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Structural changes without stable intermediate state in inelastic material. Part II. Applications to displacive and diffusional–displacive phase transformations, strain-induced chemical reactions and ductile fracture

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Abstract

A number of simple examples demonstrate the applicability of the general theory developed in Part I of this paper to various structural changes in solids, namely to displacive and generalized second-order phase transformations, twinning and reorientation of crystal lattice, ductile fracture, and strain-induced chemical reactions. The theory is extended to diffusional-displacive phase transitions. The following problems for elastic and elastoplastic materials are solved analytically: displacive and diffusional–displacive phase transitions in a spherical particle inside the space under external pressure, martensitic phase transition and twinning in ellipsoidal inclusion under applied shear stress, spherical void nucleation, crack propagation in a similar framework to the Dugdale model for a plane stress state. In most cases explicit expressions for the thermodynamic and kinetic conditions for structural changes and the geometric parameters of the nucleus are obtained and analyzed. The following typical cases in the determination of the geometric parameters of nucleus are found: solely from the principle of the minimum of transformation time and the kinetic equation without any constraints or with thermodynamic constraint; from the principle of the minimum of transformation mass and the thermodynamic criterion of structural changes (thermodynamically admissible nucleus); as an interatomic distance. For diffusional–displacive phase transformations, additional variants are related to the necessity to consider the diffusion equation (for the diffusion-controlled transformation) and constraints related to the maximum and minimum possible

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volume fraction of solute atoms. The nucleation kinetics for various nucleus geometries is compared.

Keywords: Phase transformation; Fracture; Chemo-mechanical processes; Constitutive behaviour; Kinetics

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1. Introduction

In Part I of this paper (Levitas, 2000), a general thermomechanical and kinetic approach to a very wide class of structural changes (SC) in inelastic materials is developed. The aim of this part is to illustrate an application of the general theory to various concrete phenomena, namely, martensitic phase transformations (PT), generalized second-order phase transitions, twinning, strain-induced chemical reactions in shear band, ductile fracture (void nucleation, crack propagation). Some extensions of the theory necessary for the description of diffusional–displacive PT (for example bainitic) are presented as well. In all the cases the simplest model problems are formulated in order to obtain analytical solutions which can be easily analyzed. A number of generalizations are possible.

Let us summarize the main equations and extremum principles derived in Part I (Levitas, 2000) for the parameters homogeneously distributed in the transforming volume V_n.

The local driving force for SC

$$\begin{aligned}\rho X &= \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \sigma : \mathrm{d}(\boldsymbol{\varepsilon}_\mathrm{e} + \boldsymbol{\varepsilon}_\theta + \boldsymbol{\varepsilon}_\mathrm{t}) - \rho(\psi_2 - \psi_1) - \int_{\theta_1}^{\theta_2} \rho s \mathrm{d}\theta + \int_{\mathbf{g}_1}^{\mathbf{g}_2} \frac{\partial \psi}{\partial \mathbf{g}^\mathrm{t}} : \mathrm{d}\mathbf{g} + \int_{\boldsymbol{\varepsilon}_{\mathrm{p}1}}^{\boldsymbol{\varepsilon}_{\mathrm{p}2}} \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_\mathrm{p}} : \mathrm{d}\boldsymbol{\varepsilon}_\mathrm{p} \\ &= \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \boldsymbol{\sigma} : \mathrm{d}(\boldsymbol{\varepsilon}_\theta + \boldsymbol{\varepsilon}_\mathrm{t}) - 0.5 \int_{\mathbf{E}_1}^{\mathbf{E}_2} \boldsymbol{\varepsilon}_\mathrm{e} : \mathrm{d}\mathbf{E} : \boldsymbol{\varepsilon}_\mathrm{e} - \rho\left(\psi_2^\theta - \psi_1^\theta\right) - \int_{\theta_1}^{\theta_2} \rho s \mathrm{d}\theta \\ &\quad + \int_{\mathbf{g}_1}^{\mathbf{g}_2} \rho \frac{\partial \psi}{\partial \mathbf{g}^\mathrm{t}} : \mathrm{d}\mathbf{g} + \int_{\boldsymbol{\varepsilon}_{\mathrm{p}1}}^{\boldsymbol{\varepsilon}_{\mathrm{p}2}} \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}_\mathrm{p}} : d\boldsymbol{\varepsilon}_p. \end{aligned} \tag{1}$$

The thermodynamic criterion of SC

$$\left(X - K^0\right)\rho V_n - \Gamma \Sigma_n \geqslant 0. \tag{2}$$

The kinetic equation

$$t_\mathrm{s} = t_0 \exp\left(-\frac{\left(X - K^0 - E_\mathrm{a}\right)\rho V_n - \Gamma \Sigma_n}{R\theta_\mathrm{ef}} \frac{N}{n}\right). \tag{3}$$

The principle of the minimum of the transformation time

$$t_\mathrm{s} = t_\mathrm{o} \exp\left(-\frac{\left(X^* - K^0 - E_\mathrm{a}\right)\rho^* V_n^* - \Gamma \Sigma_n^*}{R\theta_\mathrm{ef}} \frac{N}{n}\right) \to \min. \tag{4}$$

The extremum principle and kinetic equation for the case when the characteristic size of the nucleus is determined by a combination of principle (4) and the thermodynamic criterion (2) (with the sign =)

$$m_n^* = \rho^* V_n^* \rightarrow \min; \quad t_s = t_o \exp\left(\frac{\rho E_a}{R\theta_{ef}}\frac{N}{n}V_n\right). \tag{5}$$

Here $\boldsymbol{\varepsilon}_e$ is the elastic, $\boldsymbol{\varepsilon}_p$ the plastic, $\boldsymbol{\varepsilon}_\theta$ the thermal and $\boldsymbol{\varepsilon}_t$ the transformational strains; $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ are the strain and stress tensors, ρ is the mass density, s is the specific entropy, θ is the temperature, **E** is the tensor of elastic moduli, **g** is the internal variable, V_n is volume bounded by the boundary Σ_n in which SC occurs, ψ is the specific Helmholtz free energy and ψ^θ is its thermal part, Γ is the surface energy per unit area, E_a is the specific activation energy, K^0 is the athermal component of the driving force X, t_s is the transformation time, $m_n = \rho V_n$ is the mass of transforming volume V_n, $R = 8.314$ J/(K mol) is the gas constant, t_o is some characteristic time, n is the number of atoms in volume V_n which undergo thermal fluctuations, $N = 6.02 \times 10^{23}$ is Avogadro's number (number of atoms in 1 mol), θ_{ef} is the effective temperature, $\theta_{ef} = \int_0^1 \theta d\xi$, ξ is the order parameter which varies from 0 to 1 during the SC, subscripts 1 and 2 denote that parameter is defined for phase 1 (before SC) and phase 2 (after SC). For small strain approximation $\rho^* \simeq \rho$.

We will need also the following equations derived in Part I of this paper (Levitas, 2000). The local entropy production equation [Eq. (7) in Part I of this paper]

$$\tilde{S}_i := \rho\dot{s} - \rho\frac{r}{\theta} + \frac{1}{\theta}\mathrm{div}\mathbf{h} - \frac{\boldsymbol{\nabla}\theta}{\theta^2}\cdot\mathbf{h} \geqslant 0, \tag{6}$$

where **h** is the heat flux and r is the volumetric heat supply. Expression for the local rate of dissipation [Eq. (20) in Levitas, (2000)]

$$\mathcal{D} = \mathbf{X}_p : \dot{\boldsymbol{\varepsilon}}_p + \mathbf{X}_g : \dot{\mathbf{g}} + \mathbf{X}_h\cdot\mathbf{h} + X_\xi\dot{\xi} \tag{7}$$

where

$$\mathbf{X}_p = \frac{1}{\rho}\boldsymbol{\sigma} - \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p}; \quad \mathbf{X}_g = -\frac{\partial\psi}{\partial\mathbf{g}^t}; \quad \mathbf{X}_h = -\frac{1}{\rho}\frac{\boldsymbol{\nabla}\theta}{\theta} \tag{8}$$

and

$$X_\xi = \frac{1}{\rho}\boldsymbol{\sigma} : \frac{\partial(\boldsymbol{\varepsilon}_t + \boldsymbol{\varepsilon}_\theta)}{\partial\xi} - \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_t} : \frac{\partial\boldsymbol{\varepsilon}_t}{\partial\xi} - \frac{\partial\psi}{\partial\xi} \tag{9}$$

are the dissipative forces conjugated to dissipative rates $\dot{\boldsymbol{\varepsilon}}_p$, $\dot{\mathbf{g}}$, **h** and $\dot{\xi}$, respectively. Expression for entropy [Eq.$(21)_2$ in Part I of this paper]

$$s = \frac{\boldsymbol{\sigma}}{\rho} : \frac{\partial\boldsymbol{\varepsilon}_\theta}{\partial\theta} - \frac{\partial\psi}{\partial\theta}. \tag{10}$$

2. Determination of temperature. Some specifications

Temperature variation during the SC can be very significant (for example, it exceeds 1500 K for strain-induced chemical reactions in Ti–Si and Nb–Si systems, see; Nesterenko et al., 1994, 1995; Levitas et al., 1998b,c) and it has to be taken into account in the calculation of driving force and effective temperature in a kinetic equation. Generally it is impossible to obtain the local temperature evolution equation due to the term with surface energy. To obtain a simple analytical solution to a number model problems we will neglect the surface energy in dissipation inequality [Eq. (10) in Levitas (2000)] and obtain the relation $\theta\tilde{S}_{\mathrm{i}} = \mathcal{D}$ between local entropy production and dissipation rate $\mathcal{D}$. Then the combination of this relation with the local entropy production Eq. (6) and for the volumetric heat supply neglected for simplicity results in an entropy balance equation

$$\rho\theta\dot{s} = \rho\mathcal{D} - \mathrm{div}\mathbf{h} + \frac{\nabla\theta}{\theta}\cdot\mathbf{h}. \tag{11}$$

Substitution of an expression for the local rate of dissipation (7) in Eq. (11) yields

$$\theta\dot{s} = -\rho^{-1}\mathrm{div}\mathbf{h} + \mathbf{X}_{\mathrm{p}} : \dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} + \mathbf{X}_{\mathrm{g}} : \dot{\mathbf{g}} + X_{\xi}\dot{\xi}. \tag{12}$$

According to Eq. (10) we have $s = s\left(\theta, \boldsymbol{\sigma}, \mathbf{g}, \boldsymbol{\varepsilon}_{\mathrm{p}}, \xi\right)$. Substitution of this expression and generalized Fourier law $\mathbf{h} = \mathbf{f}_{\mathrm{h}}\left(-\frac{\nabla\theta}{\theta}\right)$ for the heat flux into Eq. (12) leads to the temperature evolution equation

$$\begin{aligned}\nu\dot{\theta} = {} & -\rho^{-1}\mathrm{div}\mathbf{f}_{\mathrm{h}}\left(-\frac{\nabla\theta}{\theta}\right) + \left(\mathbf{X}_{\mathrm{p}} - \frac{\partial s}{\partial\boldsymbol{\varepsilon}_{\mathrm{p}}}\theta\right) : \dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} + \left(\mathbf{X}_{\mathrm{g}} - \frac{\partial s}{\partial\mathbf{g}}\theta\right) : \dot{\mathbf{g}} \\ & + \left(X_{\xi} - \frac{\partial s}{\partial\xi}\theta\right)\dot{\xi} - \theta\frac{\partial s}{\partial\boldsymbol{\sigma}} : \dot{\boldsymbol{\sigma}}, \quad \nu := \theta\frac{\partial s}{\partial\theta},\end{aligned} \tag{13}$$

where ν is the specific heat at constant $\boldsymbol{\sigma}$, $\mathbf{g}$, $\boldsymbol{\varepsilon}_{\mathrm{p}}$ and ξ. Due to the divergence term the temperature at the given point can be determined after formulation and solution of a boundary-value problem. The situation is much simpler for the *adiabatic* process, i.e. at $\mathrm{div}\mathbf{h} = 0$, when Eq. (13) determines the temperature evolution in each material point independently, i.e. without a solution of the boundary-value problem.

Let us consider some specifications of Eq. (13). Generally $\boldsymbol{\varepsilon}_{\theta} = \boldsymbol{\alpha}(\theta - \theta_{\mathrm{o}})$, where $\boldsymbol{\alpha}(\xi, \theta - \theta_{\mathrm{o}})$ is the thermal expansion tensor and θ_{o} is the reference temperature. Assume the validity of the following decomposition for the free energy

$$\rho\psi_i = 0.5\boldsymbol{\varepsilon}_{\mathrm{e}} : \mathbf{E}_{\mathrm{i}} : \boldsymbol{\varepsilon}_{\mathrm{e}} + \rho\psi_i^{\theta} = \rho\psi_{\mathrm{i}}^{\mathrm{e}} + \rho\psi_i^{\theta}, \quad i = 1, 2, \tag{14}$$

at constant (i.e. strain and temperature independent) elastic moduli $\mathbf{E}_i$, specific heats and thermal expansion tensors in each phase. Then from the definition (13) $\nu := \theta\frac{\partial s}{\partial\theta}$ elasticity law $\boldsymbol{\sigma} = \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_{\mathrm{e}}} = \mathbf{E} : \boldsymbol{\varepsilon}_{\mathrm{e}}$ and from Eq. (10) we derive explicit expressions for the entropy and the thermal part of the free energy for each phase and for the material in the process of SC:

$$\rho s_i = \rho s_{oi} + \rho \nu_i \ln \theta/\theta_o + \boldsymbol{\sigma} : \boldsymbol{\alpha}_{\mathrm{i}}, \quad i = 1, 2; \tag{15}$$

$$\psi_i^{\theta} = \psi_{oi} - s_{oi}(\theta - \theta_o) - \nu_i \theta(\ln \theta/\theta_o - 1) - \nu_i \theta_o; \tag{16}$$

$$\rho s = \rho s_o(\xi) + \rho \nu(\xi) \ln \theta/\theta_o + \boldsymbol{\sigma} : \boldsymbol{\alpha}(\xi); \tag{17}$$

$$\psi^{\theta} = \psi_o(\xi) - s_o(\xi)(\theta - \theta_o) - \nu(\xi)\theta(\ln \theta/\theta_o - 1) - \nu(\xi)\theta_o. \tag{18}$$

Here s_{oi} and ψ_{oi} are the constants. Functions $s_o(\xi)$, $\mathbf{E}(\xi)$, $\nu(\xi)$ and $\boldsymbol{\alpha}(\xi)$ are usually unknown and we assume a linear approximation

$$\begin{aligned} s_o &= (1-\xi)s_{01} + \xi s_{02}, \quad & \mathbf{E} &= (1-\xi)\mathbf{E}_1 + \xi \mathbf{E}_2, \\ \nu &= (1-\xi)\nu_1 + \xi \nu_2, \quad & \boldsymbol{\alpha} &= (1-\xi)\boldsymbol{\alpha}_1 + \xi \boldsymbol{\alpha}_2. \end{aligned} \tag{19}$$

Then Eq. (13) can be transformed into the form

$$\nu(\xi)\dot{\theta} = \left(X_{\xi} - \theta \Delta s_o - \Delta \nu \theta \ln \frac{\theta}{\theta_o} - \rho^{-1} \boldsymbol{\sigma} : \Delta \boldsymbol{\alpha} \theta \right) \dot{\xi} - \rho^{-1} \dot{\boldsymbol{\sigma}} : \boldsymbol{\alpha}(\xi)\theta + \mathbf{X}_{\mathrm{p}} : \dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} + \mathbf{X}_{\mathrm{g}} : \dot{\mathbf{g}}, \tag{20}$$

where $\Delta \mathbf{b} := \mathbf{b}_2 - \mathbf{b}_1$ and independence of s_o of $\mathbf{g}$ and $\boldsymbol{\varepsilon}_{\mathrm{p}}$ is assumed. According to Eq. (9)

$$\begin{aligned} X_{\xi} = {} & \rho^{-1} \boldsymbol{\sigma} : \frac{\partial \boldsymbol{\varepsilon}_{\mathrm{t}}}{\partial \xi} + \rho^{-1} \boldsymbol{\sigma} : \Delta \boldsymbol{\alpha}(\theta - \theta_o) - 0.5 \rho^{-1} \boldsymbol{\varepsilon}_{\mathrm{e}} : \Delta \mathbf{E} : \boldsymbol{\varepsilon}_e - \Delta \psi_o \\ & - \Delta \nu(\theta - \theta_o) + \Delta s_o(\theta - \theta_o) + \Delta \nu \theta \ln \theta/\theta_o \end{aligned} \tag{21}$$

and Eq. (20) can be transformed into

$$\begin{aligned} \nu(\xi)\dot{\theta} = {} & \left(\rho^{-1} \boldsymbol{\sigma} : \frac{\partial \boldsymbol{\varepsilon}_{\mathrm{t}}}{\partial \xi} - \rho^{-1} \boldsymbol{\sigma} : \boldsymbol{\Delta} \ \boldsymbol{\alpha} \theta_o - 0.5 \rho^{-1} \boldsymbol{\varepsilon}_{\mathrm{e}} : \Delta \mathbf{E} : \boldsymbol{\varepsilon}_{\mathrm{e}} - \Delta \psi_o - \Delta s_o \theta_o \right. \\ & \left. - \Delta \nu(\theta - \theta_o) \right) \dot{\xi} - \rho^{-1} \dot{\boldsymbol{\sigma}} : \boldsymbol{\alpha}(\xi)\theta + \mathbf{X}_{\mathrm{p}} : \dot{\boldsymbol{\varepsilon}}_{\mathrm{p}} + \mathbf{X}_{\mathrm{g}} : \dot{\mathbf{g}}. \end{aligned} \tag{22}$$

