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PHASE TRANSITION ZONES AND TWO PHASE STRAIN FIELDS IN ELASTIC SOLIDS

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Abstract. *Conditions on the equilibrium phase boundary in a nonlinear elastic material are modeled by a system of equations that determine a one–parameter family of normals to the boundary and strains on one side of the boundary as a function of strains on the other side. Strains for which this system of equations is resolvable form the phase transition zone (PTZ) in strain space. The PTZ boundary acts as a phase diagram. The procedure for PTZ construction is developed for nonlinear elastic materials in a small strain approach. Some boundary problems for elastic bodies undergoing phase transformations are examined. The correlation between strain fields in two-phase bodies and PTZ in strain space as well as energy changes due to phase transformations, stability and stress–strain diagrams for solids on the path of the transformation are studied.*

1 INTRODUCTION

Conditions on the equilibrium phase boundary (the surface of discontinuity in deformation gradient at continuous displacement) in a nonlinear elastic material include an additional thermodynamic condition[1-4] and can be considered as the system of equations that determine the normal to the boundary as well as the strains in one phase as a function of strains in the other. This system of equations has nontrivial solution not for any hyperelastic materials and not at any deformations. The first circumstance leads to restrictions on constitutive equations, the second one leads to the concept of phase transition zone (PTZ)[5,6] formed by all strains which can coexist on the equilibrium interface in a hyperelastic material.

The importance of PTZ construction is motivated by the following reasons:

* Deformations outside PTZ cannot coexist on the interface, whatever the loading conditions. The PTZ boundary acts as a phase diagram or yield surface in strain-space.

* The problem on equilibrium two phase configuration of elastic bodies is a problem with unknown boundary and, as a rule, has no a unique solution. As is shown below, a comparison between deformation fields in different two–phase configurations of an elastic body at the same boundary conditions and PTZ allows to choose thermodynamically preferential configuration. We mean an opportunity of the following situations:

— strains in an equilibrium two–phase body are outside the PTZ except the phase boundary which corresponds to the outer PTZ boundary;

— strains in a two–phase body correspond to the PTZ interior.

The general procedure for PTZ construction was earlier developed and examined for various isotropic hyperelastic materials (finite strains)[5,6]. The purpose of the present paper is to consider phase transformations of elastic bodies in a small strain approach. First, after some remarks on constitutive equations, we show that the problem is reduced to the solution of the linear elasticity equations for heterogeneous medium with an additional (thermodynamic) condition which limits the shape of the interface. The system of conditions on the equilibrium phase boundary is split. The thermodynamic condition takes the form of an equation that determines the unit normal to the phase boundary in relation to deformation on one side of the boundary. Solvability requirements for this equation determine the PTZ boundary in strain space.

Then we study admissible directions of normal and jumps of strains on the phase boundary. While on one side of the phase boundary, any deformation from PTZ interior admits one–parametric family of normals and corresponding one-parametric family of strain jumps. This one–parametric feature disappears at the PTZ boundary. In this case strains possessed by different parts of PTZ boundary allow different kinds of phase boundary orientations and jumps of strains. So, this examination of the PTZ shows different orientations of the interface and different jumps of strains on it (i.e. different form of strain localization due to phase transitions) depending on deformation state.

All the above concerns the conditions of local equilibrium between two phases of an elastic body and means an investigation of piecewise constant two phase strain fields with plane phase boundaries. Further we investigate some features of phase transformations of elastic bodies at different stress states. By way of illustration we examine simplest boundary problems for an elastic sphere under pressure[7,8] and a tube under rotation of its lateral surface while the inner surface is held fixed. The non–uniqueness of the solution is demonstrated. Notice that such boundary problems have also been the subject of other investigations[9,10]. The goal of our paper is to study the correspondence between deformation fields in different two phase configurations of solids, energy changes due to phase transformations and the PTZ.

Another sort of problem is multiple appearance of anisotropic phase layers under the process of deformation. Dependencies of structure parameters (new phase concentration, orientation of layers, directions of anisotropy) on loading, temperature and material parameters and, as a consequence, the relationship between average stress and strain tensors are determined by the same approach.

