

Two-phase deformations within the framework of phase transition zones

A.B. Freidin, E.N. Vilchevskaya, L.L. Sharipova *

Abstract

We analyze conditions on the equilibrium interface and develop the concept of phase transition zones (PTZ) formed in strain-space by all deformations which can exist on the equilibrium interface. The importance of the PTZ construction follows from the fact that deformations outside the PTZ cannot exist on the interface, whatever the loading conditions. The PTZ boundary acts as a phase diagram or yield surface in strain-space. We develop a general procedure for the PTZ construction and give examples for various nonlinear elastic materials and in a case of small strains. We study orientations of the interface and jumps of strains on the interface and demonstrate that various points of the PTZ correspond to different types of strain localization due to phase transformations on different loading path.

1 Introduction

From the mechanical point of view phase transitions in deformable solids result in the appearance of strain fields with interfaces which are the surfaces of discontinuity in deformation gradient at continuous displacements [10, 12, 11]. We analyze conditions on the equilibrium interface and develop the concept of phase transition zones (PTZ). The PTZ is formed in strain-space by all deformations which can exist on

*Institute of Mechanical Engineering Problems, Russian Academy of Sciences, St. Petersburg, Russia (e-mail: freidin@ipme.ru)

the equilibrium interface. The PTZ is determined entirely by properties of the strain energy function of a material. The importance of the PTZ construction follows from the fact that deformations outside the PTZ cannot exist on the interface, whatever the loading conditions. The PTZ boundary acts as a phase diagram or yield surface in strain-space.

We describe a general procedure for the PTZ construction [4, 5] and give examples for various nonlinear elastic materials. Then we develop a small strain approach to the theory of phase transitions in elastic solids. The problem is reduced to the analysis of the linear elasticity equations for heterogeneous medium with an additional condition of phase equilibrium on the interface. The thermodynamic condition takes the form of an equation that determines the normal to the interface in dependence on a tensor that acts as a dislocation momentum tensor induced by new phase areas.

Since the PTZ occurs naturally in the analysis of the local equilibrium conditions, any point of the PTZ can be associated with some piece-wise linear two-phase deformations. We study characteristic features of such deformations – orientation of the interface and the jump of strains. As a result we demonstrate that different passes of deformation lead to different types of strain localization due to phase transformations.

2 Preliminaries. Equilibrium phase boundaries and phase transition zones

We are interested in equilibrium deformation fields such that the displacements are twice differentiable everywhere in a body besides a continuously differentiable surfaces (interfaces) at which the deformation gradient suffers a jump at continuous displacement.

Let Γ be the prototype of the interface in a reference (undeformed) configuration of a body, $\mathbf{m} \in \mathcal{U}$ is the unit normal to Γ , \mathcal{U} denotes a set of unit vectors. The following conditions have to be satisfied on the

equilibrium interface:

$$[[\mathbf{F}]] = \mathbf{f} \otimes \mathbf{m}, \quad (2.1)$$

$$[[\mathbf{S}]]\mathbf{m} = 0, \quad (2.2)$$

$$[[W]] = \mathbf{f} \cdot \mathbf{S}_\pm \mathbf{m}, \quad (2.3)$$

where \mathbf{F} is the deformation gradient, W is the strain energy per unit reference volume (the elastic potential), $\mathbf{S} = W_{\mathbf{F}}(\mathbf{F})$ is the Piola stress tensor related with Cauchy stress tensor as $\mathbf{T} = J^{-1}\mathbf{S}\mathbf{F}^T$, $J = \det \mathbf{F} > 0$, brackets $[[\cdot]] = (\cdot)_+ - (\cdot)_-$ denote the jump of a function across Γ , super- or subscripts “ $-$ ” and “ $+$ ” identify the values on different sides of the shock surface.

The kinematic condition (2.1) follows from the continuity of the displacement [20]. The vector $\mathbf{f} = [[\mathbf{F}]]\mathbf{m}$ is called the amplitude. The traction continuity condition (2.2) follows from equilibrium considerations.

An additional thermodynamic condition (2.3) [10, 12, 19, 11, 2, 18] arises from an additional degree of freedom produced by free phase boundaries. One could also see (2.3) in [14].

By (2.1), the conditions (2.2) and (2.3) can be rewritten as

$$\begin{aligned} (\mathbf{S}(\mathbf{F} + \mathbf{f} \otimes \mathbf{m}) - \mathbf{S}(\mathbf{F}))\mathbf{m} &= 0, \\ W(\mathbf{F} + \mathbf{f} \otimes \mathbf{m}) - W(\mathbf{F}) &= \mathbf{f} \cdot \mathbf{S}(\mathbf{F})\mathbf{m} \end{aligned}$$

where $\mathbf{F} \equiv \mathbf{F}_-$. Given \mathbf{F} , the above equations can be considered as a system of four equations for five unknowns: the amplitude $\mathbf{f} \neq 0$ and the unit normal \mathbf{m} . Those \mathbf{F} only for which the system of equations can be solved can be on the interface.

Definition [4]. *The phase transition zone is formed by all deformations which can exist on a locally equilibrium phase boundary.*

For those \mathbf{F} inside the PTZ, there in general exists an one-parameter family of solutions for \mathbf{f} and \mathbf{m} .

It is known [13, 11] that the equilibrium deformation fields with the surfaces of discontinuity which satisfy (2.1) and (2.2) at $\mathbf{f} \neq 0$ can appear only if ordinary ellipticity of the equilibrium equations fails at some deformation. It can be shown [6] that if the condition (2.3) is added to (2.2) and a material is elliptic on the both sides of the

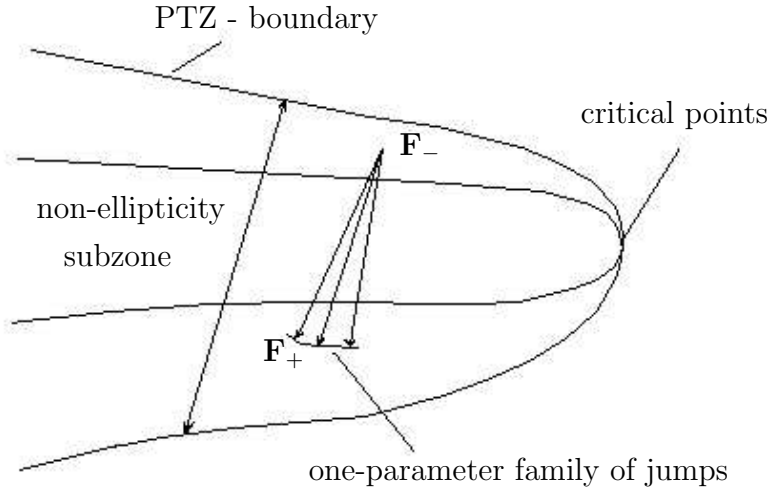


Figure 1: Phase transition zone in strain space.

interface then a material must be non-elliptic at some segment on the path

$$\mathbf{F}(\xi) = \mathbf{F}_- + \xi \mathbf{f} \otimes \mathbf{m} \quad (\xi \in (0, 1))$$

Thus, the PTZ contains the non-ellipticity sub-zone.