In contrast to (Levitas, 1998a) we did not use the simplifying assumption $X_{\xi} = K^0$. If ψ_o, Δs_o and $\Delta \nu$ are independent of $\mathbf{g}$, and $\boldsymbol{\varepsilon}_{\mathrm{p}}$, then $\mathbf{X}_{\mathrm{g}} = 0$ and $\rho \mathbf{X}_{\mathrm{p}} = \boldsymbol{\sigma}$. Using Eq. (21), the expression for X, can be transformed into

$$\begin{aligned} pX = {} & \int_{\boldsymbol{\varepsilon}_{\mathrm{t1}}}^{\boldsymbol{\varepsilon}_{\mathrm{t2}}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{t}} + \int_d^1 \boldsymbol{\sigma} : \Delta \boldsymbol{\alpha}(\theta - \theta_o) \mathrm{d}\xi - 0.5 \int_0^1 \boldsymbol{\varepsilon}_{\mathrm{e}} : \Delta \mathbf{E} : \boldsymbol{\varepsilon}_{\mathrm{e}} \mathrm{d}\xi - \rho \Delta \psi_o \\ & + \rho \Delta s_o \int_0^1 (\theta - \theta_o) \mathrm{d}\xi - \rho \Delta \nu \int_0^1 (\theta - \theta_o - \theta \ln \theta/\theta_o) \mathrm{d}\xi. \end{aligned} \tag{23}$$

At constant $\boldsymbol{\sigma}$ at $\dot{\boldsymbol{\varepsilon}}_p = \Delta\boldsymbol{\varepsilon}_p\dot{\xi}$, with a constant $\Delta\boldsymbol{\varepsilon}_p$, at $\frac{\partial\boldsymbol{\varepsilon}_t}{\partial\xi} = \Delta\boldsymbol{\varepsilon}_t$ and when the change in elastic strain due to the change of elastic constants is small Eq. (22) has a form

$$\begin{aligned}&(\nu_1 + \Delta\nu\xi)\dot{\theta} = (A - \Delta\nu\theta)\dot{\xi},\\ &A := \rho^{-1}\boldsymbol{\sigma} : \Delta\boldsymbol{\varepsilon}_t - \rho^{-1}\boldsymbol{\sigma} : \Delta\boldsymbol{\alpha}\theta_o - 0.5\rho^{-1}\boldsymbol{\varepsilon}_e : \Delta\mathbf{E} : \boldsymbol{\varepsilon}_e\\ &\quad - \Delta\psi_o - \Delta s_o\theta_o + \Delta\nu\theta_o + \rho^{-1}\boldsymbol{\sigma} : \Delta\boldsymbol{\varepsilon}_p\end{aligned} \tag{24}$$

and allows a simple analytical solution

$$\begin{aligned}&\theta = \frac{1}{\Delta\nu}\left(A - \nu_1\frac{A - \Delta\nu\theta_1}{\nu_1 + \Delta\nu\xi}\right); \qquad \theta_2 = \frac{A + \nu_1\theta_1}{\nu_2},\\ &\theta_{ef} = \frac{A}{\Delta\nu} - \frac{\nu_1(A - \Delta\nu\theta_1)}{\Delta\nu^2}\ln\frac{\nu_2}{\nu_1}.\end{aligned} \tag{25}$$

Substitution of expression for temperature (25) in expression for X (23) leads to a somewhat bulky result. At $\Delta\nu = 0$, we obtain more simple formulae

$$\theta = \theta_1 + \frac{A}{\nu}\xi; \quad \theta_2 = \theta_1 + \frac{A}{\nu}; \quad \theta_{ef} = \theta_1 + \frac{A}{2\nu} = 0.5(\theta_1 + \theta_2). \tag{26}$$

Eqs. (25) and (26) are approximately valid at variable stress as well provided that SC heat $-(\Delta\psi_o + \Delta s_o\theta_o)\dot{\xi}$ significantly exceeds all stress-dependent contributions to A. After substitution of Eq. (26) in expression (23) for X it results in

$$\begin{aligned}\rho X = &\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}}\boldsymbol{\sigma} : d\boldsymbol{\varepsilon}_t + \int_0^1\boldsymbol{\sigma} : \Delta\boldsymbol{\alpha}\left((\theta_1 - \theta_o) + \frac{A}{\nu}\xi\right)d\xi - 0.5\int_0^1\boldsymbol{\varepsilon}_e : \Delta\mathbf{E} : \boldsymbol{\varepsilon}_e d\xi +\\ &\rho\Delta s_o\left(\theta_1 - \theta_o + \frac{A}{2\nu}\right) - \rho\Delta\psi_o.\end{aligned} \tag{27}$$

3. Appearance of a spherical nucleus in an infinite elastoplastic sphere

Let us consider the PT in a spherical inclusion with the radius r in an infinite elastic — perfectly plastic sphere under applied external pressure p. Such a problem was considered from a thermodynamic point of view using different criteria in several papers (Roitburd and Temkin, 1986; Fischer et al., 1994; Levitas, 1997a,b). We will follow the paper by Levitas (1997b) and additionally take into account the temperature variation during the PT and the kinetic aspect.

Elastic properties of parent and new phases are the same, $\boldsymbol{\varepsilon}_t = 1/3\varepsilon_o\mathbf{I}\xi$ with $\varepsilon_o = \text{const}$. Then the pressure $\tilde{p}$ in a nucleus is determined by formulas (Roitburd and Temkin, 1986; Fischer et al., 1994):

$$\text{in elastic regime} \quad \tilde{p}_{\mathrm{e}} = p - \frac{\varepsilon_{\mathrm{o}}\xi}{3C}, \quad |\xi| \leqslant |\xi'|, \quad \xi' := \frac{2\sigma_{\mathrm{y}}C}{\varepsilon_{\mathrm{o}}}; \tag{28}$$

$$\text{in plastic regime} \quad \tilde{p}_{\mathrm{p}} = p - \frac{2}{3}\sigma_{\mathrm{y}}\left(\ln\frac{\varepsilon_{\mathrm{o}}\xi}{2\sigma_{\mathrm{y}}C} + 1\right), \quad |\xi| > |\xi'|. \tag{29}$$

Here $C = \frac{3(1-\nu_{\mathrm{o}})}{2E}$, E is Young's modulus, ν_{o} is Poisson's ratio, σ_{y} is the yield stress of parent phase, $\xi'\varepsilon_{\mathrm{o}}$ is the strain corresponding to the onset of plastic flow in the parent phase. Note that σ_{y} can be *positive* or *negative* and due to the condition $\frac{\varepsilon_{\mathrm{o}}}{2\sigma_{\mathrm{y}}C} > 0$ the signs of σ_{y} and ε_{o} *coincide*. Calculation of the transformation work yields

$$\int_{\boldsymbol{\varepsilon}_{\mathrm{t}1}}^{\boldsymbol{\varepsilon}_{\mathrm{t}2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{t}} = p\varepsilon_{\mathrm{o}} - \frac{\varepsilon_{\mathrm{o}}^2}{6C} \tag{30}$$

at elastic deformation and

$$\int_{\boldsymbol{\varepsilon}_{\mathrm{t}1}}^{\boldsymbol{\varepsilon}_{\mathrm{t}2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{t}} = \int_0^1 \tilde{p}\varepsilon_{\mathrm{o}}\mathrm{d}\xi = \int_0^{\xi'} \tilde{p}_{\mathrm{e}}\varepsilon_{\mathrm{o}}\mathrm{d}\xi + \int_{\xi'}^1 \tilde{p}_{\mathrm{p}}\varepsilon_{\mathrm{o}}\mathrm{d}\xi = p\varepsilon_{\mathrm{o}} - \frac{2}{3}\sigma_{\mathrm{y}}\varepsilon_{\mathrm{o}}\left(\frac{\sigma_{\mathrm{y}}C}{\varepsilon_{\mathrm{o}}} + \ln\frac{\varepsilon_{\mathrm{o}}}{2\sigma_{\mathrm{y}}C}\right) \tag{31}$$

at elastoplastic deformation. It is evidently that Eq. (30) can be obtained from Eq. (31) at $\sigma_{\mathrm{y}} = \frac{\varepsilon_{\mathrm{o}}}{2C}$ i.e. at $\xi' = 1$. Assuming that $\Delta\nu = 0$ and the term $-(\Delta\psi_{\mathrm{o}} + \rho\Delta s_{\mathrm{o}}\theta_{\mathrm{o}})\dot{\xi}$ significantly exceeds all other heat sources, we obtain from Eq. (26)

$$\theta = \theta_1 - \frac{\Delta\psi_{\mathrm{o}} + \Delta s_{\mathrm{o}}\theta_{\mathrm{o}}}{\nu}\xi; \quad \theta_2 = \theta_1 - \frac{\Delta\psi_{\mathrm{o}} + \Delta s_{\mathrm{o}}\theta_{\mathrm{o}}}{\nu}. \tag{32}$$

Using expression (27) for X we obtain

$$\begin{aligned} \rho X &= \int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{t}} - \rho\Delta\psi_{\mathrm{o}} + \rho\Delta s_{\mathrm{o}}\left(\theta_1 - \theta_{\mathrm{o}} + \frac{A}{2\nu}\right) \\ &= \int_{\boldsymbol{\varepsilon}_{\mathrm{t}1}}^{\boldsymbol{\varepsilon}_{\mathrm{t}2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{t}} + \rho\Delta s_{\mathrm{o}}(0.5(\theta_2 - \theta_1) - \theta_{\mathrm{o}}) - \rho\Delta\psi_{\mathrm{o}}; \quad A = -\Delta\psi_0 - \Delta s_o\theta_0. \end{aligned} \tag{33}$$

It follows from Eq. (33) that accounting for adiabatic heating results in the replacing of the SC start temperature θ_1 with $\theta_{\mathrm{ef}} = 0.5(\theta_2 + \theta_1)$, the same as in the dominator of kinetic Eq. (3).

As X in the solution under consideration is independent of radius r, we can repeat the same conclusions as at SC in a spherical nucleus in Part I of this paper. That is, the extremum principle (4) results in condition $r \rightarrow \min$ and the minimum value of r is determined by the thermodynamic criterion of SC (2), i.e.

$$\left(X - K^0\right)\frac{4}{3}\pi r_{\mathrm{t}}^3\rho - \Gamma 4\pi r_{\mathrm{t}}^2 = 0 \quad \text{or} \quad r_{\mathrm{t}} = \frac{3\Gamma}{\rho(X - K^0)}. \tag{34}$$

It follows from Eq. (5)

$$t_s = t_o \exp\left(\frac{\rho E_a}{R\theta_{ef}}\frac{N}{n}\frac{4}{3}\pi r_t^3\right). \tag{35}$$

Thermodynamically, PT is possible at $X \geqslant K^0$, i.e. at pressure

$$p \geqslant \frac{\varepsilon_o}{6C} + \frac{1}{\varepsilon_o}\left(K^0 + \rho\Delta\psi_o - \rho\Delta s_o(0.5(\theta_2+\theta_1)-\theta_o)\right) \tag{36}$$

for an elastic material and at

$$p \geqslant \frac{2}{3}\sigma_y\left(\frac{\sigma_y C}{\varepsilon_o} + \ln\frac{\varepsilon_o}{2\sigma_y C}\right) + \frac{1}{\varepsilon_o}\left(K^0 + \rho\Delta\psi_o - \rho\Delta s_o(0.5(\theta_2+\theta_1)-\theta_o)\right) \tag{37}$$

in the elastoplastic regime. However at small $X - K^0$ the radius of a thermodynamically admissible nucleus is large and the transformation time can significantly exceed the time of observation. Only at relatively large $X - K^0$ and small r_t can PT be observed during a reasonable time. As a kinetic PT criterion we can assume $t_s = t_{ob}$, where t_{ob} is the accepted observation time. The kinetic aspect can play a very significant role, e.g. for PT graphite–diamond treated thermodynamically in paper by Levitas (1997b).

4. Martensitic phase transition, twinning and reorientation in ellipsoidal inclusion

Let us consider PT in a thin (penny-shape) ellipsoidal inclusion of radius r and semithickness b, $r \gg b$, inside an infinite space under the action of remote shear stress τ_e (Fig. 1). The space is elastic, inclusion can be elastic or elastoplastic. All the

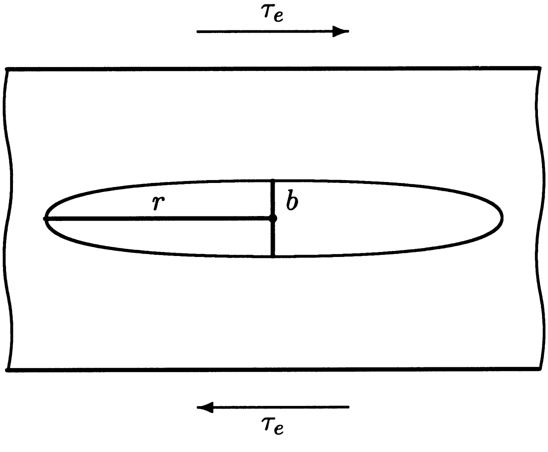

Fig. 1. Appearance of ellipsoidal nucleus.

properties are isotropic, $\mathbf{E}_1 = \mathbf{E}_2$ and temperature variation is neglected. The transformation strain contains the shear component $0.5\gamma_t$ only. It is clear that extremum principle (4) results in the orientation of a long side of inclusion r along shear stress. The thermodynamics of PT in ellipsoidal elastic inclusion has been well investigated (Christian, 1965; Olson and Cohen, 1986) using the principle of the minimum of Gibbs free energy. Kaganova and Roitburd (1989) considered elastoplastic inclusion using the same principle. This approach is analyzed in Levitas (1998a). Our thermodynamic results coincide with the known one for elastic inclusion and differ (due to the different thermodynamic approach) for elastoplastic inclusion. The kinetic analysis presented below is carried out for the first time.

4.1. Phase transformation in elastic inclusion

For an elastic material using the Eshelby (1957) solution we obtain for the shear stress in inclusion

$$\tau = \tau_e - \eta\gamma_t\frac{b}{r}; \quad \eta = \frac{\mu\pi(2-\nu_o)}{4(1-\nu_o)}, \tag{38}$$

where μ is the shear modulus. The transformation work and a local driving force are

$$\int_0^{\gamma_{t2}} \tau \mathrm{d}\gamma_t = \tau_e\gamma_{t2} - 0.5\eta\gamma_{t2}^2\frac{b}{r}; \quad \rho X = \tau_e\gamma_{t2} - \frac{1}{2}\eta\gamma_{t2}^2\frac{b}{r} - \rho\Delta\psi^\theta. \tag{39}$$

As the transformation work depends on r and b we will first try to determine them from the extremum principle (4). Minimizing with respect to r and b the transformation time, i.e.

$$\left(\tau_e\gamma_{t2} - \frac{1}{2}\eta\gamma_{t2}^2\frac{b}{r} - \rho\Delta\psi^\theta - \rho K^0 - \rho E_a\right)\frac{4}{3}\pi r^2 b - \Gamma 2\pi r^2 \rightarrow \max_{r,b}, \tag{40}$$

we obtain from conditions $\frac{\partial t_s}{\partial b} = \frac{\partial t_s}{\partial r} = 0$

$$b_k = \frac{M r_k}{\eta\gamma_{t2}^2}; \quad r_k = \frac{\eta\gamma_{t2}^2 b_k^2}{2(2Mb - 3\Gamma)}; \quad M := \tau_e\gamma_{t2} - \rho\Delta\psi^\theta - \rho K^0 - E_a. \tag{41}$$

Subscript k means that the parameter is determined from kinetic conditions. Let us analyze some variants depending on parameter M:

1. If $2Mb - 3\Gamma > 0$, then both $b > 0$ and $r > 0$. As a coefficient at r^2 in Eq. (40) is positive in this case, then r_k in Eq. (41) corresponds to the maximum rather than the minimum of the transformation time. The minimum transformation time is at $r \rightarrow \infty$ and consequently $b \rightarrow \infty$, which does not correspond to the necessity of thermal activation and the validity of kinetic equation (3).

