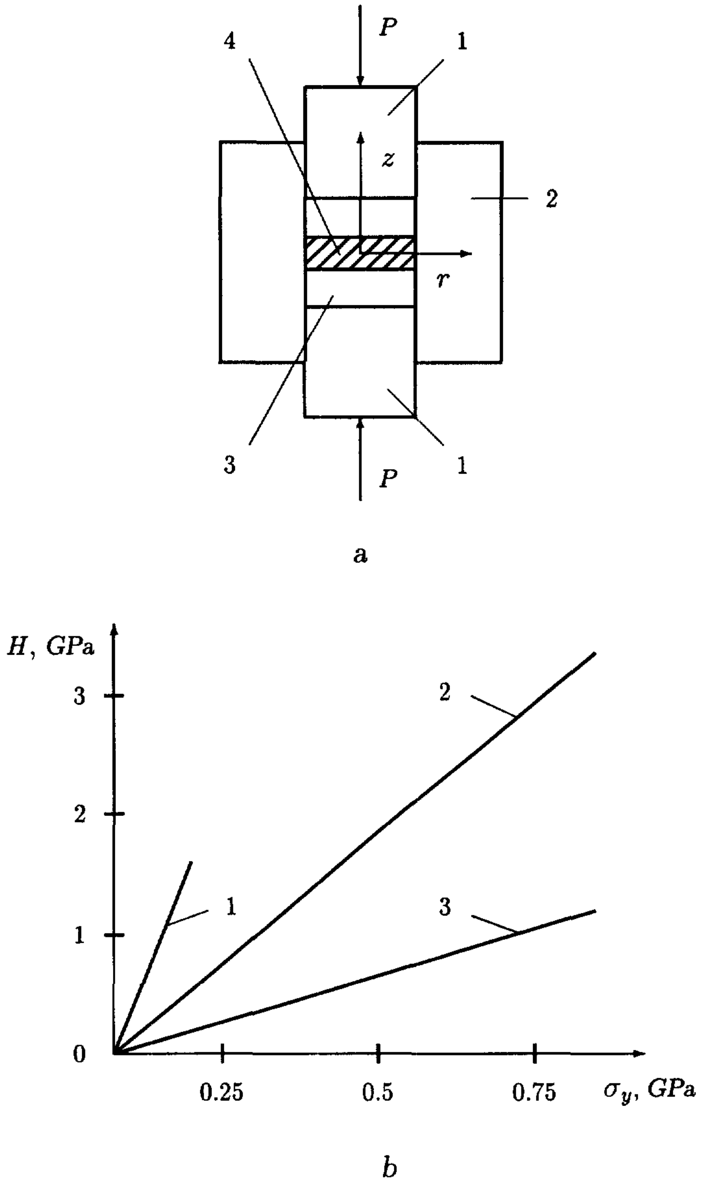

Fig. 4. (a) PT in the piston–cylinder chamber: 1—piston; 2—cylinder; 3—compressed material; 4—transformed region; (b) relation between the pressure hysteresis and the yield stress for various materials [Estrin (1993)]: 1—RbCl, KCl, KBr, KI; 2—CdS, CdSe; 3—Ce, InSb, Bi.

$$\sigma_n^{1\to 2} = \frac{\rho\,\Delta\psi^\theta}{\varepsilon_0} + \frac{\rho k}{\varepsilon_0} + \frac{2}{3}\sigma_y; \quad \sigma_n^{2\to 1} = \frac{\rho\,\Delta\psi^\theta}{\varepsilon_0} - \frac{\rho k}{\varepsilon_0} - \frac{2}{3}\sigma_y;$$

$$H := \sigma_n^{1\to 2} - \sigma_n^{2\to 1} = \frac{2\rho k}{\varepsilon_0} + \frac{4}{3}\sigma_y. \qquad (201)$$

Equation $(201)_3$ in comparison with Fig. 4(b) leads to the conclusion that

$$k = \rho^{-1} L \sigma_y \varepsilon_0 \quad \text{and} \quad H = \sigma_y(4/3 + 2L). \qquad (202)$$

The value L is equal to 5.89 for materials of group 1 [Fig. 4(b)], 1.39 for materials of group 2 and 0.11 for materials of group 3. The coefficient L is a function of the volume fraction of a new phase. Note that the pressure dependence of yield stress should be taken into account.

It follows from the obtained results that plastic work can explain only 8% of hysteresis for materials of group 1, 32% for materials of group 2 and 86% for materials of group 3; the remaining part is related to k. Consequently, the dissipative threshold k is a very important parameter in the theory of martensitic PT and knowledge about its dependence on various parameters are very important. If we assume the validity of eqn $(202)_1$ in the general case, then the dependence of k on temperature, plastic strain, plastic strain rate and history, volume fraction of martensite, grain size and so on are determined. It is known that the smaller the grain size or size of a single crystal, the worse the PT condition is, and in very small crystals temperature induced martensitic PT does not occur [Hornbogen (1984)]. The usual explanation of these results is based on the decrease in the probability of stress concentrators, e.g. dislocations which improve the PT condition, with the reduction of grain size. We can give additional reason based on the above equation. According to the Hall–Petch effect $\sigma_y = a+bd^{-0.5}$, where a and b are constants and d is some characteristic size (size of grain, subgrain, width of martensitic plate and so on [Bernstein *et al.* (1983)]. Consequently, decrease in d results in increase in σ_y and especially k, which makes the PT condition worse.

Let us discuss qualitatively the effect of strain hardening on the PT condition. Yield stresses of both parent and product (due to defects heredity) phases and, consequently, the dissipative threshold k increase with increasing plastic strain. This explains the known experimental results [Bernstein *et al.* (1983); Estrin (1993)] concerning the negative effect of preliminary plastic straining of austenite on PT.

It is necessary to mention that at logarithmic strain of order 1 strain hardening is saturated. As was shown [Levitas (1987, 1996b)] for more than 60 initially isotropic materials belonging to different classes (metals, rocks oxides, compacted powder and powder mixtures) that for monotone (without unloading) and so called quasi-monotone loading, beginning from a certain degree of deformation, materials are deformed as perfectly plastic, isotropic and strain-history independent [see also Levitas *et al.* (1994)]. Due to the relation eqn $(202)_1$ between k and σ_y it is reasonable to assume that after the same critical strain the value k is also strain and strain-history independent. This hypothesis should be verified experimentally.

8. PROBLEM FORMULATION

8.1. *Possible contradictions*

Let us consider a general formulation of quasi-static BVP for the description of PT based on the extremum principle (185) (or for example the principle of the minimum of Gibbs energy for elastic materials (189)). All surfaces across which the transformation deformation gradient $\mathbf{F}_t$ is discontinuous are the interface between the austenite and martensite or different martensite variants. Displacements are continuous in the whole body for coherent PT and have a jump across the interface for noncoherent PT (see Section 9). All deformation gradients $(\mathbf{F}, \mathbf{F}_t, \mathbf{F}_{p2}, \mathbf{F}_{p1}, \ldots)$, stress $\mathbf{T}$, temperature θ are discontinuous across the interface, normal components of stress $\mathbf{T}$ are continuous and the jump of deformation gradient meets the Hadamard compatibility conditions.