2 EQUILIBRIUM PHASE BOUNDARY IN SMALL STRAIN APPROACH

In a case of small strains a problem on equilibrium two-phase configurations of elastic body can be reduced to the determination of the phase boundary Γ and corresponding displacement field $\mathbf{u}(\mathbf{x})$, which is smooth enough at material points $\mathbf{x} \notin \Gamma$, continuous on Γ

$$[\mathbf{u}] = 0, \quad \mathbf{x} \in \Gamma \tag{1}$$

and satisfies boundary conditions, thermal condition $\theta = const$ and equilibrium conditions

$$\mathbf{x} \notin \Gamma : \quad \nabla \cdot \sigma = 0, \tag{2}$$

$$\mathbf{x} \in \Gamma : \quad [\sigma] \cdot \mathbf{n} = 0, \qquad [f] - \sigma : [\varepsilon] = 0 \tag{3}$$

where $\mathbf{n}$ is a normal to the boundary, σ and $\varepsilon = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$ are stress and linear strain tensors, θ is temperature, $f(\varepsilon, \theta)$ is free energy volume density, $\sigma = \partial f / \partial \varepsilon$, body forces are equal to zero. We use small bold letters for vectors and second order tensors, bold capitals for forth order tensors, square brackets denote the jump on the phase boundary: $[...] = (...)^+ - (...)^-$, signs "$\pm$" correspond to phases "$\pm$", " $\cdot$ " and " : " mean products[11], if $\mathbf{a}$, $\mathbf{b}$ are vectors and $\mathbf{p}$, $\mathbf{q}$, $\mathbf{K}$ are tensors, then $\mathbf{a} \cdot \mathbf{b} = a_i b_i$, $(\mathbf{p} \cdot \mathbf{a})_i = p_{ij} a_j$, $\mathbf{p} : \mathbf{q} = p_{ij} q_{ji}$, $(\mathbf{p} : \mathbf{K})_{ij} = p_{mn} K_{nmij}$, $\mathbf{p} : \mathbf{K} : \mathbf{q} = K_{nmij} p_{mn} q_{ji}$.

Thermodynamic condition $(3)_2$ follows from the conditions on the equilibrium phase boundary in a nonlinear hyperelastic material[1-4]. From (1) it follows

$$[\varepsilon] = \frac{1}{2}\left(\mathbf{n}\otimes\mathbf{a}+\mathbf{a}\otimes\mathbf{n}\right) \tag{4}$$

where $\mathbf{a}$ is an unknown amplitude vector.

In traditional small strain approach $f(\varepsilon,\theta)$ is a quadratic function of ε and representation $f(\varepsilon,\cdot)$ as a polynomial of degree more than 2 is incorrect[11]. In this case discontinuous solutions which satisfy $(3)_1$, (4) cannot exist if elasticity tensor is definite. Let us suppose that $f(\varepsilon,\cdot)$ is represented at least by two quadratic dependencies

$$f^{\pm}(\varepsilon,\theta) = f_0^{\pm}(\theta) + \frac{1}{2}(\varepsilon-\varepsilon_{\pm}^{p}) : \mathbf{C}_{\pm} : (\varepsilon-\varepsilon_{\pm}^{p}) \tag{5}$$

where parameters $\mathbf{C}_{\pm}$, $f_0^{\pm}$, $\varepsilon_{\pm}^{p}$ are elasticity tensors, free energy densities and strain tensors in unstressed phases "±". We mean the correspondence between upper and lower indexes "±". If $\varepsilon_{+}^{p}=0$, then $[\varepsilon^{p}]=\varepsilon^{p}$ is a phase transition self–strain tensor. For simplicity we do not consider thermoelastic effects.

The rule for the choice of signs "±" depending on ε follows from the consideration of the functions $f^{\pm}(\varepsilon,\cdot)$ on the path $\varepsilon(\eta)=(1-\eta)\varepsilon_{-}+\eta\varepsilon_{+}$ $(\eta\in[0,1])$[8]. If $\mathbf{C}_{\pm}$ are positive definite, the both conditions (3) can be satisfied at $\mathbf{a}\neq 0$ only if

$$f(\eta) = \min_{-,+}\{f^{-}(\eta),\, f^{+}(\eta)\}, \qquad f(\eta)=f(\varepsilon(\eta),\cdot),\;\; \eta\in[0,1] \tag{6}$$

Extended over the whole strain space or a part of strain space, (6) gives

$$f(\varepsilon,\theta) = \min_{-,+}\{f^{-}(\varepsilon,\theta),\, f^{+}(\varepsilon,\theta)\} \tag{7}$$

Notice that in fact, $f(\varepsilon,\cdot)$ is build up using a set of quadratic and linear dependencies. In particularly, a set of these functions have to correspond to the symmetry group of the material if material is anisotropic. In this paper, for the sake of simplicity, we consider only two branch free energy function (5), (7).