2. Let $2Mb-3\Gamma<0$ and $M>0$, then $b>0$ (if $r_\mathrm{k}>0$), r_k in Eq. (41) corresponds to minimum of transformation time, but it is negative. Consequently, the extremum principle (40) results in

$$b=\frac{Mr}{\eta\gamma_{\mathrm{t}2}^2};\quad r\rightarrow\min. \tag{42}$$

The minimum value of r can be found from the thermodynamic PT criterion

$$\left(\tau_\mathrm{e}\gamma_{\mathrm{t}2}-0.5\eta\gamma_{\mathrm{t}2}^2\frac{b}{r}-\rho\Delta\psi^\theta-\rho K^0\right)\frac{4}{3}\pi r^2b-\Gamma 2\pi r^2=0, \tag{43}$$

i.e. the thermodynamically admissible relation between the radius and semi-thickness is as follows

$$r=\frac{\eta\gamma_{\mathrm{t}2}^2b^2}{2\bar{A}b-3\Gamma};\quad \bar{A}:=\tau_\mathrm{e}\gamma_{\mathrm{t}2}-\rho\Delta\psi^\theta-\rho K^0=M+E_\mathrm{a}>0, \tag{44}$$

where condition $2\bar{A}b>3\Gamma$ determines external parameters at which PT can occur. Combining Eqs. (44) and (42), we have

$$b=\frac{3\Gamma}{2\bar{A}-M},\quad r=\frac{3\eta\gamma_{\mathrm{t}2}^2}{\left(2\bar{A}-M\right)M}. \tag{45}$$

Conditions $2Mb-3\Gamma<0$ and $M>0$ result in $E_\mathrm{a}<\bar{A}<3E_\mathrm{a}$. If $2Mb=3\Gamma$ and $M>0$, then the extremum principle (40) again results in $r\rightarrow\min$ and we obtain solution (45). Condition $2Mb=3\Gamma$ can be satisfied at $\bar{A}=3E_\mathrm{a}$. At $M\rightarrow 0$ we obtain

$$b=\frac{3\Gamma}{2\bar{\mathrm{A}}},\quad r\rightarrow\infty. \tag{46}$$

3. If the thickness b determined by Eq. $(45)_1$ or $(46)_1$ is smaller than interatomic distance a in direction b, then we have to put $b=a$ in Eq. (43) and obtain

$$r=\frac{\eta\gamma_{\mathrm{t}2}^2a^2}{2\bar{A}a-3\Gamma};\quad 2\bar{A}a>3\Gamma. \tag{47}$$

4. Let $M<0$ and $\bar{A}>0$, then both r_k and b_k in Eq. (41) correspond to the minimum of the transformation time, but both are negative. The extremum principle (40) results in $r\rightarrow\min$ and $b\rightarrow\min$ without any relation between r and b. Consequently, the principle of minimum of transforming volume (5) under constraint (43) or (44) has to be used. Substituting Eq. (44) in expression for V_n we obtain

$$V_n=\frac{4}{3}\pi r^2b=\frac{4}{3}\pi\eta^2\gamma_{t2}^4\frac{b^5}{(2\bar{A}b-3\Gamma)^2}\rightarrow\min_b \tag{48}$$

and an explicit expression for the thickness and radius of a thermodynamically admissible nucleus

$$b_t = 2.5\frac{\Gamma}{\bar{A}}; \quad r_t = 3.125\frac{\eta\gamma_{t2}^2\Gamma}{\bar{A}^2}; \quad \frac{r_t}{b_t} = 1.25\frac{\eta\gamma_{t2}^2}{\bar{A}}; \quad V_{nt} = 102.26\eta^2\gamma_{t2}^4\frac{\Gamma^3}{\bar{A}^5}. \tag{49}$$

Condition $\frac{r_t}{b_t} \gg 1$ results in $\eta\gamma_{t2}^2 \gg \bar{A}$ i.e. the energy of internal stresses (calculated at $b = r$) has to significantly exceed the local driving force with neglected internal stresses. For a critical nucleus, after finding a stationary (saddle) point of the left part of Eq. (43) we obtain

$$b_c = 2\frac{\Gamma}{\bar{A}}; \quad r_c = 2\frac{\eta\gamma_{t2}^2\Gamma}{\bar{A}^2}; \quad \frac{r_c}{b_c} = \frac{\eta\gamma_{t2}^2}{\bar{A}}; \quad V_{nc} = 33.51\frac{\eta^2\gamma_{t2}^4\Gamma^3}{\bar{A}^5} = 0.328\mathrm{V}_{nt}, \tag{50}$$

i.e. critical nucleus is a little bit less flat than the thermodynamically admissible one. At $\tau_e = K^0 = 0$ Eq. (50) is equivalent to those in the paper by Olson and Cohen (1986).

If the thickness b determined by Eq. $(49)_1$ is smaller than interatomic distance a, then we have to put $b = a$ and Eq. (47) is valid.

Consequently, for elastic inclusion 4 variants of determination of nucleus geometry exist: when both r and b are determined by kinetics, in this case $r \to \infty$, $b \to \infty$; when b is determined by the kinetics and r by the thermodynamic criterion; when both r and b are calculated using thermodynamic parameters; when b is equal to interatomic distance and r is determined by the thermodynamic criterion. The temperature variation can be estimated in the same way as in the previous problem, i.e. under the assumption that the transformation heat exceeds all the other heat sources. However, a more detailed analytical solution is available. Substitution of expression (39) for X and geometric parameters found in kinetic equations (3) or (5) allows us to calculate the transformation time.

4.2. Plastic inclusion

For plastic inclusion

$$\tau = \tau_e - \eta(\gamma_t - \gamma_p)\frac{b}{r}, \tag{51}$$

where γ_p is a plastic shear acting in the opposite direction to the transformation shear. During the growth of transformation strain shear stress decreases, changes the sign and reaches the yield stress τ_c in the opposite direction to the external stress

$$\tau = -\tau_c < 0 \Rightarrow \gamma_t - \gamma_p = \frac{\tau_e + \tau_c}{\eta}\frac{r}{b} = \gamma_{tc} = \mathrm{const} \leqslant \gamma_{t2}. \tag{52}$$

Here γ_{tc} is the value of the transformation shear at which plastic flow starts and it cannot exceed γ_{t2}. This causes the limitation on the ratio $\frac{r}{b}$

$$\frac{r}{b} \leqslant \frac{\eta\gamma_{t2}}{\tau_e + \tau_c}. \tag{53}$$

In order to keep the elastic state in the matrix, we assume that the yield stress of the parent phase is higher than the yield stress of the product phase. This can be the case for martensitic PT in shape memory alloys or at reverse PT in steels (provided that reverse PT foregoes the diffusional decomposition). The inelastic strain in inclusion $\gamma_{tc} := \gamma_t - \gamma_p$ remains constant during the plastic flow. Consequently, stress and plastic strain variations in the inclusion can be described by the following equations (Fig. 2)

$$\begin{aligned} \tau = \tau_e - \eta\gamma_t\frac{b}{r} \quad &\text{at} \quad \gamma_t < \gamma_{tc}; \\ \tau = -\tau_c \quad \text{and} \quad \gamma_p = \gamma_t - \gamma_{tc} \quad &\text{at} \quad \gamma_{tc} \leqslant \gamma_t \leqslant \gamma_{t2}. \end{aligned} \tag{54}$$

Calculation of the transformation work gives

$$\begin{aligned} \int_0^{\gamma_{t2}} \tau \mathrm{d}\gamma_t &= \int_0^{\gamma_{tc}} \left(\tau_e - \eta\gamma_t\frac{b}{r}\right)\mathrm{d}\gamma_t - \int_{\gamma_{tc}}^{\gamma_{t2}} \tau_c \mathrm{d}\gamma_t \\ &= \tau_e\gamma_{tc} - 0.5\eta\gamma_{tc}^2\frac{b}{r} - \tau_c(\gamma_{t2} - \gamma_{tc}) = -\tau_c\gamma_{t2} + 0.5(\tau_e + \tau_c)^2\eta^{-1}\frac{r}{b}. \end{aligned} \tag{55}$$

First, let us find the thermodynamic restriction. From the thermodynamic PT criterion

$$\left(A_1 + B\frac{r}{b}\right)\frac{4}{3}\pi r^2 b - \Gamma 2\pi r^2 \geqslant 0; \tag{56}$$

$$A_1 := -\tau_c\gamma_{t2} - \rho\Delta\psi^\theta - \rho K^0; \quad B := 0.5(\tau_e + \tau_c)^2\eta^{-1}, \tag{57}$$

follows the relation between r and b

$$2A_1 b \geqslant 3\Gamma - 2Br. \tag{58}$$

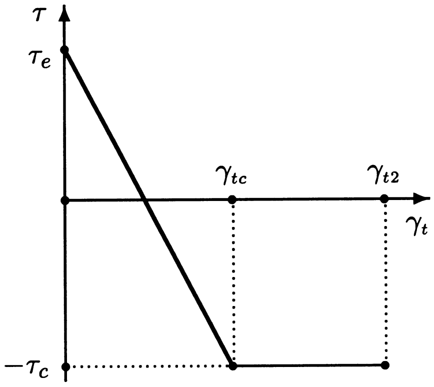

Fig. 2. Stress variation in the nucleus in the course of transformation strain growth.

Minimizing with respect to r and b the transformation time, i.e.

$$\left(M_1 + B\frac{r}{b}\right)\frac{4}{3}\pi r^2 b - \Gamma 2\pi r^2 \ \rightarrow \ \max_{\mathrm{r,b}}, \ \ M_1 := A_1 - E_a, \tag{59}$$

we obtain the following:

1. At $M_1 > 0$ we have $r \rightarrow \infty$ and $b \rightarrow \infty$, we can always satisfy the thermodynamic inequality (58), as well as constraint (53). At $M_1 = 0$ again $r \rightarrow \infty$ and as the transformation time is independent of b, we can choose $b \rightarrow \infty$ and satisfy constraint (53).
2. At $M_1 < 0, A_1 > 0$ we obtain $r \rightarrow \infty$, $b \rightarrow$ min and inequality (53) is violated, i.e. the inclusion is elastic and the above solution has to be used.
3. In order to satisfy inequality (53) we have to look for finite r. Thus, if $M_1 + B\frac{r}{b} < 0$, then $r \rightarrow$ min (as well as b) and the principle of the minimum of transforming volume under constraint (56) or (58) (with the sign =) has to be used. Substituting Eq. (58) in expression for V_n we obtain

   $$V_n = \frac{2}{3}\pi r^2 \frac{3\Gamma - 2Br}{A_1} \ \rightarrow \ \min_r \tag{60}$$

   and the expressions for the geometric parameters of a thermodynamically admissible nucleus

   $$r_t = \frac{\Gamma}{B}, \ \ b_t = \frac{\Gamma}{2A_1}, \ \ \frac{r_t}{b_t} = \frac{2A_1}{B} \leqslant \frac{\eta\gamma_{t2}}{\tau_e + \tau_c}, \ \ V_{nt} = \frac{2\pi}{3}\frac{\Gamma^3}{A_1 B^2}, \tag{61}$$

   where inequality $(61)_3$ follows from Eq. (53). Inequality $M_1 + B\frac{r}{b} < 0$ is satisfied at $3A_1 < E_a$. As the left part of Eq. (56) is linear in b, a stationary point and critical nucleus do not exist, and the larger b, the higher the driving force. According to the classical concept of a critical nucleus, the whole volume has to be transformed barrierless. Our approach predicts an explicit size of nucleus as well as the transformation time Eq. (5).
4. Let $A_1 < 0$, then b_t in Eq. (61) is less than zero. In this case condition $b \rightarrow$ min is satisfied at $b = a$. Corresponding r can be found from the thermodynamic criterion

   $$r = \frac{3\Gamma - 2A_1 a}{2B}, \ \ \frac{r}{b} = \frac{3\Gamma - 2A_1 a}{2Ba} \leqslant \frac{\eta\gamma_{t2}}{\tau_e + \tau_c}. \tag{62}$$

The last inequality determines a lower bound for A_1. Eq. (62) is valid at positive, but very large A_1 as well, when b_t determined by Eq. $(61)_2$ is smaller than lattice parameter a. In this case condition $3\Gamma > 2A_1 a$ has to be taken into account.

Comparison of elastic and elastoplastic solutions exhibits their significant differences. In particular, the case when the thickness b is determined by kinetics and the radius r is restricted by thermodynamics is lacking for plastic materials.

The reverse PT can be considered in a similar way.

4.3. Twinning and reorientation

Twinning is one of the physical mechanisms of plastic deformation of crystalline materials, especially at a low temperature, related to a jump-like shear deformation of the crystal lattice. Martensitic phase transitions are usually accompanied by twinning in order to reduce the energy of internal stresses. The significant difference between the description of dislocation plasticity (crystal slip) and twinning consists in the fact that slip shear can be infinitesimal, but the transformation shear due to twinning is always finite and its value is completely determined by crystallography. The shear stress varies significantly during the twinning (γ_t growth from zero to final value) and can even change the sign, and the variation depends on the solution of the corresponding boundary-value problem for the whole volume under consideration.

The thermodynamic theory of twinning in inelastic materials as a particular case of martensitic PT is developed by Levitas (1998a). For twinning $\psi_2^\theta = \psi_1^\theta$, $\boldsymbol{\varepsilon}_t = 0.5\gamma_t(\mathbf{mn}+\mathbf{nm})$ with γ_t for shear strain, $\mathbf{m}$ for shear direction, $\mathbf{n}$ for normal to shear plane and Eq. (1) gives

$$X = \frac{1}{\rho}\int_0^{\gamma_{t2}} \tau d\gamma_t + \frac{1}{\rho}\int_{\boldsymbol{\varepsilon}_{1\theta}}^{\boldsymbol{\varepsilon}_{2\theta}} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}_\theta - \frac{1}{2\rho}\int_{\mathbf{E}_1}^{\mathbf{E}_2} \boldsymbol{\varepsilon}_e : d\mathbf{E} : \boldsymbol{\varepsilon}_e - \int_{\theta_1}^{\theta_2} s d\theta + \int_{\mathbf{g}_1}^{\mathbf{g}_2} \frac{\partial\psi}{\partial\mathbf{g}^t} : d\mathbf{g} + \int_{\boldsymbol{\varepsilon}_{p1}}^{\boldsymbol{\varepsilon}_{p2}} \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p} : d\boldsymbol{\varepsilon}_p \tag{63}$$

with $\tau = \mathbf{m}\cdot\boldsymbol{\sigma}\cdot\mathbf{n}$ for the shear stress conjugated to γ_t. Here $\boldsymbol{\varepsilon}_p$ is related to dislocation plasticity only. 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_t and orientation of $\mathbf{e}_i$ before twinning. For $\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_p} = \frac{\partial\psi}{\partial\mathbf{g}} = 0$, isothermal processes and neglected surface energy and change in elastic moduli we obtain

$$X = \frac{1}{\rho}\int_o^{\gamma_{t2}} \tau d\gamma_t = K. \tag{64}$$

A significant difference between the Schmid law $\tau = \tau_c$ (condition of plastic shear due to dislocation motion) and Eq. (64) consists in the fact that shear stress τ varies significantly during the twinning and the variation depends on the solution of the corresponding boundary-value problem for the whole volume V. That is why the criterion of maximum shear stress, which is conventional for slip plasticity, does not describe experiments on the nucleation of a single twin under ball indentation (Boiko et al., 1986; 1991). Nevertheless, the criterion of maximum shear stress is applied to the numerical simulation of crystallographic texture during twinning and plastic slip (Kalidindi, 1998; Staroselsky and Anand, 1998).

Another approach, related to the theory of martensitic phase transformations, determines change in Gibbs free energy, a saddle point and activation energy based on solution to the problem of Eshelby elastic inclusion (Lee and Yoo, 1990; Yoo and

Lee, 1991). However, application of this approach is less clear when a dissipation due to twinning or slip plasticity have to be taken into account. Macroscopic, phenomenological, thermodynamically-based constitutive equations for twinning in elastic materials have been presented in papers by Rajagopal and Srinivasa (1995, 1997).

The results obtained in Section 4.1 describe the thermodynamics of twinning in isotropic materials at $K^0 \neq 0$, as well as the kinetics of twin nucleation. The solution to an elastoplastic problem cannot be applied to twinning, because due to equal plastic properties of material before and after twinning, plastic flow has to occur outside of inclusion as well. Numerical study of stress distributions and driving force at nucleation of martensitic plate and twin with due account of plasticity in both inclusion and surrounding and finite stains is carried out in the papers by Idesman et al. (1999, 2000).

