Phase transition zones for one class of nonlinear elastic materials

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Abstract

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. The analysis of the conditions on the equilibrium interface leads to the concept of phase transition zones (PTZ). The PTZ is formed in strain-space by all deformations which can exist on the equilibrium interface. Deformations outside PTZ cannot be on any interface whatever the loading conditions are. The PTZ boundary acts as a phase diagram or yield surface in strain-space. Various points of the PTZ boundary correspond to different types of strain localization due to phase transformations on different loading path.

We develop a procedure for the PTZ construction for nonlinear elastic materials with strain energy functions depending only on the first and third strain invariants. The procedure is specified for the case of a model material with the strain energy represented as the sum of a piece-wise linear function of the first invariant and quadratic function of the third invariant. The example demonstrates that different types of strain localization are possible due to phase transformations on different loading paths. We study in detail the competition between different types of interfaces depending on material parameters and a deformation path.

1 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, $\mathbf{m}$ is the unit normal to Γ. The following conditions have to be satisfied on the equilibrium interface:

$$[\![\mathbf{F}]\!] = \mathbf{f} \otimes \mathbf{m}, \tag{1}$$

$$[\![\mathbf{S}]\!]\mathbf{m} = 0, \tag{2}$$

$$[\![W]\!] = \mathbf{f} \cdot \mathbf{S}_{\pm}\mathbf{m}, \tag{3}$$

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 $\mathbf{T} = J^{-1}\mathbf{S}\mathbf{F}^T, \quad J = \det \mathbf{F} > 0$, 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 (1) follows from the continuity of the displacement [9]. The vector $\mathbf{f} = [\![\mathbf{F}]\!]\mathbf{m}$ is called the amplitude. The traction continuity condition (2) follows from equilibrium considerations.

An additional thermodynamic condition (3) [4, 6, 8, 5, 7] arises from an additional degree of freedom produced by free phase boundaries.

Given $\mathbf{F}_-$, the equations on the equilibrium interface (1) – (3) 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 [1]. *The phase transition zone is formed by all deformations which can exist on a locally equilibrium phase boundary.*

PTZ is determined only by the strain energy function. 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 due to phase transformations.

The conditions (1), (2), (3) can be rewritten in the actual configuration as

$$\mathbf{F}_{\pm} = \left(\mathbf{I} \pm J_{\mp}^{-1}\mathbf{c} \otimes \mathbf{n}\right) \cdot \mathbf{F}_{\mp}, \tag{4}$$

$$[\![\mathbf{T}]\!]\mathbf{n} = 0, \tag{5}$$

$$[\![W]\!] = \mathbf{c} \cdot \mathbf{T}\mathbf{n} \tag{6}$$

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

Amplitudes $\mathbf{f}$ and $\mathbf{c}$ are related as

$$\mathbf{c} \triangleq J N_1^{-1/2}\mathbf{f}, \tag{7}$$

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 [1], $[\![JN_1^{-1/2}]\!] = 0$.

Further we consider shock surfaces in isotropic materials. In this case the elastic potential depends on $\mathbf{F}$ only through the strain invariants: $W = W(I_1, I_2, J)$ and the Cauchy stress tensor is the isotropic function of $\mathbf{B}$:

$$\mathbf{T} = \mu_0 \mathbf{I} + \mu_1 \mathbf{B} + \mu_{-1} \mathbf{B}^{-1}, \tag{8}$$

$$\mu_0 = W_3 + 2J^{-1} I_2 W_2,\ \ \mu_1 = 2J^{-1} W_1,\ \ \mu_{-1} = -2JW_2, \tag{9}$$

where the strain invariants are:

$$\begin{aligned} &I_1 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = \mathrm{tr}\,\mathbf{B}, \\ &I_2 = \lambda_1^2\lambda_2^2 + \lambda_1^2\lambda_3^2 + \lambda_2^2\lambda_3^2 = J^2 \mathrm{tr}\,\mathbf{B}^{-1}, \\ &J = \lambda_1\lambda_2\lambda_3 \end{aligned} \tag{10}$$

$\lambda_i > 0$ $(i = 1, 2, 3)$ 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.