Constitutive equations take the form

$$\sigma(\varepsilon) = \mathbf{C}_{\pm} : (\varepsilon-\varepsilon_{\pm}^{p}), \quad \varepsilon\in\mathcal{E}_{\pm} \tag{8}$$

where domains of definition of phases "∓"

$$\mathcal{E}_{-}=\{\,\varepsilon:\;\varphi(\varepsilon)>0\},\;\; \mathcal{E}_{+}=\{\,\varepsilon:\;\varphi(\varepsilon)<0\}, \qquad \varphi(\varepsilon)=f^{+}(\varepsilon,\cdot)-f^{-}(\varepsilon,\cdot) \tag{9}$$

Local conditions (3) can be considered as a system of four equations for five unknowns, which determine the unit normal $\mathbf{n}$ and amplitude $\mathbf{a}$ depending on strain on one side of the phase boundary, if (4), (5), (8) are accounted for.

It follows from $(3)_1$, (4), (8), that

$$\begin{aligned} [\varepsilon] &= \mathbf{K}_{\mp}(\mathbf{n}) : \mathbf{q}_{\pm}, \quad \mathbf{q}_{\pm} = -\mathbf{C}_1 : \varepsilon_{\pm} + [\mathbf{C} : \varepsilon^p] \\ \mathbf{K}_{\pm}(\mathbf{n}) &= \{\mathbf{n} \otimes \mathbf{G}_{\pm} \otimes \mathbf{n}\}^s, \quad \mathbf{G}_{\pm} = (\mathbf{n} \cdot \mathbf{C}_{\pm} \cdot \mathbf{n})^{-1}, \quad \mathbf{C}_1 = \mathbf{C}_+ - \mathbf{C}_- \end{aligned} \tag{10}$$

(s means the symmetrization: $K_{ijkl} = \frac{1}{4}(n_i G_{jk} n_l + n_j G_{ik} n_l + n_i G_{jl} n_k + n_j G_{il} n_k)$)

Substituting of (5), (8) and (10) into $(3)_2$ brings the thermodynamic condition to the form:

$$2\gamma + [\varepsilon^p : \mathbf{C} : \varepsilon^p] + \varepsilon_{\pm} : \mathbf{C}_1 : \varepsilon_{\pm} - 2\varepsilon_{\pm} : [\mathbf{C} : \varepsilon^p] \pm \mathbf{q}_{\pm} : \mathbf{K}_{\mp}(\mathbf{n}) : \mathbf{q}_{\pm} = 0 \tag{11}$$

where $\gamma = [f_0(\theta)]$ acts as temperature in absence of thermal stresses. The system of equations is split. Equation (11) determines one-parametric family of unit normals depending on γ and strains on one side ("+" or "−") of the boundary. Strains on the other side are then computed from formulas (10).

If tensor C_1 is nonsingular, (11) can be rewritten in *$q-$ space:*

$$2\gamma_* + \mathbf{q}_{\pm} : (\mathbf{C}_1^{-1} \pm \mathbf{K}_{\mp}(\mathbf{n})) : \mathbf{q}_{\pm} = 0, \quad \gamma_* = \gamma + \frac{1}{2}[\varepsilon^p] : \mathbf{B}_1^{-1} : [\varepsilon^p] \tag{12}$$

($\mathbf{B}_1 = \mathbf{B}_+ - \mathbf{B}_-$, $\mathbf{B} = \mathbf{C}^{-1}$). Notice, that $\mathbf{q}$ is a linear transformation of ε.

3 PHASE TRANSITION ZONE

Strains for which the equation (11) or (12) can be solved for normal $\mathbf{n}$ form the *phase transition zone* in strain or $q-$ space. The PTZ is divided into sub–zones "±" with strains related by (10). Actually we have to construct only one of sub–zones.

Equation (12) can be written in a form

$$\begin{gathered} \mathcal{K}_{\mp}(\mathbf{q}_{\pm}, \mathbf{n}) = \mp\varphi(\mathbf{q}_{\pm}) \\ \mathcal{K}_{\mp}(\mathbf{q}, \mathbf{n}) = \mathbf{q} : \mathbf{K}_{\mp}(\mathbf{n}) : \mathbf{q}, \quad \varphi(\mathbf{q}) = 2\gamma_* + \mathbf{q} : \mathbf{C}_1^{-1} : \mathbf{q} \end{gathered} \tag{13}$$