Another type of inelastic deformation which is formally very close to twinning and martensitic PT is the reorientation process. For phase transformation from austenite to martensite, due to the symmetry of crystal lattice there is a finite number (e.g. 12 for the phase transformation from a cubic to monoclinic lattice) of crystallographically equivalent variants of martensite. All martensitic variants have the same components of the transformation strain tensor, but in different crystallographic basis. Transformation of one martensitic variant into another is called reorientation process. As reorientation can be considered as a *thermomechanical process* of change of transformation strain from the initial to the final value, which is accompanied by a change in all the mechanical properties, it can be treated in the similar way as twinning. There are two distinctive features of reorientation which are not important from the viewpoint of general theory in comparison with twinning: both initial and final transformation strains are nonzero and transformation strain does not necessarily represent simple shear. Some results of the micromechanical description of reorientation in elastic materials can be found in Sun and Hwang (1993), Levitas and Stein (1997). In the framework of the approach presented in this paper we can use Eq. (1) or (23) for X at $\Delta\psi^\theta = \Delta s_o = \Delta\nu = 0$ and calculate all the integrals when we vary transformation strain from its value for an initial variant $\boldsymbol{\varepsilon}_{t1}$ to the final one $\boldsymbol{\varepsilon}_{t2}$. For elastic materials the corresponding inclusion problem can be easily solved including determination of the change in the orientation of the inclusion. For plastic materials this is possible to do analytically for the reorientation in the whole inclusion without any change in its orientation.

5. Fracture in inelastic materials

We will apply now a theory developed for the description of fracture, namely void and crack nucleation and growth. We will define *fracture as a thermomechanical process of change in some region of tensile and shear elastic moduli, heat capacity, thermal expansion coefficient and yield strength from initial values to zero, which is accompanied by change in entropy, hardening rules and so on.* This process cannot be stopped at a material point in the intermediate state. After fracture, tensile stresses in the fracture region are zero.

Compression moduli cannot be decreased and tend to zero due to the peculiarity of interatomic interaction. That is why with multiaxial loading anisotropic elasticity has to be used in the general case.

Conventionally we can consider the material at each point as a mixture of vacuum with zero properties and volume fraction ξ and unfractured material. Then the fracture is a process of growth of ξ from 0 to 1. The actual fracture region and in particularly its dimension can be found from extremum principle (4). For elastic materials, at quasi-static isothermal process without dissipation due to fracture ($K = 0$), with neglected change in thermal expansion and heat capacity the fracture criterion (2) and extremum principle (4) are equivalent to those obtained using the principle of the minimum of Gibbs energy (Levitas, 1998a). Consequently in this case our approach has to give the same results as classical energetic methods in fracture mechanics (Cherepanov, 1967, 1979; Rice and Drucker, 1967; Rice, 1968a,b). At finite K^0 we take into account the athermal dissipation due to fracture even in elastic materials and this can be of principal importance. In PT theory the introduction of finite K^0 allows us to describe hysteresis and stable two-phase equilibrium under prescribed stresses (Levitas, 1998a).

Formally, at $K^0 = 0$ fracture has to be thermodynamically reversible.

For inelastic materials all energetic crack propagation criteria have the following form: some driving force has to reach its critical value. As a driving force an energy flow in an infinitesimal or finite-sized process zone (Rice, 1968a,b; Cherepanov, 1979; Hutchinson, 1983; Atluri, 1997), plastic work (Kuang and Chen, 1997), total dissipation rate (Kolednik et al., 1997; Turner and Kolednik, 1997) and so on are assumed. In most papers it is recognized that these driving forces include not only the energy necessary for a fracture process, but for plastic straining as well and it was not clear how to separate these processes. Cherepanov (1979, 1997) continues to use the same fracture criterion and kinetic relations in terms of Γ-integral for arbitrary inelastic materials neglecting the necessity of separation of plastic dissipation. Consequently, the strict thermodynamic fracture criterion was lacking.

The approach suggested in the given paper strictly separates the dissipation rate due to fracture only and expresses it as a product of dissipative force $\bar{X}$ and rate $\dot{\chi}$. Then the standard procedure in irreversible thermodynamics of connecting rate and force leads to time-independent or time-dependent fracture kinetics.

It is important that the approach developed is valid for an arbitrary dissipative material, because the material's constitutive equations are not used in the derivation. We will consider now an analytical solution of two simple problems which illustrate the method. Some preliminary results are reported in Levitas (1998b).

5.1. Void nucleation

Let us consider a spherically symmetrical problem on void nucleation in an infinite elastic — perfectly-plastic sphere under a homogeneously distributed tensile stress p. We will model this process by decreasing in a bulk modulus in a small sphere with a radius r from an initial value to zero accompanied by jump $\Delta\psi^\theta$ under isothermal conditions. The stress state for this problem can be found for example in paper by Roitburd and Temkin (1986).

Let us express integral $\int_{\mathbf{E}_1}^{\mathbf{E}_2} \boldsymbol{\varepsilon}_e : \mathrm{d}\mathbf{E} : \boldsymbol{\varepsilon}_e$ in the driving force X in terms of stresses. By definition $\boldsymbol{\varepsilon}_e = \mathbf{E}^{-1} : \boldsymbol{\sigma} = \mathbf{S} : \boldsymbol{\sigma}$, where $\mathbf{S} = \mathbf{E}^{-1}$ is the elastic compliance. From identity $\mathrm{d}(\mathbf{E} : \mathbf{S}) = \boldsymbol{0} = \mathrm{d}\mathbf{E} : \mathbf{S} + \mathbf{E} : \mathrm{d}\mathbf{S}$ we obtain $\mathrm{d}\mathbf{S} = -\mathbf{S} : \mathrm{d}\mathbf{E} : \mathbf{S}$ and

$$\int_{\mathbf{E}_1}^{\mathbf{E}_2} \boldsymbol{\varepsilon}_e : \mathrm{d}\mathbf{E} : \mathrm{d}\boldsymbol{\varepsilon}_e = \int_{\mathbf{E}_1}^{\mathbf{E}_2} \boldsymbol{\sigma} : \mathbf{S} : \mathrm{d}\mathbf{E} : \mathbf{S} : \boldsymbol{\sigma} = -\int_{\mathbf{S}_1}^{\mathbf{S}_2} \boldsymbol{\sigma} : \mathrm{d}\mathbf{S} : \boldsymbol{\sigma}. \tag{65}$$

We will assume traction continuity at the void surface, i.e. neglect the surface energy in the stress calculation. The surface tension $\frac{2\Gamma}{r}$ can be easily taken into account, but this complicates the formulae. For an elastic material we have

$$\tilde{p} = p\frac{S_1 + q}{S + q}, \tag{66}$$

where $\tilde{p}$ is the mean tensile stress inside the transforming zone (void), $S_1 = \frac{1}{3K_1}$ and $S = \frac{1}{3K}$ are the elastic bulk compliance before and during the transformation, K_1 and K are the corresponding bulk moduli, $q = \frac{1}{4\mu_1}$, μ_1 is the shear modulus before transformation. For a void after transformation $K_2 = 0$, $S_2 \to \infty$. After integration we obtain

$$\int_{\mathbf{S}_1}^{\infty} \boldsymbol{\sigma} : \mathrm{d}\mathbf{S} : \boldsymbol{\sigma} = \int_{S_1}^{\infty} \tilde{p}^2 \mathrm{d}S = p^2(S_1 + q)^2 \int_{S_1}^{\infty} \frac{\mathrm{d}S}{(S + q)^2} = p^2(S_1 + q). \tag{67}$$

As

$$S_1 + q = \frac{1}{3K_1} + \frac{1}{4\mu_1} = \frac{3}{2}\frac{(1 - \nu_o)}{E}, \tag{68}$$

where E, and ν_o are Young's modulus and the Poisson ratio of the parent material, the local driving force for an elastic material is

$$\rho X_e = 0.5p^2\left(\frac{1}{3K_1} + \frac{1}{4\mu_1}\right) - \rho\Delta\psi^\theta = p^2\frac{3}{4}\frac{(1 - \nu_o)}{E} - \rho\Delta\psi^\theta. \tag{69}$$

Let us consider a void nucleation in an elastoplastic material. During the change in compliance S in the transforming region the material deforms at the beginning in the elastic regime. Plastic flow near the transforming region starts at

$$\tilde{p}_p = p\frac{S_1 + q}{S_p + q} = p - \frac{2}{3}\sigma_y, \tag{70}$$

where σ_y is the yield stress of the parent phase, i.e. when elastic compliance S reaches the value S_p determined by equation

$$\frac{1}{S_{\mathrm{p}}+q}=\frac{p-\frac{2}{3}\sigma_{\mathrm{y}}}{p(S_1+q)}. \tag{71}$$

In the elastoplastic regime (Roitburd and Temkin, 1986)

$$\tilde{p}(S-S_1)=\frac{2}{3}\sigma_{\mathrm{y}}(S_1+q)\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right). \tag{72}$$

After differentiation of Eq. (72)

$$\begin{aligned}\mathrm{d}S&=\mathrm{d}\left[\frac{1}{\tilde{p}}\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\right]\frac{2}{3}\sigma_{\mathrm{y}}(S_1+q)\\&=\frac{2}{3}\sigma_{\mathrm{y}}(S_1+q)\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\left(\frac{1}{\tilde{p}^2}+\frac{1}{\tilde{p}2/3\sigma_{\mathrm{y}}}\right)\mathrm{d}\tilde{p}\end{aligned} \tag{73}$$

we calculate in the plastic regime

$$\begin{aligned}\int_{S_{\mathrm{p}}}^{\infty}\tilde{p}^2\mathrm{d}S=&-\frac{2}{3}\sigma_{\mathrm{y}}(S_1+q)\int_{\tilde{p}_{\mathrm{p}}}^{0}\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\mathrm{d}\tilde{p}\\&-(S_1+q)\int_{\tilde{p}_{\mathrm{p}}}^{0}\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\tilde{p}\mathrm{d}\tilde{p}.\end{aligned} \tag{74}$$

As

$$\begin{aligned}&\int_{\tilde{p}_{\mathrm{p}}}^{0}\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\tilde{p}\mathrm{d}\tilde{p}=-\frac{2}{3}\sigma_{\mathrm{y}}\int_{\tilde{p}_{\mathrm{p}}}^{0}\tilde{p}\mathrm{d}\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\\&=-\frac{2}{3}\sigma_{\mathrm{y}}\tilde{p}\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\Bigg|_{\tilde{p}_{\mathrm{p}}}^{0}+\frac{2}{3}\sigma_{\mathrm{y}}\int_{\tilde{p}_{\mathrm{p}}}^{0}\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\mathrm{d}\tilde{p},\end{aligned} \tag{75}$$

then

$$\begin{aligned}\int_{S_{\mathrm{p}}}^{\infty}\tilde{p}^2\mathrm{d}S=&\frac{2}{3}\sigma_{\mathrm{y}}(S_1+q)\tilde{p}\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\Bigg|_{\tilde{p}_{\mathrm{p}}}^{0}+\frac{8}{9}\sigma_{\mathrm{y}}^2(S_1+q)\exp\left(\frac{p-\tilde{p}}{2/3\sigma_{\mathrm{y}}}-1\right)\Bigg|_{\tilde{p}_{\mathrm{p}}}^{0}\\&=-\frac{2}{3}\sigma_{\mathrm{y}}(S_1+q)p-\frac{4}{9}\sigma_{\mathrm{y}}^2(S_1+q)+\frac{8}{9}\sigma_{\mathrm{y}}^2(S_1+q)\exp\left(\frac{p}{2/3\sigma_{\mathrm{y}}}-1\right).\end{aligned} \tag{76}$$

With an elastoplastic deformation

$$\int_{S_1}^{\infty}\tilde{p}^2\mathrm{dS}=\int_{\mathrm{S}_1}^{\mathrm{S}_{\mathrm{p}}}\tilde{p}^2\mathrm{dS}+\int_{S_{\mathrm{p}}}^{\infty}\tilde{p}^2\mathrm{dS}. \tag{77}$$

The first integral can be easily calculated with the use of Eq. (66) for the stress in the elastic regime and Eq. (71) for S_p, i.e.

$$\int_{S_1}^{S_p} \tilde{p}^2 \mathrm{d}S = -p^2(S_1+q)^2\left(\frac{1}{S+q}\right)\Bigg|_{S_1}^{S_p} = \frac{2}{3}p(S_1+q)\sigma_y. \tag{78}$$

Using Eq. (76) and (78) we obtain

$$\begin{aligned}\int_{S_1}^{\infty} \tilde{p}^2 \mathrm{d}S_2 &= \frac{8}{9}\sigma_y^2(S_1+q)\exp\left(\frac{p}{2/3\sigma_y}-1\right) - \frac{4}{9}\sigma_y^2(S_1+q) \\ &= \left(\frac{2}{3}\sigma_y^2\right)^2(S_1+q)[2\exp\left(\frac{p}{2/3\sigma_y}-1\right)-1].\end{aligned} \tag{79}$$

Consequently, for elastoplastic material we have

$$\begin{aligned}\rho X_p &= 0.5\int_{\mathbf{S}}^{\infty} \boldsymbol{\sigma} : \mathrm{d}\mathbf{S} : \boldsymbol{\sigma} - \rho\Delta\psi^{\theta} \\ &= \frac{3(1-\nu_o)}{4E}\left(\frac{2}{3}\sigma_y\right)^2\left[2\exp\left(\frac{3p}{2\sigma_y}-1\right)-1\right] - \rho\Delta\psi^{\theta}.\end{aligned} \tag{80}$$

At $p=\frac{2}{3}\sigma_y$, Eq. (80) coincides with Eq. (69) for void nucleation in an elastic material. As X is independent of radius r we can use the same conclusions as with a PT in a spherical nucleus in Section 2. That is, the extremum principle (4) results in condition $r \rightarrow \min$, the minimum value of r is determined by the thermodynamic criterion of SC (34), and the transformation time can be described by Eq. (35). Thermodynamically, fracture is possible at $X \geqslant K^0$, which determines the minimum tensile stress for void nucleation. However, only at relatively large $X-K^0$ and small r_t can void nucleation be observed during a reasonable time. As a kinetic criterion for void nucleation we can assume $t_s = t_{ob}$, where t_{ob} is the accepted observation time, i.e. the same as at PT. The thermodynamic condition for void nucleation in an elastic sphere has been studied by Cherepanov (1997). The result is obtained that the stress necessary for void nucleation monotonously decreases with the increasing void radius, i.e. nucleation of an infinite void is the most thermodynamically favorable event. Our kinetic approach determines the explicit value of the void radius and nucleation time as a function of applied pressure.

Formally the same results can be obtained for compressive pressure, which does not correspond to reality. That is why it was important to exclude decrease in compression moduli in the definition of fracture.

5.2. Crack propagation

As the next example we derive the equation for crack propagation in an elastic perfectly plastic material in a similar framework to the Dugdale (1960) model for the plane stress case (i.e. in a thin sheet). The localized plastic region OAB (Fig. 3) in front of the crack is under the action of cohesive (restraining) stresses $\sigma = \sigma_y$ on the extended crack surfaces OA and OB, the separation distance δ between these surfaces is determined by known formulae (e.g. Rice, 1968a). We will use the following interpretation: with a crack propagation by a distance Δl fracture occurs in the finite region AKLB; during this process the surface PAK (and RBL) shifts due to deformation to position PA′ (and RB′). Eq. (1) for an isothermal process at neglected $\boldsymbol{\varepsilon}_t$ and $\boldsymbol{\varepsilon}_\theta$ and the validity of Eq. (14) appears as follows

$$\rho X = \int_{\boldsymbol{\varepsilon}_{e1}}^{\boldsymbol{\varepsilon}_{e2}} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}_e + 0.5\boldsymbol{\varepsilon}_{e1} : \mathbf{E}_1 : \boldsymbol{\varepsilon}_{e1} - \rho\Delta\psi^\theta. \tag{81}$$

Here we took into account the fact that $\mathbf{E}_2 = \mathbf{0}$. Let us make additional simplifying assumptions. We will take into account the stress and elastic strain ε_e normal to the crack plane only; the work of other components is neglected. If the width of the fracture zone AA′ is small (this is really the case, as will be seen from the solution), due to zero stresses at the surface AB and the plane stress condition this is a reasonable hypothesis. Additionally we assume that during the fracture process

$$E(\xi) = E(1-\xi) \quad \text{and} \quad \sigma_y(\xi) - \sigma_y(1-\xi), \quad \text{i.e.} \quad \varepsilon_e = \frac{\sigma_y(\xi)}{E(\xi)} = \frac{\sigma_y}{E_1} = \text{const.} \tag{82}$$

Due to these assumptions the work integral in Eq. (81) disappears, elastic energy

$$0.5\boldsymbol{\varepsilon}_{e1} : \mathbf{E}_1 : \boldsymbol{\varepsilon}_{e1} = 0.5\frac{\sigma_y^2}{E_1} \tag{83}$$

is constant and the transforming volume before transformation $V_1 = b\Delta l\bar{\delta}$, where $\bar{\delta}$ is some intermediate value of the crack opening at the length Δl and b is the thickness of the thin sheet. As the local dissipation increment due to fracture $\rho X = 0.5\frac{\sigma_y^2}{E_1} - \rho\Delta\psi^\theta$ is homogeneously distributed in the fracture region and is independent of the geometry of this region, we arrive at the situation considered in Sections

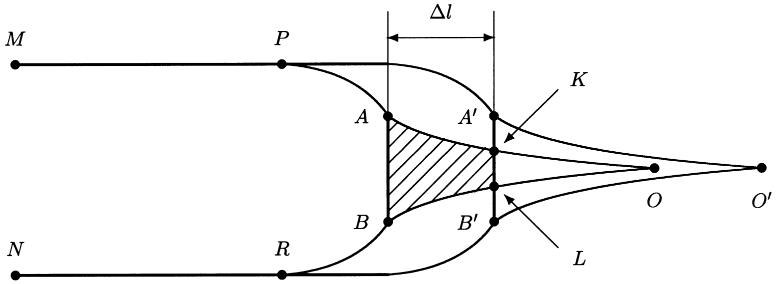

Fig. 3. The crack position MABN before and MA′B′N after crack advance by distance Δl; AOB and A′O′B′ are the localized plastic regions before and after crack advance; AKLB is the fracture zone.