Let us introduce the set $\mathscr{A}$ of admissible transformation strain tensors $\mathbf{F}_t$ at $\xi = 1$. For the PT austenite → martensite set $\mathscr{A}$ consists of tensors $\mathbf{F}_t^i = \mathbf{R}_t^i \cdot \mathbf{U}_t^i$, $i = 1, 2, \ldots, k$, where $\mathbf{U}_t^i$ is the symmetric right stretch transformation strain tensor, corresponding to ith martensitic variant, $\mathbf{R}_t^i$ is the orthogonal tensor, $\mathbf{R}_t^t : \mathbf{R}_t = \mathbf{I}$, $\det \mathbf{R}_t = 1$. All $\mathbf{U}_t^i$ are symmetry-related. Some examples of $\mathbf{U}_t^1$ for tetragonal, trigonal, orthorhombic and monoclinic martensite are given in [Bhattacharya and Kohn (1995)]. Tensors $\mathbf{U}_t^i$ for $i > 1$ may be obtained from $\mathbf{U}_t^1$ by permutating the basis.

For the transition from the ith variant with transformation gradient $\mathbf{F}_t^i = \mathbf{R}_t^i \cdot \mathbf{U}_t^i$ to the jth variant with $\mathbf{U}_t^j$ the set $\mathscr{A}$ consists of tensors $\mathbf{F}_t^j = \mathbf{R}_t^j \cdot \mathbf{U}_t^j$, $j \neq i$. For the PT martensite → austenite only the identity tensor $\mathbf{I}$ belongs to $\mathscr{A}$ due to the disappearance of transformation strain.

We assume that the PT occurs instantaneously and adiabatic approximation is valid for all points of the body under consideration. This means that if at time t and fields $\mathbf{r}(\mathbf{r}_\tau, t)$ $\mathbf{T}(\mathbf{r}, t)$, $\theta(\mathbf{r}, t)$, $\mathbf{F}_t(\mathbf{r}, t)$, $\mathbf{F}_{p1}(\mathbf{r}, t)$, $\mathbf{F}_{p2}(\mathbf{r}, t), \ldots$, the PT could occur, it will occur (according to the postulate of realizability) instantaneously, and if after finishing the PT all the above fields are stationary, the PT will not proceed. For the continuation of the PT some fields should be changed due to a change of BC or internal processes (temperature variation, creep, stress relaxation and so on). Assume that the initial data are consistent with such an instantaneous kinetic, i.e. all possible PT are finished. Let during the time Δt all or some of the fields be changed due to a change of BC or internal processes and these variations are calculated under assumptions that the PT do not occur. Let us consider these fields as new initial data ($\xi = 0$) and fix the BC (on one part of surface S_p the stress vector $\mathbf{p}$ is prescribed and on the other part S_u the displacement vector $\mathbf{u}$ is given). It is necessary to find the fields $\mathbf{F}_t(\mathbf{r}, \xi)$ for $0 \leqslant \xi \leqslant 1$ with $\mathbf{F}_t(\mathbf{r}, 1) \in \mathscr{A}$ in some unknown volume V_n (in $V - V_n$ the field $\mathbf{F}_t(\mathbf{r}, t)$ is unchanged) and corresponding to them, fields $\mathbf{r}(\mathbf{r}_\tau, t)$, $\mathbf{T}(\mathbf{r}, \xi)$, $\theta(\mathbf{r}, \xi)$, $\mathbf{F}_p(\mathbf{r}, \xi)$, $\mathbf{F}_\theta(\mathbf{r}, \xi)$, $\mathbf{F}_e(\mathbf{r}, \psi)$, $\mathbf{g}(\mathbf{r}, \xi)$ and $s(\mathbf{r}, \xi)$, satisfying the equilibrium equation $\boldsymbol{\nabla} \cdot \mathbf{T} = 0$ (or dynamic momentum balance equation), yield condition $\varphi(\mathbf{T}, \theta, \mathbf{F}_p, \mathbf{g}, \xi, \ldots) \leqslant 0$ and constitutive eqns (63), (66)–(71) as well as the PT criterion and extremum principle (190).

Since the infinitesimal variation of initial data produces finite changes in all the fields due to the PT and the material's behavior is history dependent, it is not clear how the solution of the problem depends on Δt. The main difficulty consists in the noncontradictory description of some evident physical situations, for example:

- the impossibility of transforming the whole body simultaneously under prescribed homogeneous stresses on the boundary, corresponding to a constant stress tensor;
- the existence of a two-phase equilibrium under the same BC as above;
- the existence of load or temperature hysteresis for the direct and reverse PT.

Particular cases of the above BC are realized in the PT under hydrostatic pressure (in liquid or gas) and temperature-induced PT (stress-free boundary). In experiments PT never occurs instantaneously in the whole body, even if it has a very small size. Nucleation usually takes place in some small subvolume. This is connected with the heterogeneous character of nucleation on various stress concentrators: dislocations, point defects, grain boundaries and so on. The stress concentration allows us to overcome the energy barrier (BCD) in Fig. 2. If the energy barrier is overcome by the thermal fluctuation, the probability of the fluctuation is decreased with the growth of volume as well. To increase the volume fraction of the new phase, the thermodynamic stimulus should be increased, e.g. by load or temperature variation; consequently the phase equilibrium is stable under the fixed temperature or external stresses. It is not simple to describe these results using the extremum principle (185). It is evident that in the homogeneous fields during the PT in the whole uniform body, all the continuum mechanics equations are satisfied and it is easy to show using the simplest example that the homogeneous solution maximizes the functional (185). This is related to the fact that for a nonhomogeneous solution the positive energy of internal (eigen) stresses produces the negative contribution to the driving force of PT. As the corroborating example we can use the solution of a spherically symmetrical problem of the appearance of the spherical nucleus of a new phase with the radius R in sphere with the radius R_0 loaded by homogeneously distributed pressure p [Roitburd and Temkin (1986)]. The result is obtained that for elastic (and elastoplastic) material at $k = 0$ the PT pressure monotonically decreases with the growth of radius R, and the maximum in the principle (185) will be attained at $R = R_0$. The two-phase state is unstable, because at fixed p the driving force of PT grows with the increasing radius of a new phase region.

Consequently, for elastic materials without dissipation ($k = 0$) the problem formulation based only on the principle (185) cannot describe the trivial experimental facts. This does not mean that the postulate of realizability works badly, because in this case the principle (185) coincides with the principle of the minimum of Gibbs energy (198). Let us discuss the possible ways of improving the problem formulation.

One way is the introduction of real stress concentration in material due to the distribution of various defects. In this case the PT starts in the small volume, two-phase equilibrium (at least for small values of the volume fraction of a new phase) is possible, stress or temperature hysteresis in the most cases will not occur due to the zero dissipation and reversibility of the processes. The numerical solution of such a problem becomes much more complicated than without the defects, due to the necessity to consider of very small scales. Such problems are interesting for the investigation of the effect of defects on the PT, but there is no sense in considering other macroscopic problems in this formulation.