The PTZ is illustrated schematically by Fig. 1. The elements of the PTZ are the PTZ-boundary, non-ellipticity sub-zone, critical points (a bifurcation set). Deformations outside PTZ cannot exist on any phase boundary, whatever the loading conditions are. The PTZ boundary acts as a phase diagram or yield surface in strain space. As illustrated below, different points of the PTZ boundary correspond to different orientations of the interface and different types of jumps of strains on the interface, i.e. different types of strain localization. So, we endow a strain space with a structure relating to phase transitions. Note that equilibrium interface can appear during the deformation process much more earlier than the ellipticity fails.

3 Phase transition zones for isotropic nonlinear elastic materials

The conditions (2.1), (2.2), (2.3) can be rewritten as

$$\mathbf{F}_{\pm} = (\mathbf{I} + \mathbf{a}_{\mp} \otimes \mathbf{n}) \mathbf{F}_{\mp}, \quad (3.1)$$

$$[[\mathbf{T}]]\mathbf{n} = 0, \quad (3.2)$$

$$[[W]] = \mathbf{c} \cdot \mathbf{T}\mathbf{n} \quad (3.3)$$

where \mathbf{I} denotes the unit tensor, \mathbf{n} is the normal to the interface in the deformed configuration,

$$\mathbf{n} = |\mathbf{F}_{\mp}^{-T}\mathbf{m}|^{-1}\mathbf{F}_{\mp}^{-T}\mathbf{m}, \quad \mathbf{m} = |\mathbf{F}_{\mp}^T\mathbf{n}|^{-1}\mathbf{F}_{\mp}^T\mathbf{n}. \quad (3.4)$$

Amplitudes \mathbf{f} , \mathbf{a}_{\mp} and \mathbf{c} are related as

$$\mathbf{c} \triangleq JN_1^{-1/2}\mathbf{f} = J_-\mathbf{a}_- = J_+\mathbf{a}_+, \quad (3.5)$$

where $N_{1\mp} = |\mathbf{F}_{\mp}^T\mathbf{n}|^2 = \mathbf{n} \cdot \mathbf{B}_{\mp}\mathbf{n}$, $\mathbf{B} = \mathbf{F}\mathbf{F}^T$ is the left Cauchy-Green tensor, and, as can be shown [4], $[[JN_1^{-1/2}]] = 0$.

In a case of nonlinear elastic isotropic materials

$$W = W(I_1, I_2, J), \quad \mathbf{T} = \mu_0\mathbf{I} + \mu_1\mathbf{B} + \mu_{-1}\mathbf{B}^{-1}, \quad (3.6)$$

$$\mu_0 = W_3 + 2J^{-1}I_2W_2, \quad \mu_1 = 2J^{-1}W_1, \quad \mu_{-1} = -2JW_2, \quad (3.7)$$

where

$$\begin{aligned} I_1 &= \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = \text{tr } \mathbf{B}, \\ I_2 &= \lambda_1^2\lambda_2^2 + \lambda_1^2\lambda_3^2 + \lambda_2^2\lambda_3^2 = J^2\text{tr } \mathbf{B}^{-1}, \\ J &= \lambda_1\lambda_2\lambda_3 \end{aligned} \quad (3.8)$$

are the strain invariants, $\lambda_i > 0$ ($i = 1, 2, 3$) are the principal stretches, W_1, W_2, W_3 denote $\partial W/\partial I_1, \partial W/\partial I_2$ and $\partial W/\partial J$ respectively.

3.1 Orientation invariants

Further we will see that the normal \mathbf{n} appears in relationships through the *orientation invariants*

$$G_1 = \frac{N_1}{J^2}, \quad G_{-1} = \frac{I_2}{J^2} - N_{-1} \quad (N_k = \mathbf{n} \cdot \mathbf{B}^k\mathbf{n}, \quad k = \pm 1) \quad (3.9)$$

and the amplitude \mathbf{c} can be decomposed using the vectors

$$\mathbf{t}_1 = J^{-1}\mathbf{P}\mathbf{B}\mathbf{n}, \quad \mathbf{t}_{-1} = J\mathbf{P}\mathbf{B}^{-1}\mathbf{n} \quad (3.10)$$

where $\mathbf{P} = \mathbf{I} - \mathbf{n} \otimes \mathbf{n}$ is a projector.

If values of principal stretches are different then at given \mathbf{B} a couple of invariants G_1, G_{-1} determines the normal \mathbf{n} . Relative to the basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ of eigenvectors of \mathbf{B} we have the system of equations

$$\sum n_i^2 = 1, \quad \sum n_i^2 \lambda_i^2 = J^2 G_1, \quad \sum n_i^2 \lambda_i^{-2} = \frac{I_2}{J^2} - G_{-1} \quad (3.11)$$

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

Since the solution of the system (3.11) for n_i^2 has to be non-negative, the domain \mathcal{G} of admissible values for the orientation invariants G_1, G_{-1} is a triangle with vertexes lying on the parabola $J^2 G_1^2 - I_1 G_1 + G_{-1} = 0$ (Fig. 2).

The vertexes $(\lambda_i^{-2} \lambda_j^{-2}, \lambda_i^{-2} + \lambda_j^{-2})$ ($i \neq j$) correspond to $\mathbf{n} = \mathbf{e}_k$ ($k \neq i, j$), $\mathbf{t}_1 = \mathbf{t}_{-1} = 0$. On the $i - j$ - side of the triangle

$$G_{-1} = G_1 \lambda_k^2 + \lambda_k^{-2}, \quad n_k = 0 \quad (k \neq i, j) \quad (3.12)$$

corresponding normals \mathbf{n} lie in the $i - j$ - principal plane of \mathbf{B} , $\mathbf{t}_1 \parallel \mathbf{t}_{-1}$.

The triangle \mathcal{G} degenerates into the segment if $\lambda_1 = \lambda_2 \neq \lambda_3$ or the point if $\lambda_1 = \lambda_2 = \lambda_3$. Relations with the normals in the case are evident.

Due to the kinematical condition (2.1), the invariants G_1 and G_{-1} are continuous on the interface:

$$[[G_1]] = 0, \quad [[G_{-1}]] = 0 \quad (3.13)$$

The conditions (3.13) have obvious geometrical meanings. If da and dA denote surface elements in deformed and reference configurations then it is simple to check that $G_1 = (dA/da)^2$. Then (3.13)₁ means that $[[da]] = 0$ at given dA . Analogously, (3.13)₂ means that tangent line elements are continuous across a shock surface. For the plane case one can find (3.13)₁ in [13, 1].

3.2 Kinematic compatibility

From (3.1), (3.5) follows that

$$\mathbf{B}_+ = \mathbf{B}_- + J_-^{-1} (\mathbf{c} \otimes \mathbf{B}_- \mathbf{n} + \mathbf{B}_- \mathbf{n} \otimes \mathbf{c}) + G_{-1} \mathbf{c} \otimes \mathbf{c}, \quad (3.14)$$

$$\mathbf{B}_+^{-1} = \mathbf{B}_-^{-1} - J_+^{-1} ((\mathbf{n} \otimes \mathbf{B}_-^{-1} \mathbf{c} + \mathbf{B}_-^{-1} \mathbf{c} \otimes \mathbf{n})) + J_+^{-2} (\mathbf{c} \cdot \mathbf{B}_-^{-1} \mathbf{c}) \mathbf{n} \otimes \mathbf{n}. \quad (3.15)$$

From (3.1) also follows

$$\mathbf{c} = \llbracket J \rrbracket \mathbf{n} + \mathbf{h}, \quad \mathbf{h} \triangleq \mathbf{P} \mathbf{c}. \quad (3.16)$$