2 and 4.1. The thermodynamic criterion of the beginning of fracture and the principle of the minimum of transforming mass (volume) results in

$$\left(0.5\frac{\sigma_{\mathrm{y}}^2}{E_1}-\rho\Delta\psi^{\theta}-\rho K^0\right)b\Delta l\bar{\delta}-2\Gamma\Delta lb=0;\quad \Delta l\bar{\delta}\ \rightarrow\ \min. \tag{84}$$

The minimum value of $\bar{\delta}$ can be found from the thermodynamic fracture criterion (84). Condition $\Delta l\ \rightarrow$ min results in $\Delta l=a$, where a is the interatomic distance in the direction of crack propagation. Then $\bar{\delta}=\delta$, where δ is the crack opening displacement between points A and B and the thermodynamic fracture criterion (84) reduces to the criterion of critical crack opening

$$\delta=\delta_{\mathrm{c}}:=\frac{2\Gamma}{0.5\frac{\sigma_{\mathrm{y}}^2}{E_1}-\rho\Delta\psi^{\theta}-\rho K^0}. \tag{85}$$

However, in contrast to known approaches the critical crack opening is determined in terms of known material parameters. It follows from the Dugdale model that $\delta=\frac{J}{\sigma_{\mathrm{y}}}$ (Rice, 1968a), where J is the path independent J-integral calculated over the path not passing through plastic region. Then criterion (85) can be represented as criterion of critical value of J-integral

$$J=J_{\mathrm{c}}:=\sigma_{\mathrm{y}}\delta_{\mathrm{c}}=\sigma_{\mathrm{y}}\frac{2\Gamma}{0.5\frac{\sigma_{\mathrm{y}}^2}{E_1}-\rho\Delta\psi^{\theta}-\rho K^0}. \tag{86}$$

With a growth of J which characterizes the growth in external loading at the given geometry of the system, the crack opening δ increases and when both J and δ reach corresponding threshold values, crack propagation will occur. Additional growth of δ contradicts the principle of the minimum of transforming volume; consequently during the crack propagation condition (85) is always fulfilled. Then the kinetic equation of crack growth (5) results in

$$\dot{l}=\frac{a}{t_{\mathrm{s}}}=\frac{a}{t_0}\exp\left(-\frac{\rho E_{\mathrm{a}}}{R\theta_{\mathrm{ef}}}\frac{N}{n}ba\delta_{\mathrm{c}}\right). \tag{87}$$

Eq. (87) at $\theta_{\mathrm{ef}}=\theta$ and designations $\dot{l}_{\mathrm{o}}=\frac{a}{t_{\mathrm{s}}}$, and $\bar{E}_{\mathrm{a}}=\rho E_{\mathrm{a}}\frac{N}{n}ba\delta_{\mathrm{c}}$ can be presented as the usual Arrhenius equation

$$\dot{l}=\dot{l}_{\mathrm{o}}\exp\left(-\frac{\bar{E}_{\mathrm{a}}}{R\theta}\right). \tag{88}$$

Such an equation corresponds to Zhurkov's kinetic concept of strength and experimental regularities (Zhurkov, 1965; Cherepanov, 1997). Note that in our solution the crack propagates almost continuously (atom by atom fracture), in contrast to the necessity of discrete finite crack advance in the model by Kfouri and Rice (1977). The characteristic size in our model is related to the thickness of the fractured zone δ.

Note that the numerical study of ductile fracture in a sample with edge notch is presented in a paper by Idesman et al. (2000). It is based on the same theory as here. The following typical cases in the determination of two characteristic sizes of fracture region are found: from the extremum principle and kinetic equation solely without any constraints; from the thermodynamic criterion; as an interatomic distance; as the size of a sample. In some cases crack advance is finite; however, in contrast to the model by Kfouri and Rice (1977), this advance is not a material parameter, but is determined from the extremum principle or the thermodynamic fracture criterion.

One of the remaining problems is the mass balance for fractured material. In the energetic methods of fracture mechanics the fractured material is simply removed. Physically, fracture means that atoms are separated by the distance when their interaction is negligible. For such a formulation, the volume of the fracture region has to be increased during the fracture process to some prescribed value and this condition can be considered as a kinematic constraint. In another case, for modes II and III crack surfaces can be in contact.

Another problem is related to definition of fracture: which components of elasticity tensor **E** tend to zero and in which sequences? The driving force may depend in some extend on the answer on this question.

6. Generalized second–order phase transitions

According to the classical definition (Landau and Lifshitz, 1976a), for first-order phase transformations (FOPT) in liquids or gases the thermodynamic Gibbs potential $G(p, \theta)$ is continuous along the phase equilibrium line $\theta_e(p_e)$ in the temperature θ– pressure p plane, but its first and higher derivatives have jumps. For second-order phase transformations (SOPT), the thermodynamic potential and its first derivatives are continuous along the phase equilibrium line $\theta_e(p_e)$, but its second derivatives have jumps. Temperature and pressure are equal for both phases and are considered as independent parameters. It is clear that the SOPT can be treated as a particular case of the FOPT. In particular, the well-known Clausius–Clapeyron relation derived for the FOPT can be transformed into Ehrenfest equation for the SOPT.

Generalization of the definition of SOPT and Ehrenfest equation for nonlinear elastic solids is given in paper by Grinfeld (1979). According to Grinfeld, the SOPT surface is determined in a space of strain tensor $\boldsymbol{\varepsilon}$ and temperature at which the Helmholtz free energy $\psi(\boldsymbol{\varepsilon}, \theta) = G + \boldsymbol{\sigma} : \boldsymbol{\varepsilon}$ and its first derivatives (stress tensor $\boldsymbol{\sigma}$ and entropy s) are continuous, but the second derivatives have jumps. For such SOPT, formulation in terms of Helmholtz and Gibbs free energy is equivalent due to the continuity of $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$. The main problem is related to the fact that with such a definition the SOPT cannot be considered as a particular case of the FOPT, according to their modern definitions [see Part I of this paper (Levitas, 2000) and references]. For FOPT in elastic materials, the PT condition is determined not for each material point in $\boldsymbol{\sigma}-\theta$ or $\boldsymbol{\varepsilon}-\theta$ space, but for points of the interface between two phases (Grinfeld, 1991, and references). Only three components of the stress tensor are continuous across the interface and, as the strain tensor has jump across the interface as well, it is impossible to formulate a PT condition for each material point in $\boldsymbol{\sigma}-\theta$ or $\boldsymbol{\varepsilon}-\theta$ space without solving a boundary-value problem. In the adiabatic case the temperature is also discontinuous. For PT in elastic materials with hysteresis due to interface friction, the Gibbs potential has a jump across an interface as well (Fischer et al., 1994; Levitas, 1998a,b).

For elastoplastic materials the situation is much more complicated, because a thermomechanical process in some volume has to be considered and not only the jump, but the path-dependent variation of all the parameters determines the PT conditions (Levitas 1998a).

Consequently, the definition of SOPT given by Grinfeld selects a very narrow class of phenomena in comparison with those for the FOPT. In particular, jumps of tensors of elastic moduli and thermal expansion have to be specially coordinated in order to avoid jumps in stress and strain tensors.

The aim of this Section is to define and study SOPT in inelastic solids, which are considered as a *particular case of the FOPT* treated above. We will call them generalized SOPT. The necessity of such a study is evident: some PT (e.g. ferroelectric and ferromagnetic) are considered as SOPT, but *more precisely as FOPT with a small transformation strain and jump in entropy* (Landau and Lifshitz, 1976a,b). Results of application of modern theories of FOPT and SOPT will significantly differ. Some preliminary results are reported in a short communication (Levitas, 1998b).

In order to define SOPT, we have to find the counterparts of the condition of continuity of volume (strain) and entropy. As one of these conditions we can adopt the absence of transformation strain $\boldsymbol{\varepsilon}_t=\mathbf{0}$. In order to formulate the second condition, let us introduce for FOPT the transformation entropy s_t in the following way. We define the equilibrium temperature of phases θ_e at $\boldsymbol{\varepsilon}_{ei}=\boldsymbol{\varepsilon}_{pi}=\mathbf{g}_i=\mathbf{0}$, $i=1,2$, (consequently $\boldsymbol{\sigma}_i=\mathbf{0}$) form condition $\psi_1(\mathbf{0},\theta_e,\mathbf{0},\mathbf{0})=\psi_2(\mathbf{0},\theta_e,\mathbf{0},\mathbf{0})$. Then we introduce by definition transformation entropy at $\boldsymbol{\varepsilon}_{ei}=\boldsymbol{\varepsilon}_{pi}=\mathbf{g}_i=\mathbf{0}$, $i=1,2$, as $s_t:=s_2(\mathbf{0},\theta_e,\mathbf{0},\mathbf{0})-s_1(\mathbf{0},\theta_e,\mathbf{0},\mathbf{0})$. By definition, for generalized SOPT we assume $s_t=0$.

Definition. *Generalized SOPT is a thermomechanical process of change in the thermomechanical properties of materials (elastic moduli* $\boldsymbol{E}$*, heat capacity* ν*, thermal expansion coefficient* $\boldsymbol{\alpha}$*, yield condition, hardening rules and so on) from initial to final values in some region at zero transformation strain* $\varepsilon_t=\mathbf{0}$ *and transformation entropy* $s_t=0$*. This process cannot be stopped at material point in the intermediate state.*

Of course, other more restrictive definitions are possible. We will use the above definition, because it allows us to consider a very wide class of PT and to apply the theory developed for FOPT. It is possible to define the order parameter in the following form

$$\xi := \frac{1}{3}\left(\frac{|\mathbf{E}-\mathbf{E}_1|}{|\mathbf{E}_2-\mathbf{E}_1|}+\frac{\nu-\nu_1}{\nu_2-\nu_1}+\frac{|\boldsymbol{\varepsilon}_\theta-\boldsymbol{\varepsilon}_{\theta 1}|}{|\boldsymbol{\varepsilon}_{\theta 2}-\boldsymbol{\varepsilon}_{\theta 1}|}\right), \tag{89}$$

a lot of other definitions are acceptable. It is clear that PT starts at $\xi = 0$ and finishes at $\xi = 1$; when ξ varies between 0 and 1, the parameters $\mathbf{E}$, ν and $\boldsymbol{\varepsilon}_\theta$ vary from $\mathbf{E}_i$, ν_1, $\boldsymbol{\varepsilon}_{\theta 1}$ and $\mathbf{E}_2$, ν_2, $\boldsymbol{\varepsilon}_{\theta 2}$. It is more convenient to accept for example

$$\xi := \frac{|\mathbf{E}-\mathbf{E}_1|}{|\mathbf{E}_2-\mathbf{E}_1|} \tag{90}$$

(or in terms of Young's modulus or the shear modulus) and to express all other properties $\mathbf{A}$ in terms of ξ in a such way that $\mathbf{A}(0) = \mathbf{A}_1$ and $\mathbf{A}(1) = \mathbf{A}_2$.

Equations for X_ξ, X and temperature evolution for generalized SOPT can be obtained from Eqs. (21)–(23) at $\theta_o = \theta_e$, zero transformation strain $\boldsymbol{\varepsilon}_t = \mathbf{0}$, change in the reference free energy $\Delta\psi_o = 0$ and the transformation entropy $s_t = s_{02} - s_{01} = 0$:

$$\rho X_\xi = \boldsymbol{\sigma} : \Delta\boldsymbol{\alpha}(\theta-\theta_o) - 0.5\boldsymbol{\varepsilon}_e : \Delta\mathbf{E} : \boldsymbol{\varepsilon}_e - \rho\Delta\nu(\theta-\theta_o) + \rho\Delta\nu\theta\ln\theta/\theta_o, \tag{91}$$

$$\nu(\xi)\dot{\theta} = \left(-\frac{1}{\rho}\boldsymbol{\sigma} : \Delta\boldsymbol{\alpha}\theta_o - \frac{1}{2\rho}\boldsymbol{\varepsilon}_e : \Delta\mathbf{E} : \boldsymbol{\varepsilon}_e - \Delta\nu(\theta-\theta_o)\right)\dot{\xi} - \dot{\boldsymbol{\sigma}} : \boldsymbol{\alpha}(\xi)\theta + \rho\mathbf{X}_p : \dot{\boldsymbol{\varepsilon}}_p + \rho\mathbf{X}_g : \dot{\mathbf{g}}, \tag{92}$$

$$\rho X = \int_0^1 \boldsymbol{\sigma} : \Delta\boldsymbol{\alpha}(\theta-\theta_o)d\xi - 0.5\int_0^1 \boldsymbol{\varepsilon}_e : \Delta\mathbf{E} : \boldsymbol{\varepsilon}_e d\xi - \rho\Delta\nu\int_0^1\left(\theta-\theta_o-\theta\ln\frac{\theta}{\theta_o}\right)d\xi. \tag{93}$$

The main aim in singling out the generalized SOPT is to attract the attention of researchers who work in the field of SOPT (or FOPT which are close to SOPT) in solids, but use simplified methods for liquids, to the modern theory of FOPT in inelastic solids. Additional degrees of freedom related to the effect of plastic deformation and complex multiaxial loading make it possible to find new or to intensify known SOPT, e.g. transitions in superconducting states, as is done for the FOPT. Methods of control of FOPT (Levitas, 1997a,b) will probably be useful for the generalized SOPT.

As is clear from Section 5, fracture is an intermediate case between FOPT and generalized SOPT, because $\boldsymbol{\varepsilon}_t = \mathbf{0}$ but $s_t \neq 0$. We will not limit the change in transformation entropy for fracture, because we do not know whether it corresponds to reality. Perhaps it is reasonable to exclude limitations on transformation entropy in the general case as well, because we do not know whether it corresponds to reality for any transformation.

It can be found in the physical literature on classical SOPT that they do not require nucleation and can occur under uniform fields in the whole volume homogeneously. In the framework of our theory for such SOPT an activation energy

$E_a = 0$. This condition can be used as a definition of some subclass of generalized SOPT. It is clear that this is not the case for fracture.

7. Diffusional–displacive phase transformation

7.1. General relations

Martensitic transformations are usually considered as diffusionless, i.e. solute atoms are frozen into the crystal lattice and do not redistribute during the transformation. If the temperature is high enough to allow diffusion during the PT time, redistribution of solute atoms can change the driving force, accelerate or suppress transformation of the crystal lattice or make it possible at all. Bainitic transformation and transformation from austenite to ferrite in steel belong to such diffusional–displacive PT. We do not know any continuum mechanical treatment of diffusional–displacive PT. In the physical literature (Lyubov, 1968; Umanskiy and Skakov, 1978; Olson et al., 1989, 1990) such transformations are studied as an interface propagation problem without consideration of stress and strain fields and continuum thermodynamics. It is interesting to mention that when for the determination of three unknowns two equations were available only, the maximum interface rate assumption was adopted (Olson et al., 1989). In the next paper (Olson et al., 1990), the third equation for solute trapping was used, so this principle was not necessary.