It is difficult to suggest more economical noncontradictory methods for the case without dissipation due to PT. We can assume for example that the volume V_n transformed in each step could not exceed some critical volume V_c. Then nucleation will occur in a small volume, but the phase equilibrium will be unstable. For instance, in the problem with spherical symmetry we can simulate the interface motion as subsequent nucleation of spherical layers with a volume V_c. Then the constraint $V_n \leqslant V_c$ does not play any role and the interface is unstable as in the above problem.

In the case of elastic materials with $k \neq 0$ the situation is much better. Due to the finite k dissipation and hysteresis are present. The condition $V_n \leqslant V_c$ can be substituted with the proper growing function $k = k(V_n)$ which allows the nucleation in a small volume only. This dependence introduces some characteristic scale which means that the PT criterion is nonlocal, but such an assumption does not guarantee the stability of the two-phase equilibrium due to the possibility of modeling the interface motion by subsequent nucleation. The assumption that $k = k(V_n, u_n)$ is the increasing function of interface displacement u_n does not change the situation, because instead of continuous interface propagation we can consider that new nuclei subsequently appear with the infinitesimal distance from the existing interface, consequently no one interface moves and $u_n = 0$.

We see at least two ways of getting the stable two-phase equilibrium. The first way is to assume $k = k(V_n, \mathbf{r}_\tau)$, i.e. k is nonhomogeneously distributed in the volume under consideration. The dependence $k = k(V_n, \mathbf{r}_\tau)$ can be obtained by comparing the computed and experimentally determined microstructure only, i.e. by the solution of the inverse problem. Then the field $k = k(V_n, \mathbf{r}_\tau)$ can be used for another BC.

In the second simplified variant we assume that $k = k(V_n, c)$ depends on the volume fraction (or volume) of the second phase. The place of nucleation is defined mostly by maximization of driving force X (due to homogeneity of k distribution) and sufficient increase of k with the c growth guarantees the stability of the two-phase equilibrium. The dependence of k on c is much easier to determine experimentally than the dependence of k on the $\mathbf{r}_\tau$. Such a dependence or even dependence of k on history of volume fraction variation can be borrowed from the macroscopic model [see e.g. Levitas (1994)]. In the general case, it is necessary to use different functions $k = k(V_n, c)$ for the direct, reverse PT, for different martensitic variants and for reorientation processes.

For elastoplastic materials both these variants are valid as well, but some specifications are possible. Based on eqn (202) we can assume $k = \rho^{-1} L(V_n) \sigma_y(V_n, \mathbf{F}_p, \mathbf{r}_\tau) \varepsilon_0$, i.e. the heterogeneity of k is related to the nonhomogeneity of the yield stress. In such a presentation L is the increasing function of V_n and σ_y is the decreasing function of V_n (due to the Hall–Petch effect). The field $\sigma_y(\ldots, \mathbf{r}_\tau)$ can be measured on different scales, using for example hardness, microhardness distribution or hardness measured by nanoindentor (characteristic size 0.01 μm). May be the stable two-phase equilibrium is possible at $k = L(V_n)\sigma_y(V_n, \mathbf{F}_p)$, due to heterogeneous distribution of plastic strain. In this case a second type of description is not necessary, otherwise $k = L(V_n, c)\sigma_y(V_n, \mathbf{F}_p)$.

Of course, for the prescribed displacements on the boundary S or for the nonuniformly distributed stress fields the above problems do not arise. Then the transforming volume is determined by the value of the displacements or by field $X(\mathbf{r}_\tau)$ in the neighborhood of maximum X and all the above three experimental results can be described without the introduction of the dependence of k on V_n and $\mathbf{r}_\tau$. If we consider the general formulation of the problem, we should be able to describe the worst situation.

The smallest size of the transforming region (critical nucleus) can be explicitly determined when the surface energy is taken into account. For a macroscopic region the surface energy is usually negligible in comparison with the elastic energy and dissipation and the Hall–Petch effect can play a significant role.

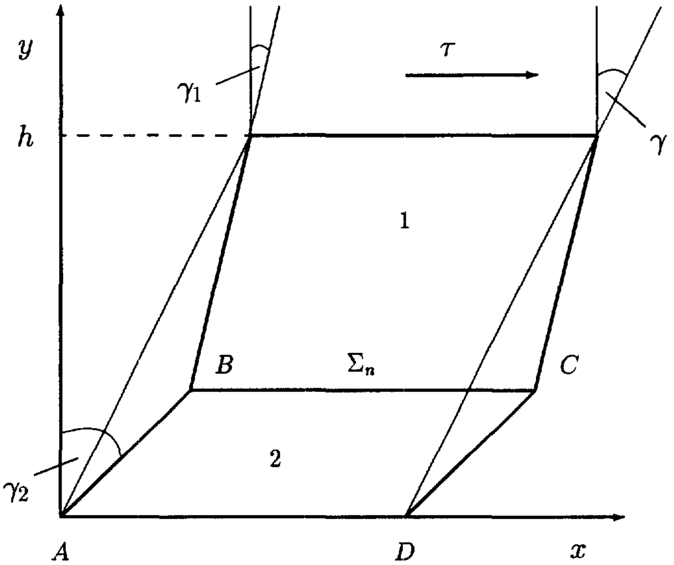

Fig. 5. Simple shear of material with PT.

8.2. *Remarks on the constitutive equations*

Let us consider, in more detail, what types of constitutive equations are used during the PT in our approach. We will start with the simplest case of elastic materials with the stress–strain diagram shown in Fig. 2, equal elastic properties of both phases and $k = 0$. Consider the simple shear of an infinite specimen (Fig. 5). At $y = 0$ velocity is zero, at $y = h$ the uniformly distributed shear stress τ is prescribed. A homogeneous field of shear stresses is the solution to the problem.

When stress reaches some critical value τ_0 determined by Maxwell condition (21), PT will occur. Consider the PT is some infinite layer ABCD as growth of homogeneously distributed transformation shear, then shear stress $\tau = \tau_0$ is fixed in each point during the PT. The main conclusion is that we do not use the part BCDEF of the initial stress–stress diagram and determine the stresses in the transforming region as a solution of quasi-static BVP for each ξ. Making an allowance for the $k \neq 0$ does not complicate the problem, shear stress is constant during the PT and is determined by the PT criterion (25).

When PT occurs in some inclusion, stress varies in the course of PT. To determine the stress variation we do not need the initial stress–strain relation. We introduce the transformation strain in the transforming region at fixed elastic properties and solve for each ξ the quasi-static BVP. Consequently, the stress variation during the PT is not determined by the initial constitutive equation, but by the properties and geometry of the system and BC. The same is valid for an elastoplastic system and different elastic properties of phases. To solve the quasi-static BVP it is necessary to know $\mathbf{E}(\xi)$ and $\sigma_y(\xi)$ for example.

Let us analyze the elastoplastic properties of materials during the PT. They are of course completely unknown and due to the very short duration of PT it is very difficult to determine them experimentally. Some plausible assumptions should be made, which after the simulation of some macroscopic situations can be checked.