Then (3.14) – (3.15) lead to the following relationships between the strain and orientation invariants on the interface and \mathbf{h} :

$$\llbracket I_1 \rrbracket = G_1 \llbracket J^2 \rrbracket + 2\mathbf{h} \cdot \mathbf{t}_1^- + G_1 \mathbf{h} \cdot \mathbf{h}, \quad (3.17)$$

$$\llbracket I_2 \rrbracket = G_{-1} \llbracket J^2 \rrbracket - 2\mathbf{h} \cdot \mathbf{t}_{-1}^- + \mathbf{h} \cdot \mathbf{B}^{-1} \mathbf{h}. \quad (3.18)$$

3.3 Traction continuity condition

Projecting the traction condition (3.2) onto the normal \mathbf{n} and the plane tangent to the shock surface and taking into account (3.6) we obtain

$$\llbracket \mu_0 \rrbracket + \llbracket \mu_1 N_1 \rrbracket + \llbracket \mu_{-1} N_{-1} \rrbracket = 0, \quad (3.19)$$

$$\llbracket \mu_1 J \mathbf{t}_1 \rrbracket + \llbracket \mu_{-1} J^{-1} \mathbf{t}_{-1} \rrbracket = 0 \quad (3.20)$$

The condition (3.19) for the normal component of the traction can be rewritten as

$$-\llbracket W_3 \rrbracket = 2 \llbracket JW_1 \rrbracket G_1 + 2 \llbracket JW_2 \rrbracket G_{-1}. \quad (3.21)$$

The equation (3.20) for the tangent component of the traction takes the form of an equation for \mathbf{h} :

$$\mathbf{A}_+ \mathbf{h} = -\llbracket W_1 \rrbracket \mathbf{t}_1^- + \llbracket W_2 \rrbracket \mathbf{t}_{-1}^-, \quad \mathbf{A}_+ \triangleq G_1 W_1^+ \mathbf{I} + W_2^+ \mathbf{P} \mathbf{B}^{-1} \quad (3.22)$$

and leads to the

Representation theorem [4]. *Assume that the material is isotropic and on the shock surface the kinematic (3.1) and traction (3.2) conditions are satisfied and*

$$D_+ = G_1 (W_1^+)^2 + G_{-1} W_1^+ W_2^+ + (W_2^+)^2 \neq 0 \quad (3.23)$$

holds. Then the amplitude \mathbf{c} is an isotropic function of the strain tensor \mathbf{B}_- and the normal \mathbf{n} and can be decomposed as follows:

$$\mathbf{c} = \llbracket J \rrbracket \mathbf{n} + \mathbf{h}, \quad \mathbf{h} = \alpha \mathbf{t}_1^- + \beta \mathbf{t}_{-1}^- \quad (3.24)$$

where the coefficients α and β are uniquely given as functions of orientation and strain invariants by the system of linear equations

$$\begin{pmatrix} G_1 W_1^+ & W_2^+ \\ -G_1 W_2^+ & G_1 W_1^+ + G_{-1} W_2^+ \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} -\llbracket W_1 \rrbracket \\ \llbracket W_2 \rrbracket \end{pmatrix}, \quad (3.25)$$

The representation (3.24) remains true for incompressible materials; one needs only to set $J \equiv 1$.

There are physical and mathematical reasons to believe that the deformations cannot be observed if the Legendre-Hadamard condition fails. The Baker-Ericksen inequalities

$$W_1 + \lambda_k^2 W_2 > 0 \quad (k = 1, 2, 3) \quad (3.26)$$

are the necessary conditions for strong ellipticity of isotropic nonlinear elastic materials. If (3.26) holds on the interface then (3.23) is satisfied at any $G_1, G_{-1} \in \mathcal{G}$ and the amplitude is represented by (3.24), (3.25) [7, 8, 9].

3.4 Thermodynamic condition. Phase transition zone

The thermodynamic condition (3.3) takes the form

$$\llbracket W \rrbracket = \tau_n \llbracket J \rrbracket + 2W_1^- \mathbf{h} \cdot \mathbf{t}_1^- - 2W_2^- \mathbf{h} \cdot \mathbf{t}_{-1}^- \quad (3.27)$$

where the normal component of the traction

$$\tau_n = \mathbf{n} \cdot \mathbf{T} \mathbf{n} = 2J(G_1 W_1 + G_{-1} W_2) + W_3 \quad (3.28)$$

can be calculated at any side of the phase boundary.

If α and β are given by the system (3.25), then substituting the representation (3.24) into (3.17), (3.18), (3.21) and (3.27) gives four equations for five unknowns I_1^+ , I_2^+ , J_+ , G_1 and G_{-1} . So, the jump

solution compatible with kinematic, traction and thermodynamic conditions, if it exists at given I_1^-, I_2^-, J_- , has a form of an one-parameter family.

If we solve three of the equations for $I_1^+ = I_1^+(G_1, G_{-1} | I_1^-, I_2^-, J_-)$, $I_2^+ = I_2^+(G_1, G_{-1} | I_1^-, I_2^-, J_-)$, $J_+ = J_+(G_1, G_{-1} | I_1^-, I_2^-, J_-)$, then the fourth equation takes the form of an equation for the one-parameter family of the orientation invariants:

$$\Psi(G_1, G_{-1} | I_1^-, I_2^-, J_-) = 0. \quad (3.29)$$

Since $G_1, G_{-1} \in \mathcal{G}_-$, the invariants J_- , I_1^- and I_2^- have to satisfy inequalities

$$\min_{G_1, G_{-1} \in \mathcal{G}_-} \Psi(G_1, G_{-1}, J_-, I_1^-) \leq 0 \leq \max_{G_1, G_{-1} \in \mathcal{G}_-} \Psi(G_1, G_{-1}, J_-, I_1^-). \quad (3.30)$$

The one-parameter family of normals is represented on the G_1, G_{-1} -plane by the intersection of the line (3.29) (the line ab on Fig. 2) with the triangle \mathcal{G} . The phase transition zone in $\lambda_1, \lambda_2, \lambda_3$ -space is formed by all principal stretches at which the intersection is non-empty. If $(\lambda_{1-}, \lambda_{2-}, \lambda_{3-})$ belongs to the PTZ boundary then the line of the solution passes through a single point of \mathcal{G}_- , i.e. passes through the vertex or externally touches the side of the triangle (the lines pq and cd on Fig. 2). In these cases the normal coincides with an eigenvector of \mathbf{B}_- or lies in a principal plane of \mathbf{B}_- ; the one-parameter character of the solution disappears.

To illustrate the PTZ in a case of finite strains construction we consider below two examples.

3.4.1 Phase transition zones for the Hadamard material

The strain energy function for the Hadamard material has the form

$$W = \frac{c}{2}I_1 + \frac{d}{2}I_2 + \Phi(J), \quad c \geq 0, \quad d \geq 0, \quad c + d \neq 0. \quad (3.31)$$

General analysis of the PTZ construction for the Hadamard material was carried out in [4]. Below we give some illustrations.