2 Orientation invariants

In the case of the isotropic material it is convenient to represent the normal $\mathbf{n}$ through the *orientation invariants*[1, 3]

$$G_1 = \frac{N_1}{J^2}, \quad G_{-1} = \frac{I_2}{J^2} - N_{-1} \quad (N_k = \mathbf{n} \cdot \mathbf{B}^k \mathbf{n}, \quad k = \pm 1) \tag{11}$$

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

$$\mathbf{t}_1 = J^{-1} \mathbf{PBn}, \quad \mathbf{t}_{-1} = J\mathbf{PB}^{-1}\mathbf{n} \tag{12}$$

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

Due to the kinematical condition (1), these invariants are continuous on the interface:

$$[\![G_1]\!] = 0, \quad [\![G_{-1}]\!] = 0 \tag{13}$$

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

$$\sum n_i^2 = 1, \quad \sum n_i^2 \lambda_i^2 = J^2 G_1, \quad \sum n_i^2 \lambda_i^{-2} = \frac{I_2}{J^2} - G_{-1} \tag{14}$$

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

Since the solution of the system (14) for n_i^2 has to be non–negative, the domain $\mathcal{G}$ of admissible values for the orientation invariants G_l, G_{-1} is a triangle with vertexes lying on the parabola $J^2 G_1^2 - I_1 G_1 + G_{-1} = 0$ (Fig. 1).

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

$$G_{-1} = G_1 \lambda_k^2 + \lambda_k^{-2}, \quad n_k = 0\ (k \neq i, j) \tag{15}$$

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

3 Phase transition zones for isotropic nonlinear elastic materials

Let us rewrite the conditions on the interface (4) — (6) in the case of the isotropic material.

It can be shown that equations (4), (7) lead to the following relationships between the strain and orientation invariants on the interface and $\mathbf{h}$:

$$[\![I_1]\!] = G_1 [\![J^2]\!] + 2\mathbf{h} \cdot \mathbf{t}_1^- + G_1 \mathbf{h} \cdot \mathbf{h}, \tag{16}$$

$$[\![I_2]\!] = G_{-1} [\![J^2]\!] - 2\mathbf{h} \cdot \mathbf{t}_{-1}^- + \mathbf{h} \cdot \mathbf{B}^{-1}\mathbf{h}. \tag{17}$$

From (4) also follows

$$\mathbf{c} = [\![J]\!]\mathbf{n} + \mathbf{h}, \quad \mathbf{h} \triangleq \mathbf{Pc}. \tag{18}$$

Projecting the traction condition (5) onto the normal we obtain [1]

$$-[\![W_3]\!] = 2\,[\![JW_1]\!]\,G_1 + 2\,[\![JW_2]\!]\,G_{-1}. \tag{19}$$

Projecting (5) onto the plane tangent to the shock surface we derive an equation for $\mathbf{h}$ [1, 3]:

$$\mathbf{A}_+ \mathbf{h} = -[\![W_1]\!]\mathbf{t}_1^- + [\![W_2]\!]\mathbf{t}_{-1}^-, \quad \mathbf{A}_+ \triangleq G_1 W_1^+ \mathbf{I} + W_2^+ \mathbf{PB}^{-1} \tag{20}$$

The thermodynamic condition (6) takes the form

$$[\![W]\!] = \tau_n [\![J]\!] + 2W_1^- \mathbf{h} \cdot \mathbf{t}_1^- - 2W_2^- \mathbf{h} \cdot \mathbf{t}_{-1}^- \tag{21}$$