Let us estimate the effect of strain rate and temperature variations on the constitutive equations in the transforming region and in its surroundings. If during the time of appearance of the nucleus ($10^{-6} \sim 10^{-10}$ s) the plastic strain rate has an order of 10^{-1} (the same as the transformation strain), then the plastic strain rate has the order of $10^5 \sim 10^9$ s^{-1} and time-dependent viscoplastic behavior should occur. If the PT duration is much smaller than the relaxation time of viscoplastic deformation, the inelastic strain and inelastic properties do not influence the PT condition, which will have the same form as for elastic materials, but all known experimental data exhibit a very strong influence of active and accommodational plastic strain on PT and a correlation between PT parameters and plastic properties. Consequently, the relaxation time of viscoplastic deformation has the same order as the PT duration.

Some of the theories of viscoplasticity are based on the assumption about the existence of the upper stress–strain diagram which corresponds to a very high (theoretically infinite) strain rate and is strain rate independent [Rabotnov (1977)]. Adopting this hypothesis we can use the rate-independent plasticity theory with the higher yield stress.

The temperature variation due to adiabatic heating (cooling) is of the order of 100 K and the problem arises as to whether it is necessary to take into account the temperature dependence of yield stress during such a short-time process. Experiments on high speed metal cuttings shows [Eremin and Rosenberg (1956)], that despite the rather high temperature increase due to plastic dissipation, the yield stress is practically temperature independent. It was related to the fact that the characteristic time of the processes which are responsible for the variation of the yield stress is much larger than the deformation time. The same can be assumed for the PT as well. The effect of temperature on thermoelastic properties should be taken into account.

Consequently, in the first approximation during the PT duration t_p we can use the strain rate and temperature independent plasticity model. After finishing the PT during a time of the order of several seconds the yield stress in the plastically deformed region will be decreased to the static value due to the decrease in the strain rate and changed due to the temperature effect. In the nontransforming region the temperature rises due to plastic dissipation and the yield stress decreases; in the transforming particles the yield stress increases (decreases) when the temperature decreases (increases). For this reason additional plastic flow and stress relaxation will occur. They can influence the next PT event in the surrounding region.

Let us consider a possible structure of inelastic constitutive equations during the PT. The first and simplest variant is a jump-like change of all the properties of the first phase to the properties of the second one at some ξ_0 (in particular at $\xi_0 = 0$ or $\xi_0 = 1$). In this case at $\xi < \xi_0$ (or $\xi > \xi_0$) the properties of the first (second) phase are used. Let the yield surface of phase 2 be $\varphi_2(\boldsymbol{\sigma}, \mathbf{g}) = 0$ (for simplicity small strains are considered). An internal variable $\mathbf{g}$ can be the back stress tensor, plastic strain $\boldsymbol{\varepsilon}_p$ or accumulated plastic strain $q(\dot{q} = (2/3\dot{\boldsymbol{\varepsilon}}_p : \dot{\boldsymbol{\varepsilon}}_p)^{1/2})$. The problem arises: what initial data should be used at $\xi = \xi_0$ for all process parameters and for $\mathbf{g}$ in our case?

We can assume $\mathbf{g}_2(\xi_0) = \mathscr{F}(\mathbf{g}_1(\xi_0), \ldots)$ with the same function $\mathscr{F}$. The case $\mathbf{g}_2 = 0$ means that the second phase completely forgets the deformation process in the first phase (complete recovery [Leblond *et al.* (1989)]. Such a situation is realized at melting and maybe at diffusive PT [Leblond *et al.* (1989)]. For martensitic PT, as follows from electronmicroscopical observations [Spasskiy *et al.* (1965); Utevskiy (1973)], the defect heredity is typical. This does not mean that $\mathbf{g}_2(\xi_0) = \mathbf{g}_1(\xi_0)$. For example, if $\mathbf{g}$ is the dislocation density, then [Streltsov (1985)]

$$\mathbf{g}_2(\xi_0) = (\det \mathbf{F}_t)^{-1} \mathbf{F}_t \cdot \mathbf{g}_1(\xi_0) \cdot \mathbf{F}_t^t. \tag{203}$$

When $\mathbf{g} \equiv q$, then in the simplest case $q_2(\xi_0) = q_1(\xi_0)$, but it is also possible that $q_2(\xi_0) = a q_1(\xi)$ with some scalar a, or $q_2(\xi_0) = q_1(\xi) - a$. Similar variants are valid for $\mathbf{g} \equiv \boldsymbol{\varepsilon}_p$.

If $\mathbf{g}$ is the back stress tensor, characterizing the internal stresses with the constitutive equation

$$\dot{\mathbf{g}}_i = \mathbf{A}_i : \dot{\mathbf{e}}_{pi}, \quad i = 1, 2 \tag{204}$$

(instead of eqn $(12)_2$) in the case without the PT, then during the PT

$$\dot{\mathbf{g}}_1 = \mathbf{A}_1 : (\dot{\mathbf{e}}_p + \dot{\mathbf{e}}_t) \quad \text{at } 0 \leqslant \xi \leqslant \xi_0;$$

$$\dot{\mathbf{g}}_2 = \mathbf{A}_2' : (\dot{\mathbf{e}}_p + \dot{\mathbf{e}}_t) \quad \text{at } \xi_0 < \xi \leqslant 1, \tag{205}$$

where $\mathbf{A}_2'$ differs from $\mathbf{A}_2$ due to a change in elastic properties, $\mathbf{A}_2'(1) = \mathbf{A}_2(1)$. Tensor $\dot{\mathbf{e}}_t$ is added to $\dot{\mathbf{e}}_p$ in eqn (205), because the total tensor of inelastic deformation is responsible for the internal stresses.

A more real situation will be when we use not the jump-like transition at some ξ_0, but some mixture of the properties of the phases 1 and 2 at $0 \leqslant \xi \leqslant 1$, considering ξ as "a volume fraction" of phase 2. In the general case we cannot mix the yield surfaces, but can write for the plastic dissipation rate $\mathscr{D}_p := \mathbf{X}_p : \dot{\boldsymbol{\varepsilon}}_p = (1-\xi)\mathscr{D}_{p1}(\dot{\boldsymbol{\varepsilon}}_p, \mathbf{g}_1) + \xi\mathscr{D}_{p2}(\dot{\boldsymbol{\varepsilon}}_p, \mathbf{g}_2)$ and then determine the yield surface corresponding to $\mathscr{D}_p$. For example, when

$$\mathscr{D}_{pi} = \sqrt{2/3}\sigma_{yi}|\dot{\mathbf{e}}_p| + \mathbf{g}_i : \dot{\mathbf{e}}_p, \quad i = 1, 2; \tag{206}$$

then

$$\mathbf{S}_i = \frac{\partial \mathscr{D}_{pi}}{\partial \dot{\mathbf{e}}_p} = \sqrt{2/3}\sigma_{yi}\frac{\dot{\mathbf{e}}_p}{|\dot{\mathbf{e}}_p|} + \mathbf{g}_i$$

and the yield condition for each phase is $|\mathbf{S} - \mathbf{g}_i| = \sqrt{2/3}\sigma_{yi}$. During the PT

$$\begin{aligned} \mathscr{D}_p &= (1-\xi)(\sqrt{2/3}\sigma_{y1}|\dot{\mathbf{e}}_p| + \mathbf{g}_1 : \dot{\mathbf{e}}_p) + \xi(\sqrt{2/3}\sigma_{y2}|\dot{\mathbf{e}}_p| + \mathbf{g}_2 : \dot{\mathbf{e}}_p); \\ \mathbf{S} &= (1-\xi)\left(\sqrt{2/3}\sigma_{y1}\frac{\dot{\mathbf{e}}_p}{|\dot{\mathbf{e}}_p|} + \mathbf{g}_1\right) + \xi(\sqrt{2/3}\sigma_{y2}|\dot{\mathbf{e}}_p| + \mathbf{g}_2) \end{aligned} \tag{207}$$