Since $[[W_1]] = [[W_2]] = 0$, the representation theorem (see (3.25)) gives

$$\mathbf{h} = 0, \quad \mathbf{c} = [[J]]\mathbf{n} \quad (3.32)$$

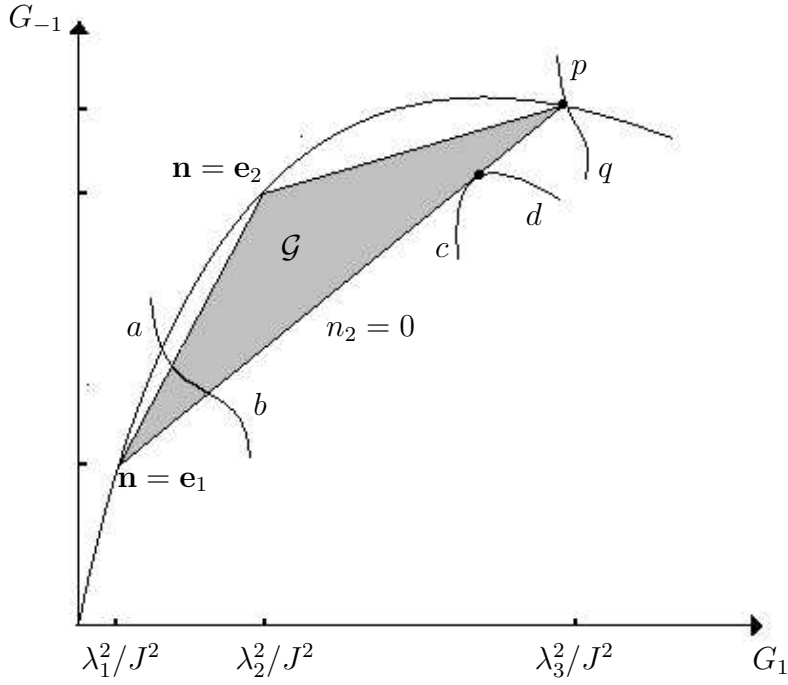


Figure 2: Admissible values domain \mathcal{G} for the orientation invariants and lines of solutions.

The condition (3.21) for the normal component of traction and the thermodynamic condition (3.27) take the form

$$cG_1 + dG_{-1} = U(J_+, J_-), \quad U(J_+, J_-) \triangleq -\frac{[\Phi']}{[J]}, \quad (3.33)$$

$$[W] = (J_-(cG_1 + dG_{-1}) + \Phi') [J] \quad (\Phi' = \frac{d\Phi}{dJ}) \quad (3.34)$$

Substituting (3.32) into kinematic relationships (3.17), (3.18) gives

$$[I_1] = [J^2]G_1, \quad [I_2] = [J^2]G_{-1} \quad (3.35)$$

Since

$$[W] = \frac{c}{2}[I_1] + \frac{d}{2}[I_2] + [\Phi(J)],$$

from (3.33) – (3.35) follows

$$\frac{1}{2}(\Phi'_+ + \Phi'_-)(J_+ - J_-) - (\Phi_+ - \Phi_-) = 0 \quad (3.36)$$

The equation (3.36) can be solved for $J_+ = J_+(J_-)$. Then (3.33) takes the form of the equation that determines the one-parameter family of normals

$$cG_1 + dG_{-1} = u(J), \quad u(J) = U(J_+(J), J), \quad G_1, G_{-1} \in \mathcal{G}_- \quad (3.37)$$

The left part of the equation (3.37) is linear in G_1, G_{-1} and reaches the minimal and maximal values in vertexes of the triangle \mathcal{G} . If $\lambda_1 < \lambda_2 < \lambda_3$ then

$$\begin{aligned} \min_{G_1, G_{-1} \in \mathcal{G}} (cG_1 + dG_{-1}) &= h(\lambda_2, \lambda_3), \quad \mathbf{n} = \mathbf{e}_1 \\ \max_{G_1, G_{-1} \in \mathcal{G}} (cG_1 + dG_{-1}) &= h(\lambda_2, \lambda_1), \quad \mathbf{n} = \mathbf{e}_3 \\ h(\lambda_i, \lambda_j) &= \frac{c}{\lambda_i \lambda_j} + d \left(\frac{1}{\lambda_i} + \frac{1}{\lambda_j} \right) \end{aligned}$$

Thus, the strains inside the PTZ satisfy the inequalities

$$h(\lambda_2, \lambda_3) \leq u(J) \leq h(\lambda_2, \lambda_1). \quad (3.38)$$

The typical PTZ cross-section by the plane $\lambda_2 = const$ is shown on the Fig. 3. For the simplicity sake we take $\Phi(J)$ in a form

$$\Phi(J) = \frac{(J - J_c)^4}{4} - \frac{A(J - J_c)^2}{2} + a(J - J_c). \quad (3.39)$$

Note that $W \rightarrow \infty$ at $J \rightarrow 0$ but one can consider (3.39) as an approximation of Φ in the vicinity of J_c . Since $J_+ > J_c$ if $J_- < J_c$ on the interface [4], we take $J_c > 1$ and do not consider the behavior of the material at small J .

Thick lines denote the PTZ boundaries, dotted lines bound the non-ellipticity sub-zone. If the point A is reached during the deformation, the interface with the normal directed as \mathbf{e}_1 becomes possible. The coexistent deformations on the interface are represented by the points

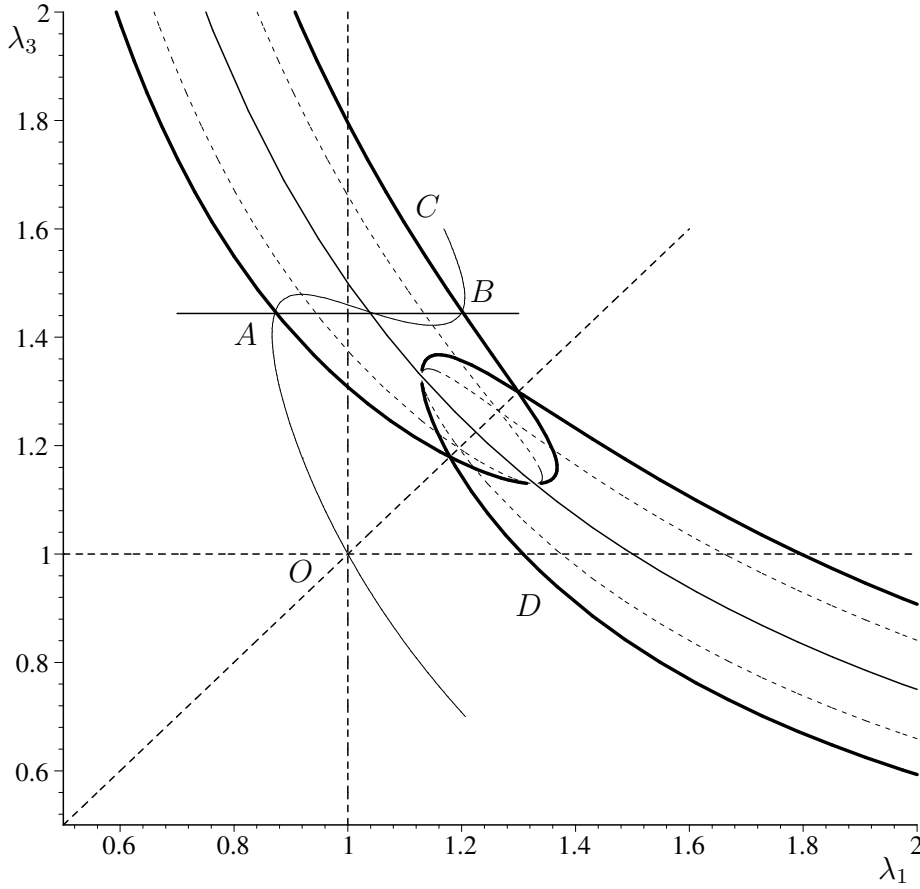


Figure 3: PTZ for the Hadamard material ($J_c = 1.45$, $A = 0.3$, $d = 0.155$, $c = 0.03$).