Tensors $\mathbf{q}$ from sub–zones $Q_{\pm}$ satisfy inequalities

$$\begin{gathered} \mathcal{K}^{\mp}_{\mathbf{min}}(\mathbf{q}) \le \mp\varphi(\mathbf{q}) \le \mathcal{K}^{\mp}_{\mathbf{max}}(\mathbf{q}) \\ \mathcal{K}^{\mp}_{\mathbf{max}}(\mathbf{q}) = \max_{\mathbf{n}} \mathcal{K}_{\mp}(\mathbf{q}, \mathbf{n}), \quad \mathcal{K}^{\mp}_{\mathbf{min}}(\mathbf{q}) = \min_{\mathbf{n}} \mathcal{K}_{\mp}(\mathbf{q}, \mathbf{n}) \end{gathered} \tag{14}$$

External and internal boundaries of $Q_{\pm}$ are determined by the equations

$$2\gamma_* + \mathbf{q} : \mathbf{C}_1^{-1} : \mathbf{q} \pm \mathcal{K}^{\mp}_{\mathbf{max}}(\mathbf{q}) = 0, \;\; 2\gamma_* + \mathbf{q} : \mathbf{C}_1^{-1} : \mathbf{q} \pm \mathcal{K}^{\mp}_{\mathbf{max}}(\mathbf{q}) = 0 \tag{15}$$

The normals to the phase boundary

$$\mathbf{n}^{\pm}_{ex}(\mathbf{q}) = \arg\max_{\mathbf{n}} \mathcal{K}_{\mp}(\mathbf{q}, \mathbf{n}), \;\; \mathbf{n}^{\pm}_{in}(\mathbf{q}) = \arg\min_{\mathbf{n}} \mathcal{K}_{\mp}(\mathbf{q}, \mathbf{n})$$

correspond to the external and internal PTZ boundaries. One–parametric feature of the solution disappears on PTZ–boundaries. Domains (9) of definition of phases are divided by the surface $\varphi_q = \{\mathbf{q} : \varphi(\mathbf{q}) = 0\}$ in q–space. This surface passes between internal PTZ boundaries $(15)_2$.

If phase "−" is isotropic, then

$$\mathbf{C}_- = \lambda_- \mathbf{E} \otimes \mathbf{E} + 2\mu \mathbf{I}, \quad \mathbf{K}_-(\mathbf{n}) = \xi_- (\mathbf{n} \otimes \mathbf{E} \otimes \mathbf{n})^s - \zeta_- \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \tag{16}$$
$$\mathcal{K}_-(\mathbf{q}, \mathbf{n}) = F(N_1, N_2)/\mu_-, \quad F(N_1, N_2) \stackrel{def}{=} N_2 - aN_1^2, \quad N_k = \mathbf{n} \cdot \mathbf{q}^k \cdot \mathbf{n} \ (k = 1, 2)$$

where $\mathbf{E}$ and $\mathbf{I}$ are second and fourth order unit tensors, λ and μ are Lame constants, $\xi = \mu^{-1}$, $\zeta = 2\mu(1-\nu)^{-1}$, ν is Poisson's ratio, $a = (2(1-\nu_-))^{-1}$.

Orientation invariants N_k determine the normal $\mathbf{n}$ if $\mathbf{q}$ is known. Using representations

$$\mathbf{q} = \sum q_i \mathbf{e}_i \otimes \mathbf{e}_i, \quad \mathbf{n} = \sum n_i \mathbf{e}_i$$

one can arrive the system of three equations

$$\sum n_i^2 = 1, \qquad \sum n_i^2 q_i^k = N_k \quad (k = 1, 2) \tag{17}$$

that is linear with respect to n_i^2 $(i = 1, 2, 3)$.

For any $\mathbf{q} \in Q_+$ equation (13) takes the form of a relationship between orientation invariants

$$F(N_1, N_2) = -\mu_- \varphi(\mathbf{q}) \tag{18}$$

and has a simple geometric interpretation on the N_1, N_2 plane. Since the solution of the system (17) has to be non–negative, the admissible value domain $\mathcal{D}$ for orientation invariants is a triangle with vertexes (q_i, q_i^2) $(i = 1, 2, 3)$. The vertexes correspond to $\mathbf{n} = \mathbf{e}_i$, points of the $i - j$ – side of the triangle correspond to $\mathbf{n}$ lying in the $i - j$ – principal plane of $\mathbf{q}$. If q_i $(i = 1, 2, 3)$ change, then vertexes of $\mathcal{D}$ move along the *skeleton curve* $N_2 = N_1^2$. On the other hand, (18) determines the parabola $N_2 = aN_1^2 - \mu_- \varphi(\mathbf{q})$ $(a > 1)$, which moves along N_2–axis if $\mathbf{q}$ changes. The line of intersection of this parabola and $\mathcal{D}$ gives one parameter family of solutions. The sub–zone Q_+ is formed by all such $\mathbf{q}$ that this intersection exists:

$$Q_+ = \{\mathbf{q} : \min_{N_1, N_2 \in \mathcal{D}} F(N_1, N_2) \leq -\mu_- \varphi(\mathbf{q}) \leq \max_{N_1, N_2 \in \mathcal{D}} F(N_1, N_2)\}$$

In Fig. 1, we show a typical cross–section of the PTZ by a plane $tr\, \mathbf{q} = const$ (a deviator section) for a case of isotropic phases. Because of isotropy we consider only one sector OAB $(q_1 \leq q_2 \leq q_3)$. Segments ab and AB correspond to external PTZ boundaries, de

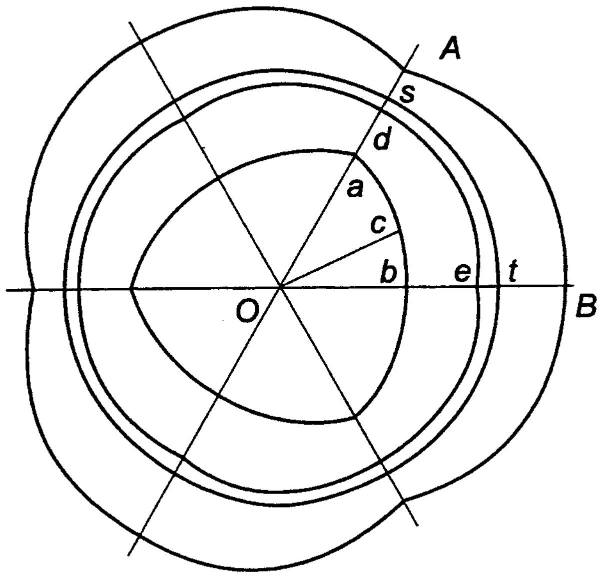

Figure 1: Deviator section of the phase transition zone in q–space

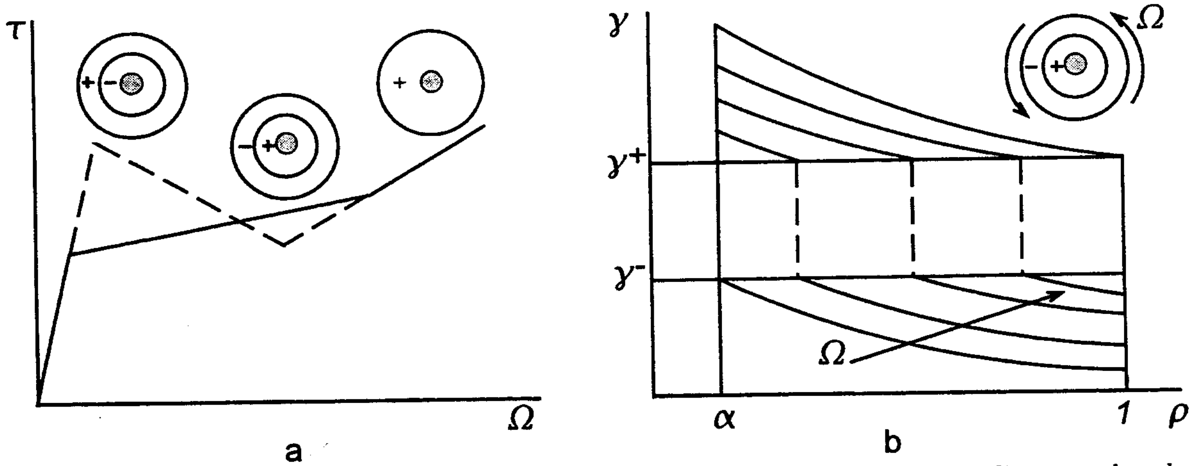

Figure 2: Phase transformation of a twisting tube ($\mu_+ < \mu_-$), a—shear stress–strain diagrams, b—shear strains distribution in a cross–section of a tube

and st are parts of the internal boundaries, the line of the intersection with the surface φ_q (not shown) passes between the lines of the internal boundaries.