and

$$|\mathbf{S} - (1-\xi)\mathbf{g}_1 - \xi\mathbf{g}_2| = \sqrt{2/3}(1-\xi)\sigma_{y1} + \sqrt{2/3}\xi\sigma_{y2}$$

with eqn (205) for $\mathbf{g}_i$. When $\sigma_{y1} = f_1(q)$, $\sigma_{y2} = f_2(q)$ for the case without PT, then besides the same dependence during the PT it is possible to adopt $\sigma_{y1} = f_1(a_1 q)$, $\sigma_{y2} = f_2(a_2 q)$ or $\sigma_{y1} = f_1(q - a_1)$, $\sigma_{y2} = f_2(q - a_2)$ with $a_i = a_i(\xi)$. It is clear that the simplest noncontradictory possibility should be used, as the assumptions cannot be checked experimentally.

8.3. *Analysis of the kinematic decomposition*

Let us consider the kinematic decomposition (29) in more detail. As the reference state for the material point we can take its state at $\xi = 0$, $\mathbf{P} = 0$ and $\theta = \theta_0$ at which $\mathbf{F}_\tau = \mathbf{F}_{e\tau} = \mathbf{F}_{\theta\tau} = \mathbf{F}_{t\tau} = \mathbf{F}_{p1\tau} = \mathbf{F}_{p\tau} = \mathbf{I}$. Before the PT $\mathbf{F}_t = \mathbf{I}$ and we can determine the thermoelastic properties of the first phase. Let $\mathbf{F}_\tau = \mathbf{F}_{e\tau} \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{p1\tau}$ after applying stresses $\mathbf{P}$ and temperature variations. The components of the deformation gradient can be determined in the following way. We will suppose that at some pathway of change in $\mathbf{P}$ to $\mathbf{P} = 0$ and θ to $\theta = \theta_0$ the plastic strain and PT do not occur. Then at elastic unloading ($\mathbf{P} = 0$) and fixed θ from the eqn (29) we get $\mathbf{F}_\tau(\mathbf{P} = 0) = \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{p1\tau}$ and determine $\mathbf{F}_{e\tau} = \mathbf{F}_\tau \cdot \mathbf{F}_\tau^{-1}(\mathbf{P} = 0)$ and the elastic properties of a parent phase at the fixed θ. Then we change θ to $\theta = \theta_0$ and get $\mathbf{F}_\tau(\mathbf{P} = 0, \theta = \theta_0) = \mathbf{F}_{p1\tau}$ and determine $\mathbf{F}_{\theta\tau} = \mathbf{F}_\tau(\mathbf{P} = 0) \cdot \mathbf{F}_{p1\tau}^{-1}$. As all the components of $\mathbf{F}_\tau$ can be determined experimentally after some variations of stress and temperature, all the material properties of the first phase, namely the thermal expansion $\mathbf{F}_{\theta\tau}(\theta)$, the thermoelasticity law $\mathbf{F}_{e\tau}(\mathbf{P}, \theta)$ and flow rule can be determined as well.

Let the PT occur and all components of deformation gradient be present in the given point after applying stresses $\mathbf{P}$ and temperature variations. The term $\mathbf{F}_{p1\tau}$ is known as it can be determined before the PT. The remaining components of the deformation gradient can be determined in the following way. We will suppose that some pathway of change in $\mathbf{P}$ to $\mathbf{P} = 0$ and θ to $\theta = \theta_0$ without the reverse PT and plastic strain exists. Then in the same way as for the first phase we can define $\mathbf{F}_{e\tau}$, $\mathbf{F}_{\theta\tau}$ and consequently $\mathbf{F}_{t\tau} \cdot \mathbf{F}_{p\tau}(1)$ and the thermoelastic properties of the second phase. After that we vary $\mathbf{P}$ and θ in such a way that the reverse PT without additional plastic strain takes place in exactly the opposite direction (i.e. the lattice is reconstructed into its initial state), and the state with $\mathbf{P} = 0$ and $\theta = \theta_0$ can be reached without the direct PT. The remaining strain is $\mathbf{F}_{p\tau}(1) \cdot \mathbf{F}_{p1\tau}$ and we determine $\mathbf{F}_{t\tau}$ and $\mathbf{F}_{p\tau}(1)$ as well.

Let us discuss the sequences of tensors in the decomposition (29). For materials without PT the sequences $\mathbf{F}_\tau = \mathbf{F}_{e\tau} \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{p\tau}$ in the generalized Lee (1969) decomposition is substantiated in books by Levitas (1987, 1992b, 1996b). In brief, the elastic deformation gradient $\mathbf{F}_e$ should always be first from the left-hand side, because in the opposite case it is impossible to derive from the second law of thermodynamics the elasticity law which is independent of temperature and plastic strain. If we designate the thermoelastic strain $\mathbf{F}_{e\theta\tau} := \mathbf{F}_{e\tau} \cdot \mathbf{F}_{\theta\tau}$, then in the decomposition $\mathbf{F}_\tau = \mathbf{F}_{e\theta\tau} \cdot \mathbf{F}_{p\tau}$ again $\mathbf{F}_{e\theta}$ should be from the left-hand side, as in the opposite case it is impossible to derive the thermoelasticity law which is independent of plastic strain. Moreover, if we are interested in studying the thermoelastic behavior of preliminary plastically deformed material, then we consider the motion $\mathbf{r} = \mathbf{r}(\mathbf{r}_p, t)$ with respect to a plastically deformed reference configuration V_p, formed by vectors $\mathbf{r}_p = \mathbf{r}_p(\mathbf{r}_\tau, t)$, $\mathbf{r}_p = \mathbf{F}_{p\tau} \cdot \mathbf{r}_\tau$. The configuration V_τ can be unknown; when we have a piece of material we do not always know how it was previously deformed. Consequently, eqn (29) for materials without PT should be reduced to $\mathbf{F}_\tau = \mathbf{F}_{e\tau} \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{p1\tau}$, or for phase 2 relative to the configuration V_f to $\mathbf{F}_f = \mathbf{F}_{ef} \cdot \mathbf{F}_{\theta f} \cdot \mathbf{F}_{p2f}$ (again, we do not always know whether the material in hand had the PT and plastic strain before or not). Considering the PT relative to the configuration V_{p1}, we again should have elastic and thermoelastic strain from the left and inelastic strain $\mathbf{F}_{t\tau} \cdot \mathbf{F}_{p\tau}(\xi)$ from the right. The problem only remains which of decomposition, $\mathbf{F}_{tp} \cdot \mathbf{F}_{p\tau}(\xi)$ or $\mathbf{F}_{p\tau}(\xi) \cdot \mathbf{F}_{tp}$, is noncontradictory.