A and B . Only λ_1 jumps on the interface. If the point D is reached, the normal is directed as \mathbf{e}_3 , λ_3 jumps on the interface.

The line OAC represents the path of plane stretching in the “3”-direction in a case of uniform deformation - without the separation into two phases. In this case

$$\lambda_2 = 1, \quad \lambda_1 = \Lambda(\lambda_3)\lambda_3, \quad \tau_1(\lambda_1, \lambda_3) = 0 \quad (3.40)$$

where τ_1 is the principal Cauchy stress and the function $\Lambda(\lambda_3)$ is found from the condition $(3.40)_3$.

One can see that instead of passing through the non-ellipticity

sub-zone the sample can be divided into two phases before the non-ellipticity zone is reached. If A corresponds to the deformation on one side of the interface, then $\mathbf{n} = \mathbf{e}_1$ and B corresponds to the deformations on the other side. Since τ_1 remains to be zero after the plane interface (interfaces) appear, the condition (3.40)₃ does not fail because of internal stresses. Thus, the point B must belong to the curve OAC . The role of internal stresses produced by phase transformations is demonstrated in the example given below.

3.4.2 Phase transition zones construction for compressible materials with strain energy depending on two strain invariants

Let $W = W(I_\alpha, J)$ ($\alpha = 1$ or 2). Then, by (3.24), (3.25), (3.17) and (3.18)

$$\mathbf{h} = -\frac{[[W_\alpha]]}{W_{\alpha+}^+ G_1} \mathbf{t}_1^-, \quad (3.41)$$

$$[[I_1]] = G_1 [[J^2]] - \frac{[[W_\alpha^2]]}{W_{\alpha+}^2} L_1^-, \quad [[I_2]] = G_{-1} [[J^2]] - \frac{[[W_\alpha^2]]}{W_{\alpha+}^2} L_2^-, \quad (3.42)$$

$$L_1 = I_1 - J^2 G_1 - G_{-1} G_1^{-1}, \quad L_2 = I_2 - J^2 G_{-1} - G_1^{-1}, \quad (3.43)$$

If $W = W(I_1, J)$ then the conditions (3.21) and (3.27) take the form

$$2G_1 [[JW_1]] = -[[W_3]], \quad (3.44)$$

$$[[W]] = \frac{W_1^- W_3^+ + W_1^+ W_3^-}{W_1^- + W_1^+} [[J]] + \frac{2W_1^- W_1^+}{W_1^- + W_1^+} [[I_1]]. \quad (3.45)$$

Relationships (3.42)₁, (3.44) and (3.45) are three equations for the four unknowns J_+ , I_1^+ , G_1 and G_{-1} . If we solve (3.44) and (3.45) to obtain

$$J_+ = J_+(G_1, J_-, I_1^-), \quad I_1^+ = I_1^+(G_1^-, J_-, I_1^-), \quad (3.46)$$

and substitute the expressions into (3.42), we derive an equation in the form

$$\Psi \triangleq \Psi_1(G_1, J_-, I_1^-) + \Psi_2(G_1, J_-, I_1^-) G_{-1} = 0. \quad (3.47)$$

The equation (3.47) determines a line of one-parameter solutions on the G_1, G_{-1} -plane.

The invariants J_- and I_1^- have to satisfy inequalities

$$\begin{aligned}\Psi_{min}(J_-, I_1^-) &\leq 0 \leq \Psi_{max}(J_-, I_1^-), \\ \Psi_{min}(J_-, I_1^-) &= \min_{G_1, G_{-1} \in \mathcal{G}_-} \Psi(G_1, G_{-1}, J_-, I_1^-), \\ \Psi_{max}(J_-, I_1^-) &= \max_{G_1, G_{-1} \in \mathcal{G}_-} \Psi(G_1, G_{-1}, J_-, I_1^-).\end{aligned}$$

Since $\Psi(G_1, G_{-1}, J_-, I_1^-)$ is linear in G_{-1} , its maximal and minimal values are reached at the boundary of \mathcal{G}_- . The corresponding normal lies in the principal planes of \mathbf{B}_- or coincide with the eigenvector of \mathbf{B}_- . Thus, three types of strain localization due to phase transitions can be expected if the interface corresponds to the PTZ boundary: (1) the interface is analogous to the shear band, plane jump of strains takes place on the interface, (2) the interface is perpendicular to the direction of the maximal stretch, only the maximal stretch suffers a jump on the phase boundary, (3) the interface is perpendicular to the direction of the minimal stretch that suffers a jump.

Materials with a potential $W = W(I_2, J)$ may be considered analogously.

Let

$$W(I_1, J) = V(I_1) + \Phi(J) \quad (3.48)$$

where

$$\begin{aligned}V(I_1) &= \begin{cases} c_1 I_1, & I_1 \in (0, I_c) \\ c_2(I_1 - I_c) + c_1 I_c, & I_1 \in (I_c, \infty) \end{cases}, \quad c_1 > c_2, \\ \Phi(J) &= aJ^2 + bJ + c\end{aligned} \quad (3.49)$$

where the coefficient $a > 0$ characterize the reaction of the material with respect to volume changing. A ‘‘kink’’ in a point $I_1 = I_c$ replaces the non-ellipticity sub-zone.

The conditions on the equilibrium interface (3.42)₁, (3.44) and (3.45) take the form

$$[I_1] = (\gamma^2 - 1)G_1 J_-^2 + (k^2 - 1)L_1^- \quad (3.50)$$

$$-A(\gamma - 1) = (\gamma - k)G_1 \quad (3.51)$$

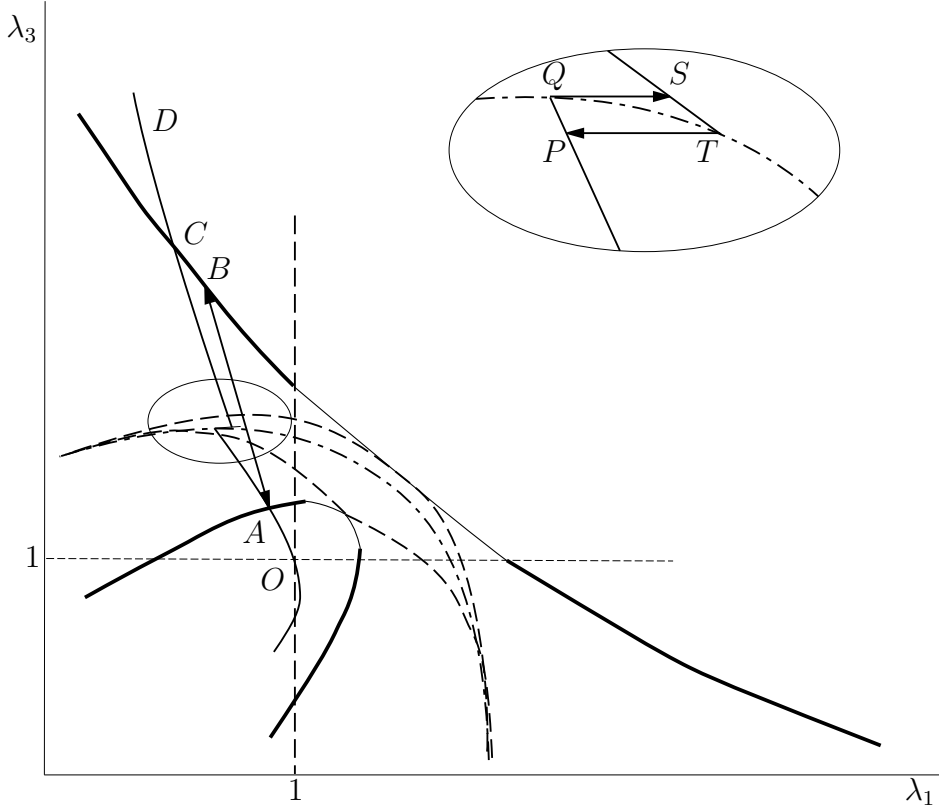


Figure 4: PTZ for the model material in a plane case.

$$[I_1] = (k + 1)(I_c - I_1^-) - AJ_-^2(\gamma - 1)^2 \quad (3.52)$$

where $\gamma = J_+/J_-$, $k = c_1/c_2$, $A = a/c_2$ and L_1 is determined by (3.43)₁.