In this section we will extend and apply our continuum approach for the description of diffusional–displacive PT. We will consider the simplest case of diffusion of one solute component with the mass fraction c in a solvent material. In this case the energy balance equation (3) or (5) in Part I (Levitas, 2000) remains the same

$$\int_{V_n}\left(\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}-\rho\dot{U}-\mathrm{div}\mathbf{h}+\rho r\right)\mathrm{d}V_n-\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Sigma_n}\Gamma\,\mathrm{d}\Sigma_n=0, \tag{94}$$

but in the entropy production [Eq.(4) in Part I] we have to include additional flux $\mathbf{j}$

$$S_i:=\frac{\mathrm{d}}{\mathrm{d}t}\int_{V_n}\rho s\,\mathrm{d}V_n-\int_{V_n}\rho\frac{r}{\theta}\mathrm{d}V_n+\int_{\Sigma_n}\frac{\mathbf{h}}{\theta}\cdot\mathbf{n}\,\mathrm{d}\Sigma_n-\int_{\Sigma_n}\frac{\mu\mathbf{j}}{\theta}\cdot\mathbf{n}\,\mathrm{d}\Sigma_n\geqslant 0. \tag{95}$$

Here U is the specific internal energy, μ is the chemical potential of the solute component and $\mathbf{j}$ is the flux of solute atoms which satisfies the balance equation

$$\rho\dot{c}+\mathrm{div}\mathbf{j}=0. \tag{96}$$

Then instead of Eq.(7) in (Levitas, 2000) for the local entropy production we obtain from Eq.(95)

$$\tilde{S}_i:=\rho\dot{s}-\rho\frac{r}{\theta}+\frac{1}{\theta}\mathrm{div}\mathbf{h}-\frac{\boldsymbol{\nabla}\theta}{\theta^2}\cdot\mathbf{h}-\mathrm{div}\left(\frac{\mu\mathbf{j}}{\theta}\right)\geqslant 0. \tag{97}$$

Using the balance Eq. (96) we transform

$$\mathrm{div}\left(\frac{\mu \mathbf{j}}{\theta}\right)=\frac{\mu}{\theta}\mathrm{div}\mathbf{j}+\mathbf{j}\cdot\nabla\left(\frac{\mu}{\theta}\right)=-\frac{\rho\mu}{\theta}\dot{c}+\mathbf{j}\cdot\nabla\left(\frac{\mu}{\theta}\right). \tag{98}$$

Excluding the expression div**h** – ρr from Eq. (97) and substituting it in Eq. (94) we receive after evident transformations an inequality

$$\bar{\mathcal{D}}:=\int_{V_\mathrm{n}}\rho\theta\tilde{S}_i \mathrm{d}V_\mathrm{n}=\int_{V_\mathrm{n}}\rho\mathcal{D}\mathrm{d}V_\mathrm{n}-\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Sigma_\mathrm{n}}\Gamma \mathrm{d}\Sigma_\mathrm{n}\geqslant 0, \tag{99}$$

with

$$\begin{aligned}\rho\mathcal{D}&:=\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}-\rho\dot{U}+\rho\theta\dot{s}-\frac{\nabla\theta}{\theta}\cdot\mathbf{h}+\rho\mu\dot{c}-\theta\mathbf{j}\cdot\nabla\left(\frac{\mu}{\theta}\right)\\&=\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}-\rho\dot{\psi}-\rho s\dot{\theta}-\frac{\nabla\theta}{\theta}\cdot\mathbf{h}+\rho\mu\dot{c}-\theta\mathbf{j}\cdot\nabla\left(\frac{\mu}{\theta}\right)\end{aligned} \tag{100}$$

for the local rate of dissipation per unit volume and $\bar{\mathcal{D}}$ for the total dissipation rate. In an additive decomposition of a total strain tensor

$$\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}_\mathrm{e}+\boldsymbol{\varepsilon}_\mathrm{p}+\boldsymbol{\varepsilon}_\theta+\boldsymbol{\varepsilon}_\mathrm{t}+\boldsymbol{\varepsilon}_\mathrm{c} \tag{101}$$

we take into account the misfit strain $\boldsymbol{\varepsilon}_\mathrm{c}$ which is proportional to the change in the solute fraction during the diffusion, i.e. $\boldsymbol{\varepsilon}_\mathrm{c}=\mathbf{b}(\xi)(c-c_1)$, $\mathbf{b}(0)=\mathbf{b}_1$, $\mathbf{b}(1)=\mathbf{b}_2$. Substituting $\psi=\psi(\boldsymbol{\varepsilon}_\mathrm{e},\theta,\boldsymbol{\varepsilon}_\mathrm{p},\mathbf{g},\boldsymbol{\varepsilon}_\mathrm{t},c,\xi)$ and decomposition (101) in Eq. (100) and using the same procedure as to derive Eqs.(20) and (22) for the dissipation rate in Part I, we obtain

$$\begin{aligned}\mathcal{D}=\mathbf{X}_\mathrm{p}:\dot{\boldsymbol{\varepsilon}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\dot{\mathbf{g}}+\mathbf{X}_\mathrm{h}\cdot\mathbf{h}+X_\xi\dot{\xi}+\left(\mu+\frac{\boldsymbol{\sigma}}{\rho}:\frac{\partial(\boldsymbol{\varepsilon}_\mathrm{c}+\boldsymbol{\varepsilon}_\mathrm{t}+\boldsymbol{\varepsilon}_\theta)}{\partial c}-\frac{\partial\psi}{\partial_c}\right)\dot{c}\\-\frac{\theta}{\rho}\mathbf{j}\cdot\nabla\left(\frac{\mu}{\theta}\right)\end{aligned} \tag{102}$$

with the designations given in Eq. (8) and

$$X_\xi=\frac{1}{\rho}\boldsymbol{\sigma}:\frac{\partial(\boldsymbol{\varepsilon}_t+\boldsymbol{\varepsilon}_\theta+\boldsymbol{\varepsilon}_c)}{\partial\xi}-\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_t}:\frac{\partial\boldsymbol{\varepsilon}_t}{\partial\xi}-\frac{\partial\psi}{\partial\xi}. \tag{103}$$

It is usually assumed that when $\dot{c}$ does not change due to chemical reaction, the rate of dissipation is independent of $\dot{c}$ (similar to when it is independent of $\dot{\theta}$). This condition defines the chemical potential

$$\mu=-\frac{\boldsymbol{\sigma}}{\rho}:\frac{\partial(\boldsymbol{\varepsilon}_\mathrm{c}+\boldsymbol{\varepsilon}_\mathrm{t}+\boldsymbol{\varepsilon}_\theta)}{\partial c}+\frac{\partial\psi}{\partial c} \tag{104}$$

in a form similar to the entropy in Eq. (10). The kinetic equation $\mathbf{j}=\mathbf{f}_\mathrm{j}\left(\theta\boldsymbol{\nabla}\left(\frac{\mu}{\theta}\right)\right)$ between the additional dissipative rate $\mathbf{j}$ and force $\theta\boldsymbol{\nabla}\left(\frac{\mu}{\theta}\right)$ represents the generalized Fick's law and its substitution in balance Eq. (96) results in the diffusion equation

$$\rho\dot{c}=-\mathrm{div}\left(\mathbf{f}_j\left(\theta\boldsymbol{\nabla}\left(\frac{\mu}{\theta}\right)\right)\right). \tag{105}$$

For the driving force for PT $\bar{X}:=\dfrac{1}{m_\mathrm{n}}\left(\displaystyle\int_{V_\mathrm{n}}\int_0^1\rho X_\xi \mathrm{d}\xi\mathrm{d}V_\mathrm{n}-\Delta\bar{\Gamma}\right)$ we obtain

$$\bar{X}m_\mathrm{n}=\int_{V_\mathrm{n}}\int_{\boldsymbol{\varepsilon}_{\mathrm{t}1}}^{\boldsymbol{\varepsilon}_{\mathrm{t}2}}\rho\left(\frac{\boldsymbol{\sigma}}{\rho}-\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_\mathrm{t}}\right):\mathrm{d}\boldsymbol{\varepsilon}_\mathrm{t}\mathrm{d}V_\mathrm{n}+\int_{V_\mathrm{n}}\int_0^1\rho\left(\frac{\boldsymbol{\sigma}}{\rho}:\frac{\partial(\boldsymbol{\varepsilon}_\theta+\boldsymbol{\varepsilon}_\mathrm{c})}{\partial\xi}\right)-\frac{\partial\psi}{\partial\xi}\mathrm{d}\xi\mathrm{d}V_\mathrm{n}-\Delta\bar{\Gamma}. \tag{106}$$

Let us consider the alternative expressions for $\bar{X}$. From Eqs. (100) and (102) it follows

$$\begin{aligned}X_\xi\dot{\xi}&=\mathcal{D}-\mathbf{X}_\mathrm{p}:\dot{\boldsymbol{\varepsilon}}_\mathrm{p}-\mathbf{X}_\mathrm{g}:\dot{\mathbf{g}}-\mathbf{X}_\mathrm{h}\cdot\mathbf{h}+\rho^{-1}\theta\mathbf{j}\cdot\boldsymbol{\nabla}\left(\frac{\mu}{\theta}\right)\\&=\rho^{-1}\boldsymbol{\sigma}:\dot{\boldsymbol{\varepsilon}}-\dot{\psi}-s\dot{\theta}-\mathbf{X}_\mathrm{p}:\dot{\boldsymbol{\varepsilon}}_\mathrm{p}-\mathbf{X}_\mathrm{g}:\dot{\mathbf{g}}+\mu\dot{c};\end{aligned} \tag{107}$$

$$\begin{aligned}\bar{X}=&\frac{1}{m_\mathrm{n}}\int_{V_\mathrm{n}}\left(\int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2}\boldsymbol{\sigma}:\mathrm{d}\boldsymbol{\varepsilon}-\rho\Delta\psi-\int_{\theta_1}^{\theta_2}\rho s\mathrm{d}\theta-\int_0^{t_\mathrm{s}}\rho\left(\mathbf{X}_\mathrm{p}:\dot{\boldsymbol{\varepsilon}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\dot{\mathbf{g}}+\mu\dot{c}\right)\mathrm{d}t\right)\mathrm{d}V_\mathrm{n}\\&-\frac{\Delta\bar{\Gamma}}{m_\mathrm{n}}.\end{aligned} \tag{108}$$

Taking into account the decomposition (101) and Eq. $(8)_1$ for $\mathbf{X}_\mathrm{p}$ we obtain

$$\begin{aligned}\bar{X}=&\frac{1}{m_\mathrm{n}}\int_{V_\mathrm{n}}\left(\int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2}\boldsymbol{\sigma}:\mathrm{d}(\boldsymbol{\varepsilon}_\mathrm{e}+\boldsymbol{\varepsilon}_\theta+\boldsymbol{\varepsilon}_\mathrm{t}+\boldsymbol{\varepsilon}_\mathrm{c})-\rho(\psi_2-\psi_1)-\int_{\theta_1}^{\theta_2}\rho s\mathrm{d}\theta+\int_{\mathbf{g}_1}^{\mathbf{g}_2}\rho\frac{\partial\psi}{\partial\mathbf{g}^\mathrm{t}}:\mathrm{d}\mathbf{g}\right.\\&\left.+\int_{\boldsymbol{\varepsilon}_{\mathrm{p}1}}^{\boldsymbol{\varepsilon}_{\mathrm{p}2}}\rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}_\mathrm{p}}:\mathrm{d}\boldsymbol{\varepsilon}_\mathrm{p}+\int_{c_1}^{c_2}\rho\mu\mathrm{d}c\right)\mathrm{d}V_\mathrm{n}-\frac{\Delta\bar{\Gamma}}{m_\mathrm{n}}.\end{aligned} \tag{109}$$

The same procedure as used to derive Eqs. (11)–(13) leads to

$$\rho\theta\dot{s}=\rho\mathcal{D}-\mathrm{div}\mathbf{h}+\frac{\boldsymbol{\nabla}\theta}{\theta}\cdot\mathbf{h}-\rho\mu\dot{c}; \tag{110}$$

$$\theta\dot{s}=-\rho^{-1}\mathrm{div}\mathbf{h}+\mathbf{X}_\mathrm{p}:\dot{\boldsymbol{\varepsilon}}_\mathrm{p}+\mathbf{X}_\mathrm{g}:\dot{\mathbf{g}}+X_\xi\dot{\xi}-\mu\dot{c}; \tag{111}$$

$$\begin{aligned}\nu\dot{\theta}=&-\rho^{-1}\mathrm{div}\mathbf{f}_\mathrm{h}\left(-\frac{\boldsymbol{\nabla}\theta}{\theta}\right)+\left(\mathbf{X}_\mathrm{p}-\frac{\partial s}{\partial\boldsymbol{\varepsilon}_\mathrm{p}}\theta\right):\dot{\boldsymbol{\varepsilon}}_\mathrm{p}+\left(\mathbf{X}_\mathrm{g}-\frac{\partial s}{\partial\mathbf{g}}\theta\right):\dot{\mathbf{g}}\\&+\left(X_\xi-\frac{\partial s}{\partial\xi}\theta\right)\dot{\xi}-\theta\frac{\partial s}{\partial\boldsymbol{\sigma}}:\dot{\boldsymbol{\sigma}}-\left(\mu+\frac{\partial s}{\partial c}\theta\right)\dot{c},\end{aligned} \tag{112}$$

i.e. the term proportional to $\dot{c}$ appears in the temperature evolution equation. Assume the validity of the following decomposition for the free energy

$$\rho\psi_i = 0.5\boldsymbol{\varepsilon}_{\mathrm{e}i} : \mathbf{E}_i : \boldsymbol{\varepsilon}_{\mathrm{e}i} + \rho\psi_i^{\theta}(\theta) + \rho\psi_i^{\mathrm{c}}(c,\theta) = \rho\psi_i^{\mathrm{e}} + \rho\psi_i^{\theta}(\theta) + \rho\psi_i^{\mathrm{c}}(c,\theta), \quad i = 1,2, \tag{113}$$

with the same elastic and thermal energies as for the case without diffusion and additional term ψ^{c} due to solute atoms. We neglect the dependence of elastic and thermal constants on c. In an approximation of the regular solution the following expression is valid (Christian, 1965; Lyubov, 1981)

$$\rho\psi_i^{\mathrm{c}} = \Omega_i^{-1}(e_{\mathrm{o}i}c + k\theta(c\ln c + (1-c)\ln(1-c))) + 0.5u_{\mathrm{o}i}c^2. \tag{114}$$

Here Ω_i is the atomic volume of a solvent atom, k is the Boltzmann constant, constants e_{0i} and u_{o} characterize the self-energy and interaction energy of solute atoms. We assume a linear approximation

$$\psi^{\theta} = (1-\xi)\psi_1^{\theta} + \xi\psi_2^{\theta}, \quad \psi^{\mathrm{c}} = (1-\xi)\psi_1^{\mathrm{c}} + \xi\psi_2^{\mathrm{c}}, \quad \mathbf{b} = (1-\xi)\mathbf{b}_1 + \xi\mathbf{b}_2. \tag{115}$$

Then according to Eq. (103)

$$\begin{aligned}\rho X_{\xi} = {} & \boldsymbol{\sigma} : \frac{\partial \boldsymbol{\varepsilon}_{\mathrm{t}}}{\partial \xi} + \boldsymbol{\sigma} : \Delta\boldsymbol{\alpha}(\theta-\theta_{\mathrm{o}}) + \boldsymbol{\sigma} : \Delta\mathbf{b}(c-c_1) - 0.5\boldsymbol{\varepsilon}_{\mathrm{e}} : \Delta\mathbf{E} : \boldsymbol{\varepsilon}_{\mathrm{e}} \\ & - \rho\Delta\psi^{\theta}(\theta) - \rho\Delta\psi^{\mathrm{c}}(c,\theta);\end{aligned} \tag{116}$$

$$\begin{aligned}\rho X = {} & \int_{\boldsymbol{\varepsilon}_{\mathrm{t}1}}^{\boldsymbol{\varepsilon}_{\mathrm{t}2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{t}} + \int_0^1 \boldsymbol{\sigma} : \Delta\boldsymbol{\alpha}(\theta-\theta_{\mathrm{o}})\mathrm{d}\xi + \int_0^1 \boldsymbol{\sigma} : \Delta\mathbf{b}(c-c_1)\mathrm{d}\xi \\ & - 0.5\int_0^1 \boldsymbol{\varepsilon}_{\mathrm{e}} : \Delta\mathbf{E} : \boldsymbol{\varepsilon}_{\mathrm{e}}\mathrm{d}\xi - \int_0^1 \big(\rho\Delta\psi^{\theta}(\theta) + \rho\Delta\psi^{\mathrm{c}}(c,\theta)\big)\mathrm{d}\xi.\end{aligned} \tag{117}$$

It is important to mention that the change in free energy due to diffusion affects the PT only when there is a difference between free energy parts $\Delta\psi^{\mathrm{c}}$ related to solute atoms. The misfit strain affects PT in two ways: first, due to the third term in Eq. (117) proportional to the change in misfit strain during the PT; second, even at $\Delta\mathbf{b} = 0$ misfit strain changes the stress distribution and contributes to the first, second and fourth terms in Eq. (117). If ψ_i^{c} and $\mathbf{b}_i$ are the same for both phases and the stress variation due to misfit strain is negligible, diffusion does not change the driving force for PT, because the change in free energy due to diffusion and work $\boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_{\mathrm{c}}$ in Eq. (108) is completely compensated for by the term $\mu\mathrm{d}c$.