We choose the first one, because the tensor $\mathbf{F}_{c\tau} := \mathbf{F}_{e\tau} \cdot \mathbf{F}_{\theta\tau} \cdot \mathbf{F}_{t\tau}$ describes the deformation of a crystal lattice and in some theories (e..g Landau theory) it is not decomposed into its components. In this case during the PT $\mathbf{F}_\tau = \mathbf{F}_{c\tau} \cdot \mathbf{F}_{p\tau}(\xi) \cdot \mathbf{F}_{p1\tau}$ (otherwise it is impossible to derive the "elasticity" law $\mathbf{F}_{c\tau}(\mathbf{P}, \ldots)$ independently of plastic strain) and using the decomposition of $\mathbf{F}_{c\tau}$ we obtain eqn (30). Consequently, eqns (29) and (30) are noncontradictory and all other combinations have some drawbacks.

For polycrystals there are several possibilities of description. First, we can formally apply the same approach as for a single crystal for an initially isotropic material point (similar to phenomenological plasticity theory). The same experimental procedure for the determination of all the components of $\mathbf{F}$ is valid. The problem related to the correct allowance of the finite rotations for each intermediate configuration arises, because there is no explicit privileged orientation as in the case with a crystal lattice. For the solution of the problem it is possible to use the approach developed earlier for finite elastoplasticity [Levitas (1986, 1987, 1992b, 1996b)].

Second, it is possible to consider the representative volume of polycrystalline material under macroscopically homogeneous BC. Using PT theory for a single crystal, solution of the BVP and averaging procedure over the representative volume, we can describe the PT progress and macroscopic constitutive equations numerically. Decomposition (29) for the macroscopic deformation gradient can be applied, but parameter ξ is now the volume fraction of the second phase, i.e. the phase equilibrium is possible for arbitrary $0 < \xi < 1$. There is no contradiction with the derivation of the PT criterion (17) based on the assumption that at $0 < \xi < 1$ phase equilibrium is impossible. We use the PT criterion (17) in this approach not for the whole volume, but for each point of the representative volume. The procedure for the determination of all the components of the macroscopic deformation gradient is the same as for a single crystal, with the difference that all necessary thermomechanical processes can always be realized, because we carry out them not in the real experiment, but numerically.

Third, we can develop a formal phenomenological description of PT in terms of the volume fraction of the new phase. Equations (29), (30), (32)–(38) are valid in this case if parameter ξ is the volume fraction of the second phase. As the phase equilibrium is possible for arbitrary $0 < \xi < 1$, there is no necessity to average over the ξ and the PT criterion is valid in the form $X_\xi = k_\xi$ with k_ξ for the dissipative threshold. The postulate of realizability gives the following extremum principle

$$X_\xi(\mathbf{b}_\xi) - k_\xi(\mathbf{b}_\xi) = 0 > X_\xi(\mathbf{b}_\xi^*) - k_\xi(\mathbf{b}_\xi^*). \tag{208}$$

For a polycrystal it is difficult to determine experimentally $\mathbf{F}_{t\tau}$ and $\mathbf{F}_{p\tau}(\xi)$ separately, because due to the microheterogeneity of the stress state, the plastic strain will be changed during the reverse PT.

It is not always possible to realize the above thermomechanical processes for the separation of all components of the deformation gradient for a single crystal as well and some additional methods are needed. For a single crystal the terms $\mathbf{F}_{e\tau}$, $\mathbf{F}_{\theta\tau}$ and $\mathbf{F}_{t\tau}$ describe the deformation of the crystal lattice, which can be measured independently using for instance X-rays. There are a finite number of possible variants of the transformation strain gradient $\mathbf{F}_{t\tau}$ (to within RBR). The plastic strain does not affect the crystal lattice and consequently the thermoelastic properties and transformation strain gradient $\mathbf{F}_{t\tau}$. Varying the thermomechanical treatment (temperature and plastic strain history) it is possible to significantly change the value k, hysteresis of PT and the region of stability of each phase. If the state with $\mathbf{P} = 0$ and $\theta = \theta_0$ in the second phase can be reached after some treatment, we can determine the thermoelastic properties and the lattice parameters of the second phase and consequently $\mathbf{F}_{t\tau}$. Then in an arbitrary real situation the terms $\mathbf{F}_{e\tau}$ and $\mathbf{F}_{\theta\tau}$ can be calculated under the given $\mathbf{P}$ and θ, one of the possible tensors $\mathbf{F}_{t\tau}$ can be determined by X-rays and $\mathbf{F}_{p\tau}(1)$ can be defined from eqn (29) under the given $\mathbf{F}$.

For arbitrary $0 < \xi < 1$ it is impossible to determine the component of $\mathbf{F}_\tau$ in eqn (29) due to the very short time of the PT and the impossibility of controlling the stress and temperature. Determination of the thermoelastic and plastic properties during the PT is also doubtful. In this case eqn (29) is a convenient assumption for the development of approximate theories.

9. DISPLACEMENT DISCONTINUITIES: NONCOHERENCE AND FRACTURE

One of the mechanisms for getting more profitable stress variation in the transforming particle is related to the possibility of displacement discontinuities on the moving or fixed (at nucleation) interface. The tangential to the interface jump of displacements produces so-called noncoherence and is connected with the generation and sliding of dislocations on the interface with the Burgers vector tangential to the interface. The jump of the normal to interface displacement is a fracture. Earlier [Christian (1965); Roitburd (1972); Boguslavskiy (1985)] the possibility of noncoherent PT in elastic materials was estimated by comparing the energy of a coherent nucleus (displacements are continues) and a noncoherent nucleus while taking into account the energy of dislocations. Now it is clear that the sliding along the interface is a dissipative process and comparison of energies is not sufficient. The dissipative concept in the theory of noncoherent PT in elastoplastic materials at the small noncoherence and in the reference configuration was developed in papers by Levitas (1992a, 1995a, 1997a). A very complex theory was developed by Cermelli and Gurtin (1994b). We will present a modified version of our approach for arbitrary noncoherence and in the actual configuration. Manipulations in the actual configuration allow us to find the contacting points easily and to satisfy the traction continuity condition in them, which are difficult and sometimes impossible (at multiple intersections of many displacement discontinuity surfaces) in the reference configuration. The sliding along the interface can be considered as a contact problem and there is not any limitation on the value of sliding. At incremental solution of BVP in the actual configuration we do not need an information about reference configuration.