The equation (3.51) can be solved for $\gamma = \gamma(G_1)$. Then substituting (3.50) into (3.52) leads to the following relationship for the orientation invariants

$$\frac{J_-^2 G_1^2}{A + G_1} + L_1^- = \frac{I_c - I_1^-}{k - 1} \quad (3.53)$$

The “-”- PTZ subzone is determined by the inequalities

$$\min_{G_1, G_{-1} \in \mathcal{G}} \frac{J_-^2 G_1^2}{A + G_1} + L_1^- \leq \frac{I_c - I_1^-}{k - 1} \leq \max_{G_1, G_{-1} \in \mathcal{G}} \frac{J_-^2 G_1^2}{A + G_1} + L_1^- \quad (3.54)$$

The “+”- subzone is constructed analogously.

The PTZ cross-section for the material (3.48) is shown at Fig. 4 at $A > k$. The dot-and-dash line corresponds to $I_1 = I_c$. Thick lines correspond to “shear bands”. In this case the normal to the interface lies in a plane of maximal and minimal stretches. A shear parameter contributes to the jump of strains.

If thin lines are reached then the interfaces may appear which are perpendicular to the direction of the maximal principal stretch, and only this stretch suffers a jump.

Dotted lines denote internal PTZ boundaries. Corresponding interfaces are perpendicular to the direction of minimal stretching. Thus, depending on the deformation path various types of strain localization are possible due to phase transformations.

The competition between the types of the interfaces also depends on the material parameters. If $A \gg k$ then interfaces of shear band type are preferential if the PTZ boundary is reached. The angle between the interface and the direction of the maximal stretch is about $\pi/4$. If the parameter A decreases then the angle increases, and interfaces perpendicular to the direction of maximal stretching can also appear.

At $A \approx k$ the difference between two types of the interfaces disappears. If $A < A_*$ then only the interfaces perpendicular to the maximal stretching correspond to the PTZ boundary, where A_* depends on k and I_c .

The line $OACD$ represents plane stretching in the “3”- direction in a case of uniform deformation - without the separation into two phases. Note that in the vicinity of the line $I = I_c$ the behavior at loading and unloading includes hysteresis $PQST$. Similar to the Hadamard material, two-phase deformation can appear before the line $I = I_c$ is reached.

Since the PTZ construction arises from the analysis of the local equilibrium conditions, every point of the PTZ corresponds to some piece-wise linear two-phase deformation with plane interfaces. Points A and B represent such a deformation. If the point A is reached on the path OAQ , one can suppose that a thin layer of the phase “+” appears in an unbounded media and the point B corresponds to the deformation inside the layer.

Because of internal stresses acting in the “1” - direction inside the layer, the condition (3.40)₃ fails. That is why the point B does not

belong to the curve DCS , in contrast to the Hadamard material. Analogously, if the point C is reached on the path DCS , appearance of the layer of the phase “-” surrounded by the phase “+” can be assumed.

In conclusion note that we do not study here how the phase “-” transforms into the phase “+”. In a case of heterogeneous deformation due to multiple appearance of a new phase areas average deformations are prescribed by boundary conditions. Two-phase structures have to be found but the local deformations on the interfaces belong to the PTZ.

4 Equilibrium phase boundaries in a case of small strains

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

$$[[\mathbf{u}]] = 0, \quad \mathbf{x} \in \Gamma \quad (4.1)$$

and satisfying boundary conditions, thermal condition $\theta = \text{const}$, and equilibrium conditions

$$\mathbf{x} \notin \Gamma : \quad \text{Div } \boldsymbol{\sigma} = 0, \quad (4.2)$$

$$\mathbf{x} \in \Gamma : \quad [[\boldsymbol{\sigma}]]\mathbf{n} = 0, \quad [[f]] - \boldsymbol{\sigma} : [[\boldsymbol{\varepsilon}]] = 0 \quad (4.3)$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the stress and strain tensors, θ is the temperature, $f(\boldsymbol{\varepsilon}, \theta)$ is the volume free energy density represented by a number of quadratic function of $\boldsymbol{\varepsilon}$.

Further, for the sake of simplicity, we consider two-branches free energy function

$$f(\boldsymbol{\varepsilon}, \theta) = \min_{-,+} \{f^-(\boldsymbol{\varepsilon}, \theta), f^+(\boldsymbol{\varepsilon}, \theta)\}, \quad (4.4)$$

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

The constitutive equations take the form:

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}) = \mathbf{C}_\pm : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_\pm^p) \quad (4.5)$$

Parameters \mathbf{C}_\pm , f_0^\pm , $\boldsymbol{\varepsilon}_\pm^p$ are the elasticity tensors, free energy densities and strain tensors in unstressed phases “ \pm ”. If $\boldsymbol{\varepsilon}_+^p = 0$, then $[\boldsymbol{\varepsilon}^p] \equiv \boldsymbol{\varepsilon}^p$ is the self-strain tensor. Body forces and thermoelastic effects are not taken into account. Twinning also is not studied here.

It follows from (4.1), (4.3)₁, (4.5), that [16, 6]

$$\begin{aligned} [\boldsymbol{\varepsilon}] &= \mathbf{K}_\mp(\mathbf{n}) : \mathbf{q}_\pm, \quad \mathbf{q}_\pm = -\mathbf{C}_1 : \boldsymbol{\varepsilon}_\pm + [\mathbf{C} : \boldsymbol{\varepsilon}^p], \\ \mathbf{K}_\pm(\mathbf{n}) &= \{\mathbf{n} \otimes \mathbf{G}_\pm \otimes \mathbf{n}\}^s, \quad \mathbf{G}_\pm = (\mathbf{n} \cdot \mathbf{C}_\pm \cdot \mathbf{n})^{-1}, \quad \mathbf{C}_1 = \mathbf{C}_+ - \mathbf{C}_-, \end{aligned} \quad (4.6)$$

s means the symmetrization: $K_{ijkl} = n_{(i}G_{j)(k}n_{l)}$. Substituting (4.4), (4.5) and (4.6) into (4.3)₂ brings the thermodynamic condition to the form [15, 6]

$$2\gamma + [\boldsymbol{\varepsilon}^p : \mathbf{C} : \boldsymbol{\varepsilon}^p] + \boldsymbol{\varepsilon}_\pm : \mathbf{C}_1 : \boldsymbol{\varepsilon}_\pm - 2\boldsymbol{\varepsilon}_\pm : [\mathbf{C} : \boldsymbol{\varepsilon}^p] \pm \mathbf{q}_\pm : \mathbf{K}_\mp(\mathbf{n}) : \mathbf{q}_\pm = 0 \quad (4.7)$$

where $\gamma = [f_0(\theta)]$ acts as temperature in absence of thermal stresses. So, the system of equations is split. Given γ , any of two equations (4.5) determines one-parametric family of unit normals depending on strains on one side (“+” or “-”) of the interface. Strains on the other side can be computed by formulas (4.6).