The solute volume fraction c and temperature variation during the PT are determined by the solution of coupled temperature evolution and diffusion equations. If we assume for simplicity $c - c_1 = \Delta c\xi$ and an isothermal process at $\theta = \theta_0$ then Eq. (117) transforms into

$$
\begin{aligned}
pX = {} & \int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_t + \int_0^1 \boldsymbol{\sigma} : \Delta \mathbf{b} \Delta c \xi \mathrm{d}\xi - 0.5 \int_0^1 \boldsymbol{\varepsilon}_e : \Delta \mathbf{E} : \boldsymbol{\varepsilon}_e \mathrm{d}\xi - \rho \Delta \psi^{\theta}(\theta_o) \\
& - f(c_2, c_1, \theta_o),
\end{aligned}
\tag{118}
$$

where

$$
\begin{aligned}
f(c_2, c_1, \theta_o) := {} & \Delta c^{-1} \int_{c_1}^{c_2} \rho \Delta \psi^{c}(c, \theta_o) \mathrm{d}c = \frac{1}{2} \Delta c^{-1} \Big[\Delta\big(\Omega^{-1} e_o\big)\big(c_2^2 - c_1^2\big) \\
& + \frac{1}{3} \Delta u_o \big(c_2^3 - c_1^3\big) + \Delta \Omega^{-1} k \theta_o \bigg(c_2^2 \ln c_2 - c_1^2 \ln c_1 - \frac{1}{2}\big(c_2^2 - c_1^2\big) \\
& + (1 - c_2)^2 \ln(1 - c_2) - (1 - c_1)^2 \ln(1 - c_1) - \frac{1}{2}\big((1 - c_2)^2 - (1 - c_1)\big) \bigg) \Big].
\end{aligned}
\tag{119}
$$

When the volumetric transformation strain is zero, then $\Delta\Omega^{-1} = 0$ and the first two terms in Eq. (119) remain only. At small c or Δc the second term can be neglected as well.

7.2. Appearance of a spherical nucleus

As the simplest example we consider the nucleation of a spherical particle with the radius r in an infinite elastic-perfectly plastic sphere under applied external pressure at diffusional–displacive PT. Let the misfit strain $\boldsymbol{\varepsilon}_c = \frac{1}{3}\varepsilon_c \mathbf{I}$ be purely dilatational, where ε_c is the volumetric misfit strain, i.e. $\varepsilon_c = b(\xi)(c - c_1) = b(\xi)\Delta c \xi = b_1 \Delta c \xi + \Delta b \Delta c \xi^2$. We assume that solute atoms are homogeneously distributed in the nucleus. The work integrals in expression for X are bulky in the general case. Approximating the quadratic with respect to the ξ term in ε_c with the linear one, i.e. $\Delta b \Delta c \xi^2 \approx 0.5 \Delta b \Delta c \xi$, we obtain

$$
\boldsymbol{\varepsilon}_t + \boldsymbol{\varepsilon}_c = \frac{1}{3}(\varepsilon_o + 0.5(b_1 + b_2)\Delta c)\xi \mathbf{I} = \frac{1}{3}\varepsilon_{tc}\xi \mathbf{I}. \tag{120}
$$

Now we can use Eqs. (28) and (29) for stress variation, in which transformation strain ε_o has to be replaced with the ε_{tc}. Then

$$
\begin{aligned}
\int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}_t + 0.5 \int_0^1 \boldsymbol{\sigma} : \Delta \mathbf{b} \Delta c \mathrm{d}\xi & = \int_0^1 p(\varepsilon_{tc}\xi) \mathrm{d}(\varepsilon_0 \xi) + 0.5 \int_0^1 p(\varepsilon_{tc}\xi) \Delta b \Delta c \mathrm{d}\xi \\
& = \int_0^1 p(\varepsilon_{tc}\xi) \mathrm{d}(\varepsilon_{tc}\xi) \left(1 - \frac{b_1 \Delta c}{\varepsilon_{tc}}\right).
\end{aligned}
$$

Calculating the last integral with the help of Eq. (31) with ε_{tc} instead of ε_0, we obtain for X

$$
pX = \left(p\varepsilon_{tc} - \frac{2}{3}\sigma_y \left(\sigma_y C + \varepsilon_{tc} \ln \frac{\varepsilon_{tc}}{2\sigma_y C}\right)\right)\left(1 - \frac{b_1 \Delta c}{\varepsilon_{tc}}\right) - \rho \Delta \psi^{\theta}(\theta_o) - f(c_2, c_1). \tag{121}
$$

Formally the kinetic equation has the same form

$$\left(X - K^0 - E_a\right)\frac{4}{3}\pi\rho r^3 - \Gamma 4\pi r^2 - \frac{n}{N}R\theta_{ef}\ln\frac{t_o}{t_s} = 0, \tag{122}$$

as without diffusion, but X depends on c_2. As c_1 before PT in the parent phase is known Eq. (122) contains three unknowns: r, c_2 and t_s. The following relation

$$r_d^2 = 2D\frac{c_1 - c_{1r}}{c_2 - c_{1r}}t, \tag{123}$$

is the consequence of the solution of the diffusion equation, where D is the diffusion coefficient, t is the diffusion time and c_{1r} is the solute volume fraction in the parent phase at the interface (Christian, 1965; Lyubov, 1981). This equation determines the radius r_d of a sphere in which during the time t the volume fraction c_2 can be reached. Additionally, the constraint

$$c_{min} \leqslant c_2 \leqslant c_{max} \tag{124}$$

must be taken into account. It means, in particular, that the fraction of solute cannot exceed some possible maximum value, determined by the type of crystal lattice and the difference in atomic size of solute and solvent atoms. The minimum value can be zero or determined from the thermodynamic condition for solute atoms across the interface. For example, if the solute has a very high mobility, the equality of the solute chemical potential in phase 1 and phase 2 can be assumed which relates c_2 and c_{1r}

If during time t the nucleus with the radius r with the volume fraction c_2 of solute atoms appears, then the inequality

$$r \leqslant r_d = \left(2D\frac{c_1 - c_{1r}}{c_2 - c_{1r}}t\right)^{0.5} \tag{125}$$

has to be valid. In the opposite case the fraction c_2 cannot be reached in the nucleus with radius r during the nucleation time. If $r < r_d$ then diffusion can guarantee fraction c_2 during the nucleation time in the sphere larger than the nucleus, i.e. diffusion does not limit the transformation kinetics. This can take place for example when $c_2 = c_{max} > c_1$ or $c_2 = c_{min} < c_1$ i.e. when the solute volume fraction in the nucleus reaches the maximum or minimum possible values. Consequently, if the solution obtained satisfies the inequality $r < r_d$ then the process is transformation controlled and we do not need Eq. (123); in the case $r = r_d$ the kinetics is diffusion controlled.

To illustrate the approach only, we assume for simplicity that c_{1r} is known from the solution of the diffusion equation and is independent of c_2. Let us consider the following cases.

Let diffusion be a limiting process, i.e. $r = r_d$ and constraint (124) is satisfied. Finding c_2 from Eq. (123)

$$c_2 = 2D(c_1 - c_{1r})\frac{t}{r^2} + c_{1r}, \tag{126}$$

substituting this c_2 in X (and probably in K^0 and E_a) and maximizing the left part of Eq. (122) with respect to r (i.e. minimizing transformation time), we derive an additional equation

$$-\frac{\partial\left(X - K^0 - E_a\right)}{\partial c_2}\frac{4D(c_1 - c_{1r})\rho t}{3} + \left(X - K^0 - E_a\right)\rho r^2 - 2\Gamma r = 0. \tag{127}$$

Eqs. (122) and (127) after substitution of expression (126) for c_2 in them represent two equations with respect to two unknowns r and t. After substitution of t from Eq. (127) into Eq. (122), we get the nonlinear algebraic equation to find r.

Let us analyze the results obtained:

1. In the case without diffusion ($D = 0$ or when X, K^0 and E_a do not depend on c_2) the first term in Eq. (127) is zero, this equation has no positive solution [as $\left(X - K^0 - E_a\right) < 0$] and we arrive at the same situation as for displacive PT, i.e. $r \rightarrow$ min and r is determined from the thermodynamic PT criterion. If diffusion promotes the PT and increases the difference $X - K^0 - E_a$, i.e. the first term $\frac{\partial\left(X-K^0-E_a\right)}{\partial r}$ in Eq. (127) is negative, then again this equation has no positive roots. In this case $r \rightarrow$ min, the PT criterion (34), the kinetic equation (35) and diffusion Eq. (126) are three equations for the determination of three unknowns r, c_2 and t. Substituting t from Eq. (126) in kinetic equation (35), and then r from Eq. (34) in Eq. (35), we obtain a nonlinear equation with respect to c_2. Substituting c_2 found in Eq. (34) we can find r, and then t from Eq. (126). Then we have to check inequality (124).
2. If diffusion suppresses the PT and decreases the difference $X - K^0 - E_a$, i.e. the first term $\frac{\partial\left(X-K^0-E_a\right)}{\partial r}$ in Eq. (127) is positive, then a solution of Eq. (127) for "optimal" r exists. If it exceeds the thermodynamically admissible radius and inequality (124) is in fact satisfied, then it is the actual solution.
3. Let the solution obtained not satisfy the thermodynamic PT criterion (2), i.e. $r < r_t$. Then we should repeat the same procedure as in item (1).
4. Let one of the inequalities (124) be violated, e.g. $c > c_{max}$. Then we put $c = c_{max}$ and substitute it in Eq. (122). As in this case X is independent of r, the principle of the minimum of transformation time reduces to the $r \rightarrow$ min and the minimum value of r is determined from the PT criterion (34), and the transformation time can be found from kinetic equation (35). If $r \leqslant r_d$, then we have obtained the actual solution.
5. Let us obtain for the case $c = c_{max}$ considered in item $4 r > r_d$, i.e. diffusion is a limiting process. Then we put $r = r_d$ and two Eqs. (122) and (126) determine

two unknowns r and t and an additional extremum principle is not necessary. If r satisfies PT criterion (2), then the solution obtained is the actual one. In the opposite case, a solution does not exist.

8. Strain–induced chemical reactions in shear band

Strain-induced chemical reactions were observed recently (Nesterenko et al., 1994, 1995) in experiments in the shear band in both Ti–Si and Nb–Si mixtures. The first attempt of continuum thermomechanical finite strain modeling of this phenomenon and explanation of the possible reasons for the acceleration of chemical reactions due to intense plastic shear is made in (Levitas et al., 1998b,c). In particular, the reaction-induced plasticity (RIP) phenomenon, similar to transformation-induced plasticity (TRIP) for PT was derived. These considerations were based on a simplified kinetic equation without correctly accounting for actual transforming volume. Here we will combine a new kinetic equation with the results of the solution of the corresponding problem in (Levitas et al., 1998b,c) and will demonstrate a significant difference in final results.

Formally chemical reactions can be considered in the same way as PT. We assume that the transformation strain is a spherical tensor. Consider an infinite rigid-plastic half-space with prescribed normal σ_n and shear τ stresses on the whole surface (Fig. 4) under plane strain condition. We assume the existence of a region with localized plastic shear deformation, i.e. shear band, along the whole surface. The material outside of the shear band is rigid. It is assumed that a coherent SC occurs in the layer inside the shear band. For coherent SC the displacements are continuous across the interface. The problem formulation is reduced to one considered in the paper by Levitas (1997), namely coherent SC in parallel to the external surface infinite layer inside the rigid half-space (Fig. 5). In Fig. 5a transformed particle is shown after transformation strain which is pure volumetric. In order to satisfy the displacement continuity across the interface AB and independence of the solution of x, additional plastic strain is needed (Fig. 5b). As is shown in (Levitas et al., 1998b,c), such a reaction-induced plasticity can be very significant and leads to very intensive heating. We assume that total, transformation and plastic deformation gradients are homogeneous in a layer and that the stress field is homogeneous and time-independent.

For the local driving force X, the temperature during and after the end of the chemical reaction as well as for the effective temperature is obtained (Levitas et al., 1998b,c):

$$X = \left(\frac{1}{2\rho}\left(2\sigma_n - \sqrt{\sigma_y^2 - 4\tau^2}\right)\varepsilon_0 + 0.5\Delta s_o(\theta_1 + \theta_2) - \Delta U_o\right), \tag{128}$$

$$\theta = \theta_1 + \frac{A}{\nu}\xi; \quad \theta_2 := \theta(1) = \theta_1 + \frac{A}{\nu}, \quad \theta_{ef} = 0.5(\theta_1 + \theta_2); \tag{129}$$

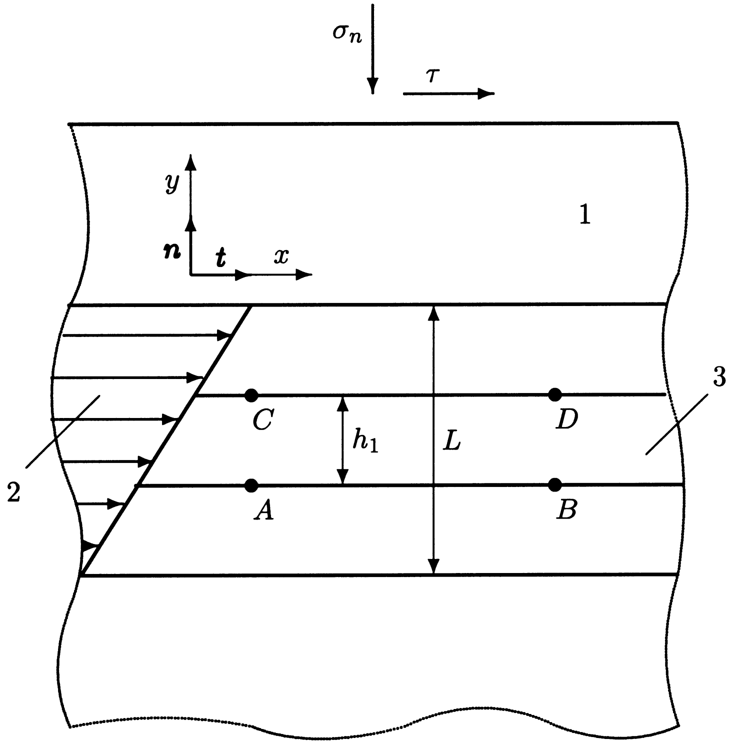

Fig. 4. Schematic illustration of chemical reactions in a shear band: 1, half space; 2, shear band with displacement; 3, layer with chemical reactions.

$$A := \frac{\varepsilon_0}{\rho}\left(\sigma_{\rm n} + \frac{2\tau^2}{\sqrt{\sigma_{\rm y}^2 - 4\tau^2}}\right) - \Delta U_{\rm o}, \tag{130}$$

where $\Delta U_{\rm o}$ is the jump in the reference internal energy, ρ and h is the mass density and the thickness of the layer in the reference configuration (before the chemical reaction), A is the heat source due to the reaction heat $\Delta U_{\rm o}$ and reaction-induced plasticity. It is clear from Eqs.(128)–(130) that at $\tau \rightarrow 0.5\sigma_{\rm y}$ the heat source due to reaction-induced plasticity tends to infinity and the temperature tends to melting temperature.

Minimizing with respect to h the reaction time, i.e.

$$\frac{n}{N}R\theta_{\rm ef}\ln\frac{t_{\rm o}}{t_{\rm s}} = \rho\left(X - K^0 - E_{\rm a}\right)hlb - \Gamma 2lb \rightarrow \max_h, \tag{131}$$

where l and b are the length and width of the interface surface, we obtain $h \rightarrow$ min. It follows from the thermodynamic PT criterion

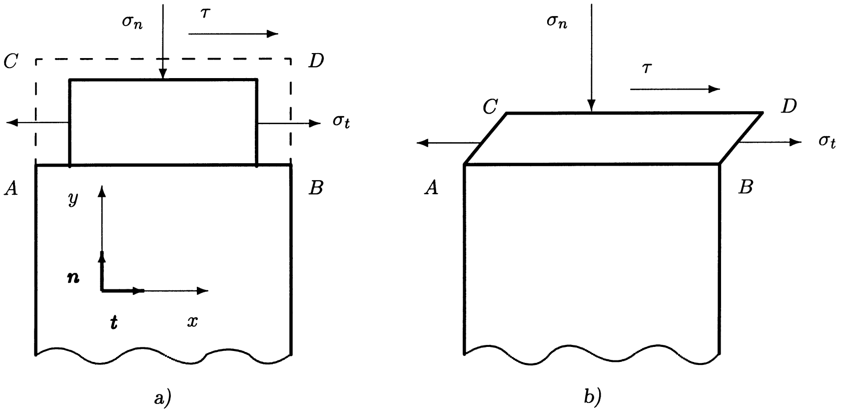

Fig. 5. Scheme of chemical reaction in a thin layer.

$$h = \frac{2\Gamma}{\rho(X - K^0)}. \tag{132}$$

Substitution of Eq. (132) in kinetic equation (5) results in

$$t_s = t_0 \exp\left(\frac{E_a}{R\theta_{ef}} \frac{N}{n} \frac{2\Gamma}{(X - K^0)} lb\right). \tag{133}$$

As the kinetic criterion of the initiation of the chemical reaction it is assumed that the reaction time t_s is less than the time of deformation in the shear band.