For the points of a noncoherent interface the rate of dissipation due to sliding takes the form

$$\mathscr{D}_s = \boldsymbol{\tau} \cdot [\mathbf{v}_s] - \dot{\psi}_s([\mathbf{u}_s]) \geqslant 0, \tag{209}$$

where $[\mathbf{u}_s]$ is the displacement discontinuity, $[\mathbf{v}_s] = [\dot{\mathbf{u}}_s]$, $\boldsymbol{\tau} = -\mathbf{m} \cdot \mathbf{T} \cdot \mathbf{nm}$ the shear stress and ψ_s is the energy of the displacement discontinuity (dislocations). After obvious transformations we obtain

$$\mathscr{D}_s = \left(\boldsymbol{\tau} - \frac{\partial \psi_s}{\partial [\mathbf{u}_s]}\right) \cdot [\mathbf{v}_s] = \mathbf{X}_s \cdot [\mathbf{v}_s] = \mathscr{D}_s([\mathbf{v}_s], [\mathbf{u}_s]), \tag{210}$$

where $\mathbf{X}_s = \boldsymbol{\tau} - (\partial \psi_s / \partial [\mathbf{u}_s])$ is the dissipative force conjugated with $[\mathbf{v}_s]$. The dissipation function $\mathscr{D}_s([\mathbf{v}_s], [\mathbf{u}_s])$ should be determined experimentally; for time-independent martensitic transformations it is a homogeneous function of degree one in $[\mathbf{v}_s]$. Using the postulate of realizability [Levitas (1992a, 1995b)] (or in the given case other postulates of irreversible thermodynamics or plasticity theory) it is easy to obtain relations, formally similar to ones in the plasticity theory;

$$\mathbf{X}_s([\mathbf{v}_s], [\mathbf{u}_s]) \cdot [\mathbf{v}_s]^* - \mathscr{D}_s([\mathbf{v}_s]^*, [\mathbf{u}_s]) < 0 = \mathbf{X}_s([\mathbf{v}_s], [\mathbf{u}_s]) \cdot [\mathbf{v}_s] - \mathscr{D}_s([\mathbf{v}_s], [\mathbf{u}_s]); \tag{211}$$

$$\mathbf{X}_s \cdot [\mathbf{v}_s] > \mathbf{X}_s^* \cdot [\mathbf{v}_s] \quad \text{at } \varphi_s(\mathbf{X}_s^*, [\mathbf{u}_s]) \leqslant 0 = \varphi_s(\mathbf{X}_s, [\mathbf{u}_s]); \tag{212}$$

$$\mathbf{X}_s = \frac{\partial \mathscr{D}_s}{\partial [\mathbf{v}_s]}; \quad [\mathbf{v}_s] = h_s \frac{\partial \varphi_s}{\partial \mathbf{X}_s}, \tag{213}$$

where $\varphi_s = 0$ is the sliding condition (similar to the yield condition) and scalar h_s is determined from the consistency condition

$$\dot{\varphi}_s = \frac{\partial \varphi_s}{\partial \mathbf{X}_s} \cdot \dot{\mathbf{X}}_s + \frac{\partial \varphi_s}{\partial [\mathbf{u}_s]} \cdot [\mathbf{v}_s] = 0. \tag{214}$$

Taking into account eqn (213) we obtain

$$h_s = -\frac{\partial \varphi_s}{\partial \mathbf{X}_s} \cdot \dot{\mathbf{X}}_s \left(\frac{\partial \varphi_s}{\partial [\mathbf{u}_s]} \cdot \frac{\partial \varphi_s}{\partial \mathbf{X}_s} \right)^{-1}. \tag{215}$$

For the function φ_s independent of $[\mathbf{u}_s]$ the scalar h_s is undetermined (as the plastic strain rate for perfectly plastic materials). For the isotropic case we get

$$\mathscr{D}_s = \tau_s |[\mathbf{v}_s]|, \quad \mathbf{X}_s = \tau_s \frac{[\mathbf{v}_s]}{|[\mathbf{v}_s]|}, \quad \varphi_s = |\mathbf{X}_s| - \tau_s = 0 \quad \text{and} \quad [\mathbf{v}_s] = |[\mathbf{v}_s]| \frac{\mathbf{X}_s}{\tau_s}, \tag{216}$$

where τ_s is the dissipative threshold for the occurrence of sliding, at $|\mathbf{X}_s| < \tau_s$ sliding is impossible and the interface is coherent.

In the first approximation we assume that the processes of PT and sliding along the interface are thermodynamically independent, i.e. the driving force X in PT criterion (73) is independent of $[\mathbf{v}_s]$ and the driving force $\mathbf{X}_s$ in sliding criterion (216) is independent of the rate of PT $\dot{\chi}$. Then these processes will interact through the stress field variation due to both of them.

The scheme of application of criteria (122) and (216) is as follows. We model the appearance of a new nucleus in some volume by growth of transformation strain (parameter ξ) and variation of material properties. If for a given ξ the sliding criterion is not met, then the interface is coherent. If for a given ξ the sliding criterion (216) is satisfied, we admit the sliding in this point until a value where the criterion (216) is violated. After completing the PT we check with the criterion (122) whether it is thermodynamically admissible. Consequently, growing transformation strain produces the stresses which are necessary for the appearance of noncoherence and noncoherence changes the stress variation in the transforming particle.

Let us consider the moving interface, using the expression for the rate of dissipation per unit surface of a noncoherent interface

$$\mathscr{D}_\Sigma = -\mathbf{p} \cdot [\mathbf{v}] - \rho_2 [\psi] v_{n2} \geqslant 0. \tag{217}$$

Equation (217) is a counterpart of the equation, obtained for example in papers by Levitas (1992a, 1995a) in the reference configuration. The velocity jump is decomposed $[\mathbf{v}] = [\mathbf{v}_1] + [\mathbf{v}_2]$, where $[\mathbf{v}_1]$ is the velocity jump when $[\mathbf{r}] = 0$, i.e. for a coherent interface,

($[\mathbf{v}_1] := -(\mathbf{I}-\mathbf{F}_{12})\cdot\mathbf{n}v_{n2}$), and $[\mathbf{v}_2] := [\mathbf{v}]-[\mathbf{v}_1]$ is the jump of $[\mathbf{v}]$ at a fixed interface (at $v_{n2}=0$ $[\mathbf{v}_2]=[\mathbf{v}]$). Then

$$[\mathbf{v}_2] = a\mathbf{n}+[\mathbf{v}_s], \tag{218}$$

where a is the normal to the interface component of $[\mathbf{v}_2]$ which characterizes fracture. Consequently,

$$\mathscr{D}_\Sigma = (\mathbf{n}\cdot\mathbf{T}\cdot(\mathbf{I}-\mathbf{F}_{12})\cdot\mathbf{n}-\rho_2[\psi])v_{n2}-\mathbf{n}\cdot\mathbf{T}\cdot\mathbf{n}a+\boldsymbol{\tau}\cdot[\mathbf{v}_s] \geqslant 0. \tag{219}$$

The infinitesimal interface displacement $v_{n2}\,\Delta t$ is modeled by the appearance of the nucleus with the volume $v_{n2}\,\mathrm{d}\Sigma\,\Delta t$ and at the fixed interface the sliding according to eqn (213) is considered. We assume for simplicity thermodynamic independence between the interface motion and sliding (fracture) on the interface. Thermodynamic coupling between $[\mathbf{v}_s]$ and v_n is considered [Levitas (1992a, 1995a)].

The jump of the normal to interface displacement or fracture can be considered in a similar way as noncoherence. We assume that PT and fracture criteria are mutually independent and these processes are coupled through the stress fields only. If, in the course of growth of transformation strain (parameter ξ) and variation of material properties in the nucleus, some chosen fracture criterion is met in some point of the interface (or in other points), the crack should be introduced. Practically this results in the introduction of a new boundary with zero normal and shear stresses. After completing the PT we check with the criterion (122) as to whether PT is in fact possible. Consequently, growing transformation strain generates the stresses which are necessary for fracture and fracture changes the stress variation in the transforming particle. We should not take into account the variation of surface energy due to fracture in PT criterion, because it should be taken into account in the fracture criterion. Thermodynamical coupling between a and $[\mathbf{v}_2]$ can be considered in the standard way.