If tensor \mathbf{C}_1 is nonsingular, the equations (4.7) can be rewritten in q -space:

$$\begin{aligned} K_\mp(\mathbf{q}_\pm, \mathbf{n}) &= \mp\varphi(\mathbf{q}_\pm), \\ K_\pm(\mathbf{q}, \mathbf{n}) &= \mathbf{q} : \mathbf{K}_\pm(\mathbf{n}) : \mathbf{q}, \quad \varphi(\mathbf{q}) = 2\gamma_* + \mathbf{q} : \mathbf{C}_1^{-1} : \mathbf{q}, \\ \gamma_* &= \gamma + \frac{1}{2}[\boldsymbol{\varepsilon}^p] : \mathbf{B}_1^{-1} : [\boldsymbol{\varepsilon}^p], \quad \mathbf{C}_1 = \mathbf{C}_+ - \mathbf{C}_-, \quad \mathbf{B}_1 = \mathbf{B}_+ - \mathbf{B}_-, \quad \mathbf{B} = \mathbf{C}^{-1}. \end{aligned} \quad (4.8)$$

Strains for which the equation (4.7) or (4.8) can be solved for the unit normal \mathbf{n} form the phase transition zone in $\boldsymbol{\varepsilon}$ - or q -space. Note that the equation $\varphi(\mathbf{q} = 0)$ determines the surface of discontinuity in the derivative of $f(\boldsymbol{\varepsilon})$ where $f^+(\boldsymbol{\varepsilon}) = f^-(\boldsymbol{\varepsilon})$.

The PTZ is divided into sub-zones \mathcal{Q}_\pm . By (4.8), tensors $\mathbf{q}_\pm \in \mathcal{Q}_\pm$ satisfy inequalities

$$\begin{aligned} \mathcal{K}_{\min}^\mp(\mathbf{q}_\pm) &\leq \mp\varphi(\mathbf{q}_\pm) \leq \mathcal{K}_{\max}^\mp(\mathbf{q}_\pm), \\ \mathcal{K}_{\max}^\mp(\mathbf{q}_\pm) &= \max_{\mathbf{n}} \mathcal{K}_\mp(\mathbf{q}, \mathbf{n}), \quad \mathcal{K}_{\min}^\mp(\mathbf{q}_\pm) = \min_{\mathbf{n}} \mathcal{K}_\mp(\mathbf{q}_\pm, \mathbf{n}). \end{aligned} \quad (4.9)$$

The normals $\mathbf{n}_{ex}^{\pm}(\mathbf{q})$ and $\mathbf{n}_{in}^{\pm}(\mathbf{q})$ afford a maximum and a minimum to $\mathcal{K}_{\mp}(\mathbf{q}_{\pm}, \mathbf{n})$, respectively, and correspond to the external and internal boundaries of the sub-zones \mathcal{Q}_{\pm} [17, 6]. Note that the tensor \mathbf{q}^+ can be related with the tensor of the dislocation moments induce by new phase areas [16].

If phase “-” is isotropic, maximal and minimal values of $\mathcal{K}_-(\mathbf{q}^+, \mathbf{n})$ as well as corresponding normals depend on relations between the eigenvalues q_i of \mathbf{q}_+ [3, 17, 6]. Let $q_1 \leq q_2 \leq q_3$, $q_1 \neq q_3$, $|q|_{\min}$, $|q|_{\max}$ are the minimal and maximal absolute values of the eigenvalues, $\mathbf{e}_{|q|_{\min}}$, $\mathbf{e}_{|q|_{\max}}$ are the corresponding eigenvectors, n_i are the components of the normal \mathbf{n} in the basis of eigenvectors of \mathbf{q}_+ .

If $q_1 q_3 < 0$ or $q_1 q_3 > 0$, $(1 - \nu_-)|q|_{\min} < \nu_-|q|_{\max}$, then

$$n_3^2 = \frac{(1 - \nu_-)q_3 - \nu_-q_1}{q_3 - q_1}, \quad n_2 = 0,$$

$$\mu_- \mathcal{K}_{\max}^-(\mathbf{q}_+) = \frac{1 - \nu_-}{2}(q_1^2 + q_3^2) - \nu_-q_1q_3.$$

The plane jump of strains similar to shearing takes place on the interface.

In the other case

$$\mathbf{n}_{ex}(\mathbf{q}_+) = \mathbf{e}_{|q|_{\max}}, \quad \mathcal{K}_{\max}^-(\mathbf{q}_+) = \frac{1 - 2\nu_-}{2\mu_-(1 - \nu_-)}|q|_{\max}^2. \quad (4.10)$$

Only maximal eigenvalue of the strain tensor suffers a jump on the interface.

At minimal value of $\mathcal{K}_-(\mathbf{q}^+, \mathbf{n})$

$$\mathbf{n}_{in}(\mathbf{q}_+) = \mathbf{e}_{|q|_{\min}}, \quad \mathcal{K}_{\max}^-(\mathbf{q}_+) = \frac{1 - 2\nu_-}{2\mu_-(1 - \nu_-)}|q|_{\min}^2. \quad (4.11)$$

Only minimal eigenvalue of the strain tensor suffers a jump.

Thus, if \mathbf{q}_+ on the interface belongs to the external PTZ boundary then, depending on a relation between eigenvalues of \mathbf{q}_+ , the normal \mathbf{n} lies in the 1 – 3 – principal plane of the tensor \mathbf{q}_+ or coincides with the eigenvector $\mathbf{e}_{|q|_{\max}}$. On the internal PTZ boundary (4.11) holds. Thus, only plane or one-dimensional jumps of strains take place on the interface if the interface corresponds to the PTZ boundary.