If strains on the phase boundary belong to the external PTZ boundaries, then the normal $\mathbf{n}$ lies in the $1-3$ – principal plane of tensor $\mathbf{q}$ and depends on q_1, q_3 (segment ac) or coincides with eigenvector $\mathbf{e}_{|q|\max}$ corresponding to $\max\{|q_1|, |q_2|, |q_3|\}$ (segment cb), depending on a relation between eigenvalues of $\mathbf{q}$. If the phase boundary corresponds to the internal PTZ boundaries, then $\mathbf{n} = \mathbf{e}_{|q|\min}$. Jumps of strains can be computed from formulas (10), (16).

4 TWO PHASE STRAIN FIELDS

To study the correspondence between deformation fields in various two phase configurations of elastic bodies and the PTZ we consider phase transformations of a sphere under pressure[7,8], a tube under rotation of its lateral surface while the inner surface is held fixed and unbounded medium in homogeneous average strain field.

In a case of a sphere and a tube the material is supposed to be isotropic. Two phase states with a single phase boundary (with a spherical boundary in a case of a sphere and cylindrical one in a case of a tube) are examined. The radius of the phase boundary is determined by the thermodynamic condition (12) (or (11)). The non–uniqueness of the solution is demonstrated even at this class of two phase configurations. The equilibrium conditions can be satisfied if a new phase area propagates from the interior as well as from the outer boundaries of the bodies.

The relationship between external pressure p and average volume strain ϑ_0 on the path of the transformation of the sphere takes the form

$$-p = k_* \left(\vartheta_0 - \vartheta_*\right) + p_*$$

where $k_* = -\frac{4}{3}\mu_e \leq 0$ is an "effective" bulk modulus of a sphere, μ_e is a shear modulus of the material of the external phase, ϑ_* and p_* depend on material parameters. From the macroscopic point of view the sphere demonstrates a behavior of a trilinear material with a strain softening effect.

Energy estimates show that the competition between above mention solutions is determined by the shear modulus μ_- and μ_+ of the phases. More rigid phase is located in an internal part of the sphere. For the both solutions strains on the phase boundaries correspond to the PTZ boundary, but the other strains are outside the PTZ in a case of thermodynamically preferential configuration, otherwise strains are inside the PTZ.

On the path of the transformation of a tube the relationship between shear stress τ and tangent displacement Ω on the external surface takes the form

$$\tau = \tau_0 + G_* \left(\Omega - \Omega_0\right), \quad G_* = \frac{D}{\mu_e - \alpha^2 \mu_i}$$

where α is a ration of internal and external radiuses of a tube, τ_0, Ω_0 and D depend on material parameters and α, μ_e and μ_i are shear modules of external and internal phases. Shear stress τ increases on the path of the transformation if $\mu_i < \mu_e$, otherwise "effective shear modulus" $G_* < 0$ (Fig. 2a) or two phase deformation is unstable. The first way of the phase transformation is thermodynamically more preferential and shear strains γ in the tube are outside the PTZ except the phase boundary ($\gamma = \gamma^{\pm}$) which corresponds to the outer PTZ boundary (Fig. 2b). Shear strains in the two phase tube are inside the PTZ if $\mu_i > \mu_e$.

Our next example is a phase transformation of unbounded medium due to multiple appearance of new phase layers. Equilibrium volume concentration of a new phase, orientation of layers, directions of the anisotropy inside the layers are determined in the dependence on average strains. Energy changes and stability analysis shows that thermodynamically preferential piecewise constant strain fields correspond to the PTZ boundary. It is proved that the effective elasticity tensor can be not positive definite on the path of phase transformation.

5 CONCLUSIONS

On the whole presented considerations of heterogeneous deformation of solids due to phase transformations demonstrate the following:

– a phase transition zone can be constructed in strain space; the PTZ boundary acts as a phase diagram in strain space

– equilibrium new phase areas appearance is thermodynamically preferential in comparison with keeping one-phase state under the same boundary condition in displacements; a comparison between deformation fields in different two–phase configurations of an elastic body and PTZ gives additional reasons for the choice of the thermodynamically preferential configuration

– strains and stresses on the interface remain constant during the process of quasi–static phase transformation of an elastic body and equal to those ones in one-phase configurations at the beginning and at the end of transformation

– stress–strain diagrams for elastic solids undergoing phase transformations has the form of diagrams for an elastic–plastic materials; a body can demonstrate the strain softening effect on the path of phase transformation.

The developed models can be used in studies of martensite transformations and shape memory effects in smart materials, strain localization in the form of crazes and shear bands in glassy polymers.

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