The next question arises: when a jump of displacements across the interface occurs, does it remain after the shifting of the interface to the next position? The crack remains in the initial position, because there is no physical mechanism of the moving of the crack as a whole. For the sliding along the interface due to generation of the dislocations three variants are possible:

(a) the dislocations remain completely at the initial position;
(b) the dislocations move with the interface;
(c) one part of the dislocations remains and another moves with the interface.

The last two cases are related to nonconservative (not in their slip plane) motion of dislocation and should be accompanied by the diffusion of point defects [Kosevich (1978)]. Nonconservative dislocation motion can occur at diffusive PT, but is too slow for diffusionless martensitic PT. Consequently, dislocations remain at the initial positions and represent the "memory" of the moving noncoherent interface. When shear stresses change the sign and reach the critical value for the sliding inside the second phase then the displacement discontinuity can be decreased.

At the numerical solution of BVP the time step Δt as well as the volume covered by interface $v_{n2}\,\Delta t$ are finite and the solution can depend on the value Δt. There are two typical situations. If the sliding criterion is satisfied at Δt exceeding some critical value Δt_c and at smaller Δt the interface is coherent, then we should use $\Delta t < \Delta t_c$ and obtain a discrete set of noncoherent interfaces. If the sliding criterion is met for arbitrary small Δt, we cannot obtain solution independent of Δt in framework of the model developed. Then sliding on the discrete interfaces should be substituted with the continuous plastic shear in the layer covered by interface $v_{n2}\,\Delta t$. For the simplest isotropic case this results in introduction of the addition yield condition and associated flow rule for the transforming layer:

$$\varphi_s = |\tau| - \tau_s = 0 \quad \text{and} \quad \dot{\gamma}_p = |\dot{\gamma}_p| \frac{\tau}{\tau_s}, \tag{220}$$

where $\dot{\gamma}_p$ is the additional plastic shear strain rate component due to noncoherence, conjugated to τ.

It is known that when the interface loses its coherence, its mobility decreases sharply. The usual explanation of this phenomenon is that it is difficult to shift the interface dislocation, but why can the PT not occur in an infinitesimal neighborhood to a noncoherent interface which is possible without the shifting of the dislocations? It seems to us that the low mobility of a noncoherent interface is related to a sharp change of stress state and decrease in the driving force of PT X. For coherent PT the appearance of the first martensitic nucleus improves the PT condition for the next one or for the growth of the nucleus (the so-called autocatallytic effect), because the energy of internal stresses at the appearance of the first nucleus is higher than at the appearance of the next one or at the growth of the first nucleus.

Noncoherence decreases the energy of internal stresses of the first nucleus, improves the condition of its appearance and reduces the help of these internal stresses the growth of the nucleus. From the other side the remaining displacement discontinuity increases the energy of internal stresses after the shifting of the interface. That is why the appearance of a new nucleus is more profitable thermodynamically than motion of the noncoherent interface. The numerical study of noncoherent interface propagation based on the theory suggested [Levitas *et al.* (1997a)] confirms this qualitative analysis. Note, that noncoherent interface without friction was considered by Grinfeld (1991) and Leo and Sekerka (1989). Detailed kinematics of noncoherent interface is presented by Cermelli and Gurtin (1994b).

10. CONCLUDING REMARKS

The theory developed of PT in the material point of an inelastic continuum allows a consistent derivation of nucleation and interface propagation conditions for quite general situations. The advantages of the proposed approach are as follows. 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. The derivation of the extremum principle is based on the postulate of realizability, which is checked for various thermodynamic systems. We do not consider the whole body, but only material points in which the PT occurs at the current time. For points without PT evidently $X \equiv 0$, which is why it is senseless to study them. They affect the PT through the stress field, because the stress variation in the transforming region in the course of PT is determined by the solution of the BVP for the whole body.

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. All equations of Section 2 are valid for dynamic processes, because the expressions for dissipation increment used are the same as in the quasi-static case. The inertia terms should be taken into account when the Gauss theorem is used in Section 4 and in the jump condition for the traction vector in Section 5.

Consideration of the transforming volume only allows us to simplify the procedure of average description of PT [Levitas (1995b)], because it is not necessary to determine the free energy for the whole representative volume [e.g. in Levitas (1992b); Bhattacharya and Weng (1994)]. At the same time it is possible to determine the stress variation in the transforming region more precisely and distinguish, for example, cases of the appearance of a new nucleus and interface propagation [Levitas and Stein (1996)].

It is possible that under the given increment of BC the local PT conditions for nucleation and interface propagation and the postulate of realizability allows several solutions, e.g. nucleation in different places or deformation process without PT. Then the stability analysis should be used. The stable solution can be chosen using the extremum principle for the whole volume, using again the postulate of realizability [Levitas (1992a, 1995a)]. This means that the fulfilment of the local PT criteria is not enough for the occurrence of PT and only the global criterion will give the final solution. An example of noncoincidence of the local ad global PT criteria is considered [Levitas (1992a, 1995a); Idesman *et al.* (1997)].

Despite some difficulties in problem formulation, some simple BVPs were formulated and solved analytically [Levitas (1995c, 1995d, 1996a, 1996c, 1997)]: PT in a thin layer (horizontally and optimally inclined) in a rigid-plastic half-space under the action of applied pressure and shear stresses; PT under compression and shear of materials in Bridgman anvils; the appearance of the spherical nucleus in an infinite elastoplastic sphere under applied pressure (without and with fracture on an interface) with application to temperature-induced PT in steel and pressure-induced PT graphite–diamond; noncoherent PT in a rigid-plastic half-space. A number of experimental results are explained and some of the interpretations are completely unexpected. Some methods to control of PT by means of the purposeful control of stress–strain fields are suggested. A numerical study of the PT based on the theory proposed was made [Levitas *et al.* (1996b, 1997a); Idesman *et al.* (1997)].

At the same time, it is not completely clear how a material knows before PT that after finishing the PT criterion (73) will be met. For an elastic material without dissipation due to PT it is possible to imagine that direct and reverse PT occur due to fluctuations and the phase equilibrium corresponds to an equal activation barrier (e.g. equal areas (BCD) and (DEF) in Fig. 2) [see Abeyaratne and Knowles (1993); Levitas *et al.* (1996b)]. If direct PT due to some fluctuations occurs at a stress smaller than the Maxwell stress τ_0 in Fig. 2, then the reverse PT returns the particle to the parent phase, because at a stress smaller than the Maxwell stress the activation barrier for the reverse PT is smaller that for the direct PT. Due to the complete reversibility of processes nothing will change in the system after numerous fluctuational direct and reverse PT. Consequently, the phase transition (equilibrium) condition has in this case a statistical interpretation. When $k \neq 0$, after the fluctuational direct PT at $0 < X < k$ the condition for the reverse PT at the same k will be worse and the material with the higher probability will be in phase 2 rather than in phase 1. If direct and reverse PT occur fluctuationally, then heat generation will take place. For plastic materials additionally the plastic strain will be accumulated. All these contradictions indicate, that for materials with threshold type dissipation statistical interpretation of the PT condition is impossible.

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