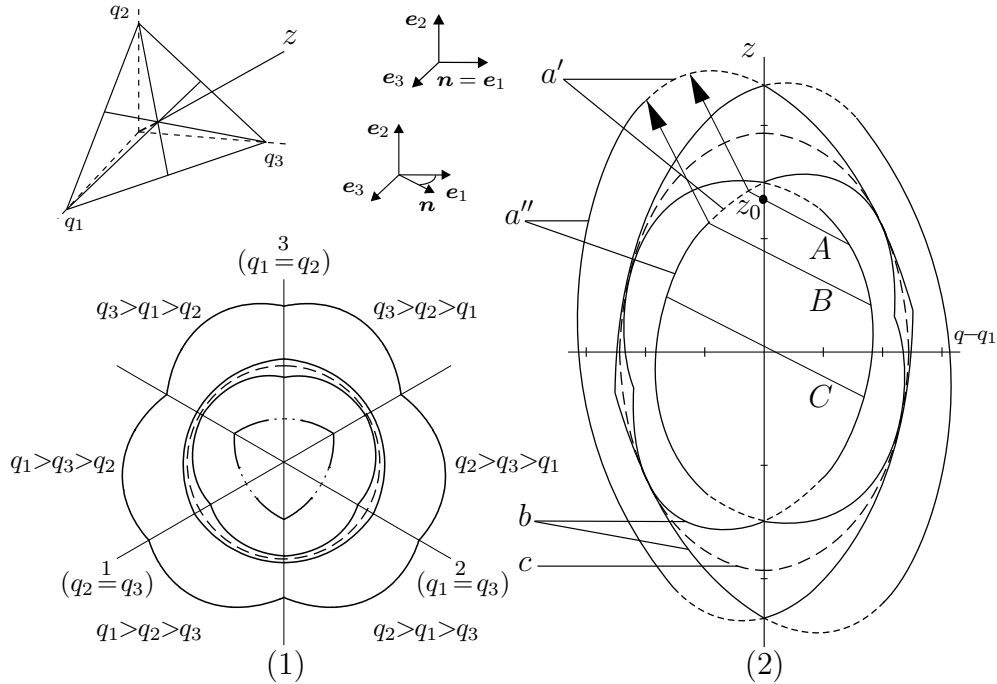


Figure 5: PTZ cross-sections: (1) - by the plane $tr \mathbf{q} = const$, (2) - by the plane $q_2 = q_3 = q$; a' and a'' - external PTZ boundaries; b - internal PTZ boundaries; c - the surface of discontinuity in the derivative of $f(\boldsymbol{\varepsilon})$; z_0 corresponds to the undeformed state.

The PTZ cross-sections for the case of isotropic phases ($\boldsymbol{\varepsilon}^p$ is a spherical tensor) are shown in Fig. 5. Depending on strain state, different orientations of the interface and different types of jumps of strains are possible. The line A in the Fig. 5(2) corresponds to uniaxial stretching – compression. When the path of deformation crosses the PTZ boundary, the interface perpendicular to the direction of stretching can appear at stretching and the “shear band” type interface appears at uniaxial compression. The lines B and C correspond to uniaxial deformations under pressure. Only “shear band” type interfaces can appear if pressure is more than some critical value.

Acknowledgements

The help of the student M. Stepanenko is gratefully acknowledged. This work is supported by the Russian Foundation for Basic Research (Grants No. 01-01-00324, 02-01-06263) and the Program of Ministry of Industry and Sciences of Russian Federation (Project No. 40.010.1 1.1195).

References

- [1] R. Abeyaratne and J.K. Knowles, *Equilibrium shocks in plane deformation of incompressible elastic materials*. J. Elasticity **22** (1989) 63–92.
- [2] R.L. Fosdick and B. Hertog, *The Maxwell relation and Eshelby's conservation law for minimizers in elasticity theory*. J. Elasticity **22** (1989) 193–200.
- [3] A.B. Freidin, *Crazes and shear bands in glassy polymer as layers of a new phase*. Mekhanika Kompozitnih Materialov, No. 1, 3-10 (1989). (Mechanics of Composite Materials, 1-7 (1989)).
- [4] A.B. Freidin and A.M. Chiskis, *Phase transition zones in nonlinear elastic isotropic materials. Part 1: Basic relations*. Izv. RAN, Mekhanika Tverdogo Tela (Mechanics of Solids) **29** (1994) No. 4, 91–109.
- [5] A.B. Freidin and A.M. Chiskis, *Phase transition zones in nonlinear elastic isotropic materials. Part 2: Incompressible materials with a potential depending on one of deformation invariants*. Izv. RAN, Mekhanika Tverdogo Tela (Mechanics of Solids) **29** (1994) No. 5, 46–58.
- [6] A.B. Freidin, *Small strains approach to the theory on solid-solid phase transformations under the process of deformation*. Studies on Elasticity and Plasticity (St. Petersburg State University) **18** (1999) 266-290 (in Russian).
- [7] A.B. Freidin, E.M. Croitoro *deformations with discontinuous gradients and ellipticity of isotropic hyperelastic materials*. 1st Canadian Conference on Nonlinear Solids Mechanics. Victoria, BS, Canada, June 16–June 20, 1999. Proceedings. Vol. 2, 670-681.

- [8] A.B. Freidin, *On phase equilibrium in nonlinear elastic materials*. Nonlinear problems of continuum mechanics. Izvestia Vuzov. North-Caucasus region (2000) 150-168 (in Russian)
- [9] A.B. Freidin, *Two-phase deformation fields and ellipticity of nonlinear elastic materials*. Proceed. of the XXVIII Summer School "Actual Problems in Mechanics", St.Petersburg, Russia, June 1-10, 2000. Vol. 1, 219-235 (2001)
- [10] M.A. Grinfeld, *On conditions of thermodynamic equilibrium of the phases of a nonlinear elastic material*. Dokl. Acad. Nauk SSSR **251** (1980) 824–827.
- [11] M.E. Gurtin, *Two-phase deformations of elastic solids*. Arch. Rat. Mech. Anal. **84** (1983) 1–29.
- [12] R.D. James, *Finite deformation by mechanical twinning*. Arch. Rat. Mech. Anal. **77** (1981) 143–177.
- [13] J.K. Knowles and E. Sternberg, *On the failure of ellipticity and the emergence of discontinuous deformation gradients in plane finite elastostatics*. J. Elasticity **8** (1978) 329–379.
- [14] J.K. Knowles, *On the dissipation associated with equilibrium shocks in finite elasticity*. J. Elasticity **9** (1979) 131–158.
- [15] L.B. Kublanov and A.B. Freidin, *Solid phase seeds in a deformable material*. Prikladnaia Matematika i Mekhanika, **52** (1988), 493-501. (Journal of Applied Mathematics and Mechanics (PMM U.S.S.R.), **52** (1988), 382-389).
- [16] I.A.Kunin. *Elastic Media with Microstructure II*. Springer-Verlag, Berlin, New York, etc. (1983).
- [17] N.F. Morozov and A.B. Freidin, *Phase transition zones and phase transformations of elastic solids under different stress states*. Proceedings of the Steklov Mathematical Institute **223** (1998) 220–232.
- [18] V.G. Osmolovsky, *Variational problem on phase transitions in mechanics of solids*. St. Petersburg State University, St. Petersburg (2000) (in Russian).

- [19] L. Truskinovsky, *Equilibrium interphase boundaries*. Dokl. Acad. Nauk SSSR **265** (1982) 306–310.
- [20] G. Truesdell, *A First Course in Rational Continuum Mechanics*. The Johns Hopkins University, Baltimore, Maryland (1972).

Dvofazne deformacije unutar zona faznih prenosa

UDK 531.01, 532.59, 536.76

Analiziramo uslove na ravnotežnu medjugranicu i razvijamo koncept zone faznog prenosa (PTZ) koja se formira u deformacionom prostoru za sve deformacije koje postoje na ravnotežnoj medjugranici. Važnost PTZ-konstrukcije sledi iz činjenice da deformacije van PTZ ne mogu da koegzistiraju na medjugranici bez obzira kakvi su uslovi opterećenja. PTZ-medjugranica deluje kao fazni dijagram ili površ tečenja u deformacionom prostoru. Dalje razvijamo opšti postupak za PTZ-konstrukciju i dajemo primere za različite nelinearne elastične materijale kao i slučaj malih deformacija. Proučavamo orijentacije medjugranice i skokove deformacija na medjugranici. Takođe pokazujemo da različite tačke na PTZ odgovaraju različitim tipovima deformacione lokalizacije uzrokovanim faznim transformacijama na različitim putevima opterećenja.