Let us compare our results with those obtained in (Levitas et al., 1998b,c). The following kinetic equation is used there

$$t_s = t_{po} \exp - \frac{X - K^0 - 2\Gamma/(ph) - E_a}{R\theta_{ef}}, \tag{134}$$

i.e. the actual activation energy is determined per mol without duly accounting for the actual transforming volume. It is shown that the main reason for the acceleration of reaction kinetics due to shear stress or strain is related to the increase in effective temperature in the denominator of Eq. (134) due to reaction-induced plasticity. The increase in the driving force X due to shear stresses has practically no effect on the kinetics. Note that the effective temperature in the driving force (128) is eliminated by the effective temperature in the denominator of Eq. (134). The results obtained here (133) predict a much stronger effect of the driving force and increase in effective temperature due to reaction-induced plasticity on transformation time (see Fig. 7).

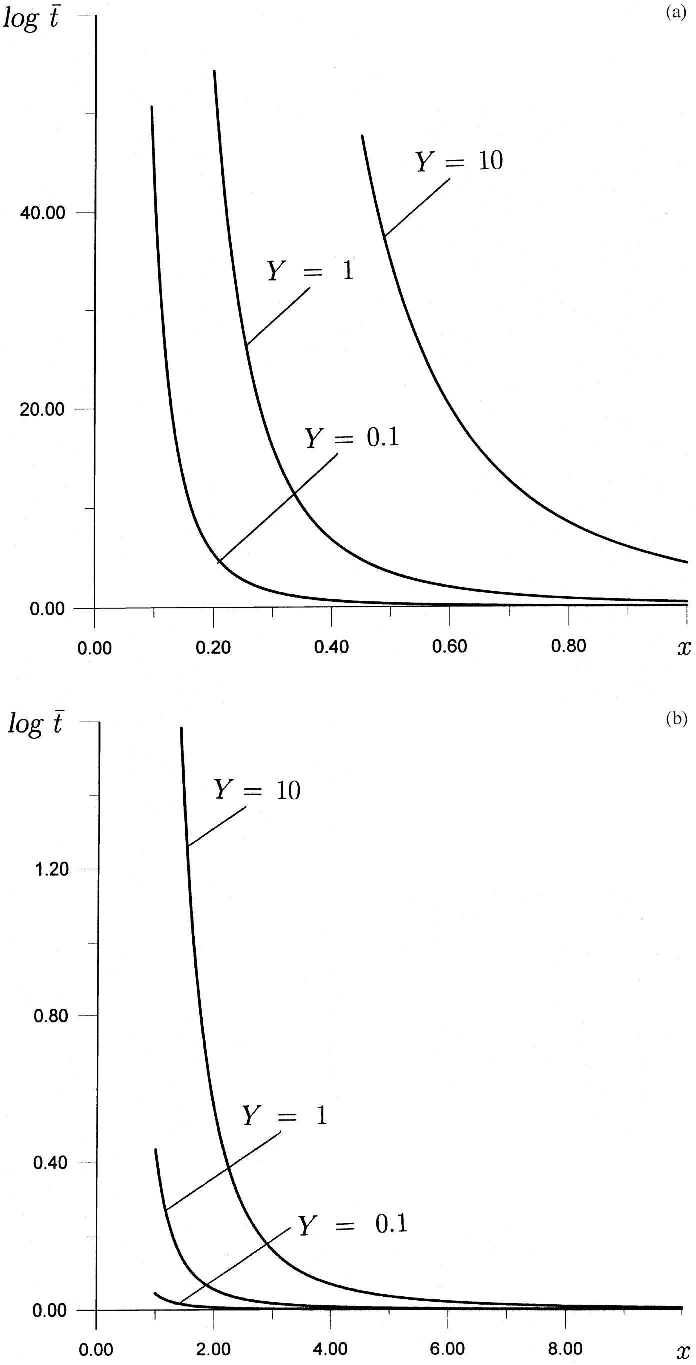

Fig. 6. Relation between modified time of structural change and driving force [Eq.(135)] for $m = -3$ and various Y.

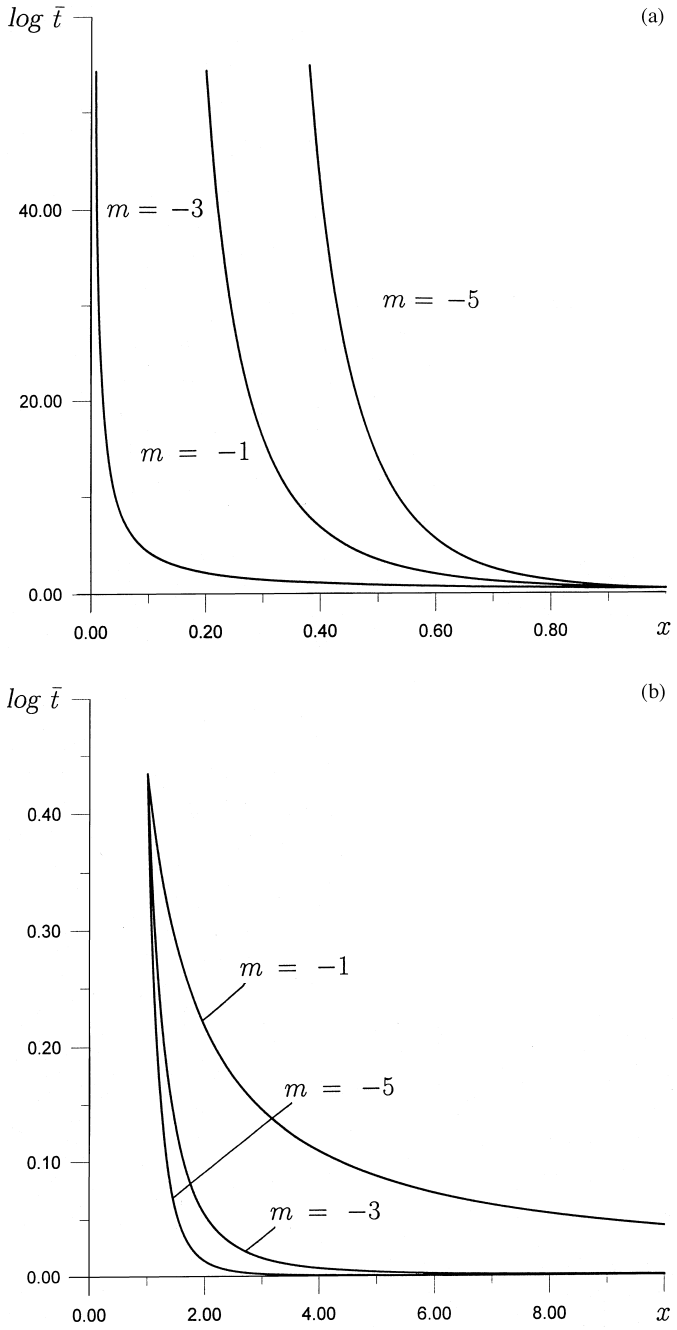

Fig. 7. Relation between modified time of structural change and driving force [Eq.(135)] for $Y = 1$ and various m (nucleus geometries).

9. Comparison of nucleation kinetics for various nucleus geometries

For a thermodynamically admissible nucleus, the transformation time depends very strongly on the transforming volume [Eq. (5)]. The transforming volume is a power function of the difference between the local driving force and the athermal threshold $x := X - K^0$:

$$V_{\mathrm{nt}} = Lx^{\mathrm{m}}, \quad L = P\Gamma^{\mathrm{p}}. \tag{135}$$

The power m is equal to -3 for a spherical nucleus [Eqs. (34) and (35)]; $m = -1$ for a plastic ellipsoidal nucleus [Eq. (61)], for crack propagation [Eqs. (85) and (87)] and for a nucleus in the form of thin infinite layer [Eq. (133)]; $m = -5$ for an elastic ellipsoidal nucleus [Eq. (49)]. Note that for elastic ellipsoidal inclusion the transforming volume is affected by the driving force when energy of internal stresses is excluded [see Eqs. (44) and (49)]. For plastic ellipsoidal inclusion the mechanical and thermal parts of the driving force influence the transforming volume separately; power -1 is valid at the fixed external stress.

Power p is equal to 1 for crack propagation and for an infinitely thin layer and $p = 3$ for all other cases under consideration. The parameter P is independent of x and Γ and for each case can be found in the above formulae.

Let us represent the expression for transformation time Eq. (5) with the help of Eq. (135) in the form

$$\bar{t} = \exp(Yx^{\mathrm{m}}); \quad \bar{t} := \frac{t_{\mathrm{s}}}{t_{\mathrm{o}}}; \quad Y = \frac{\rho E_{\mathrm{a}} L}{R\theta_{\mathrm{ef}}} \frac{N}{n}. \tag{136}$$

The parameter $\bar{t}$ is proportional to the transformation time and Y is a combination of the activation energy, temperature and surface energy. To get a feeling of how the driving force affects the transformation time, the relation between $\log \bar{t}$ and x (i.e. $\log \bar{t} = Yx^m \log e$) is plotted in Fig. 6 for $m = -3$ and three different values of Y. What is typical is a very strong dependence of $\log \bar{t}$ on x at small x with a sharp transition to weak dependence between these parameters at large x. If we prescribe some observation time t_{ob}, then the condition $t = t_{\mathrm{ob}}$ (or $\bar{t} = \bar{t}_{\mathrm{ob}}$) determines a driving force x necessary for nucleation. Fig. 6 supports the idea of the importance of heterogeneities in driving force distribution and heterogeneous nucleation at different defects (for example, for martensitic PT; Olson and Cohen, 1986) at small driving forces. An increase in driving force due to stress concentration at defects can decrease the transformation time by several orders of magnitude. At relative high driving forces heterogeneities are not so important, due to the weak dependence of the transformation time on the driving force, and homogeneous nucleation is possible. The smaller the activation and surface energy, the smaller the driving force necessary for nucleation and the sharper the transition from high driving force sensitivity to a low one. At relatively high $X - K^0$ the transformation time is insensitive to the effective temperature and activation energy, i.e. Eq. (133) describes the transition to athermal kinetics.

In Fig. 7 the same relations are plotted for $Y = 1$ and different m. At $x < 1$ the smaller $|m|$ the smaller the driving force necessary for nucleation and the less the nucleation is sensitive to heterogeneities. For $x > 1$ the smaller $|m|$ the higher the driving force necessary for nucleation.

Note that an alternative kinetic description, based on the choice of $\dot{m}_{\mathrm{n}}$ as a generalized rate (Levitas, 1998b), kinetic equation

$$\dot{m} = \dot{m}_{\mathrm{o}} \exp\left(\frac{\left(X - K^0 - E_{\mathrm{a}}\right)\rho V_{\mathrm{n}} - \Gamma\Sigma_{\mathrm{n}}}{R\theta_{\mathrm{ef}}}\frac{N}{n}\right); \quad t_{\mathrm{p}} = \frac{\rho V_{\mathrm{n}}}{\dot{\mathrm{m}}_{\mathrm{n}}}. \tag{137}$$

and the principle of the maximum of the transformation rate $\dot{m} \rightarrow \max$ results in an equation for the transformation time in the following form

$$\tilde{t} = x^{\mathrm{m}} \exp(Yx^{\mathrm{m}}); \quad \tilde{t} := \frac{t_{\mathrm{p}}\dot{m}_{\mathrm{o}}}{\rho L}. \tag{138}$$

We have $\log \tilde{t} = m \log x + \log \bar{t}$. For the values m under consideration both descriptions lead to the same qualitative and slightly different quantitative results. However, for diffusional–displacive PT a qualitative difference was observed.

10. Concluding remarks

In the present paper, a number of simple examples demonstrate the applicability of the general theory developed in the paper (Levitas, 2000) to various SC in solids, namely to displacive and generalized second-order phase transformations, twinning and reorientation of martensitic variants, ductile fracture, and strain-induced chemical reactions. The theory is extended to diffusional–displacive phase transitions. The following problems for elastic and elastoplastic materials are solved analytically: displacive and diffusional–displacive phase transitions in a spherical particle inside the space under external pressure, martensitic phase transition and twinning in ellipsoidal inclusion under applied shear stress, spherical void nucleation, crack propagation in a framework similar to the Dugdale model for a plane stress state. In most cases explicit expressions for the thermodynamic and kinetic conditions for SC and the geometric parameters of the nucleus are obtained and analyzed. The following typical cases in the determination of the geometric parameters of the nucleus are found: solely from the principle of the minimum of transformation time and the kinetic equation without any constraints or with a thermodynamic constraint; from the principle of the minimum of transformation mass and the thermodynamic criterion of structural changes (thermodynamically admissible nucleus); as an interatomic distance. For diffusional–displacive PT, additional variants are related to the necessity to consider the diffusion equation (for the diffusion-controlled PT) and constraints related to the maximum and minimum possible volume fraction of solute atoms.

It is clear that assumptions related to the plane strain state or SC in an infinite layer are unreal from a kinetic point of view. A small three dimensional nucleus will appear for such problems with the higher transformation rate; however, analytical solutions for such cases are not available.

Hopefully, other structural changes, like dislocation nucleation, static and dynamic recrystallization, oxidation, deformation of amorphous materials, can be described in the same way. Electromagnetic phenomena can be included in the general scheme as well.

The transition to atom by atom growth indicates that atomistic rather than continuum mechanic treatment is necessary. However, like in dislocation theory, continuum description can give reasonable estimates. Atomistic calculations also allows us to determine variation of material properties along the ξ-variation (e.g. Krasko and Olson, 1989) and the actual activation energy.

The kinetics of individual events proposed can be used in combination with a statistical hypothesis and the micro- to macro- transition for the derivation of equations for macroscopic kinetics in terms of the volume fraction of the transformed phase.

The next important problem is related to the mutual effect of various structural changes, their competition and mutual assistance. As examples we can consider an interaction between PT and plasticity, fracture and PT, twinning and PT and so on. Here we described plasticity using the continuum flow theory. Even in this case the interaction between plasticity and PT can lead to ambiguity. It is possible that under the given increment of boundary conditions the PT criterion and extremum principle allow several solutions, e.g. transformation in different places or propagation of different interfaces. At least two solutions are always possible: first, the solution without the PT (because it satisfies all the equations of continuum mechanics), second, the solution with the PT. Such a situation was revealed in papers by Levitas (1992; 1995) and Levitas et al. (1998c). It was suggested that the best unique solution among all those possible is the stable one. To formulate the stability criterion again the *postulate of realizability* is applied. Using it, the extremum principle for the whole volume is derived to choose the stable solution. These results were obtained for time-independent materials and kinetics of SC. For time-dependent kinetics the principle of minimum of transformation time will probably be sufficient to choose the best solution, i.e. the scenario which will be observed as the first in time. The interaction between PT and fracture and sliding (incoherence) at the interface was considered in papers by Levitas (1997a,b, 1998a), Levitas et al. (1998a) and Idesman et al. (1997) using simplified criteria of maximum normal stress for fracture and maximum shear stress for sliding. The interaction between PT and fracture in elastoplastic materials based on the theory developed in this paper is studied by Idesman et al. (2000).

In the framework of the approach considered in the present paper plasticity and sliding along the interface can be considered as structural changes as well, namely as generation and motion of dislocations. Then these phenomena have to be described using the above criterion, kinetic equation and extremum principle, as is done for PT, fracture, twinning and others. In particular, problems of dislocation nucleation during the PT inside the phases and at the interface, similar to the problem of dislocation nucleation near the crack tip (Rice and Beltz, 1994; Xu et al,. 1995; Cherepanov, 1997) arise. All the interacting SC have to be considered simultaneously and transformation times for each of them have to be calculated. If the transformation time for one of the processes is considerably smaller than for others, then this process will occur only. In the case of comparable transformation times all the SC can occur simultaneously. The minimization of transformation time for each SC can lead to conflict. Some new extremum principle, probably based on stability analysis, may be considering all SC as one compound SC, have to be derived and we hope that the postulate of realizability will be helpful again. Note that consideration of the same SC in two interacting regions is part of the same problem.

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