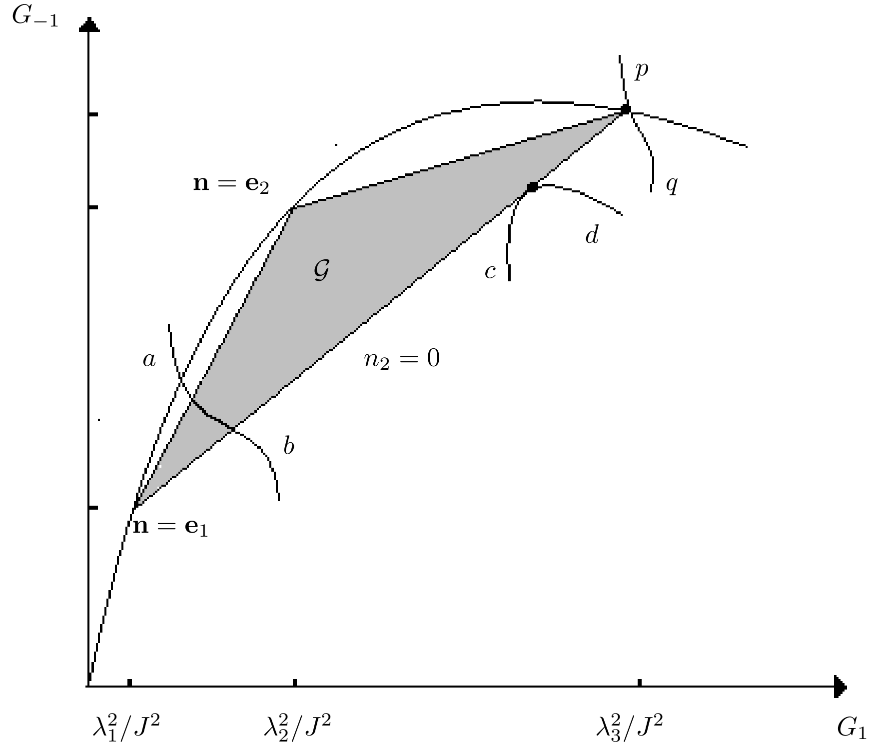

Figure 1: Admissible values domain $\mathcal{G}$ for the orientation invariants and lines of solutions.

where the normal component of the traction

$$\tau_n = \mathbf{n} \cdot \mathbf{Tn} = 2J\,(G_1 W_1 + G_{-1} W_2) + W_3 \tag{22}$$

can be calculated at any side of the phase boundary.

If $\mathbf{h}$ is given by the system (20), then substituting the representation (18) into (16), (17), (19) and (21) 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 $I_i^+ = I_i^+(G_1, G_{-1}|I_1^-, I_2^-, J_-)$, $i = (1,2)$, $J_+ = J_+(G_1, G_{-1}|I_1^-, I_2^-, J_-)$, then the forth equation takes the form of an equation for the one-parameter family of the orientation invariants:

$$\Psi(G_1, G_{-1}\,|\,I_1^-, I_2^-, J_-) = 0. \tag{23}$$

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

$$\min_{G_1, G_{-1} \in \mathcal{G}_-} \Psi(G_1, G_{-1}, J_-, I_1^-) \le 0 \le \max_{G_1, G_{-1} \in \mathcal{G}_-} \Psi(G_1, G_{-1}, J_-, I_1^-). \tag{24}$$

The one-parameter family of normals is represented on the G_1, G_{-1}–plane by the intersection of the line (23) (the line ab on Fig. 1) 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. 1). 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.

4 PTZ construction for compressible materials with the strain energy depending on two strain invariants

Let $W = W(I_1, J)$. Then, by (20), (16) and (17)

$$\mathbf{h} = -\frac{[\![W_1]\!]}{W_1^+ G_1}\mathbf{t}_1^-, \tag{25}$$

$$[\![I_1]\!] = G_1 [\![J^2]\!] - \frac{[\![W_1^2]\!]}{W_{1+}^2} L_1^-, \tag{26}$$

$$L_1 = I_1 - J^2 G_1 - G_{-1} G_1^{-1}, \tag{27}$$

and the conditions (19) and (21) take the form

$$2G_1\,[\![JW_1]\!] = -\,[\![W_3]\!]\,, \tag{28}$$

$$[\![W]\!] = \frac{W_1^- W_3^+ + W_1^+ W_3^-}{W_1^- + W_1^+}[\![J]\!] + \frac{2W_1^- W_1^+}{W_1^- + W_1^+}[\![I_1]\!]. \tag{29}$$

Relationships (26), (28) and (29) are three equations for the four unknowns J_+, I_1^+, G_1 and G_{-1}. If we solve two of them and substitute the result into the third we derive an equation in the form

$$\Psi \triangleq \Psi_1(G_1, J_-, I_1^-) + \Psi_2(G_1, J_-, I_1^-)G_{-1} = 0. \tag{30}$$

The equation (30) determines a line of an one-parameter family solutions on the G_1, G_{-1}–plane.

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

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

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 an eigenvector of $\mathbf{B}_-$. It follows from (20) that if the material is elliptic on the both sides of the interface, then in the first case plane jump of strains takes place on the interface, in the second case only corresponding principal stretches suffers a jump.

As an example we apply the developed procedure to a material with a special potential that is represented as the sum of the Treloar potential with a kink [2] and a term depending on the third strain invariant. This term characterizes deformation at pure hydrostatic state. For this material it is possible to obtain the analytical expression for the PTZ boundaries in the compact form.

Let

$$W(I_1, J) = V(I_1) + \Phi(J) \tag{31}$$

where

$$V(I_1) = \begin{cases} c_1 I_1, & I_1 \in (0, I_c) \\ c_2(I_1 - I_c) + c_1 I_c, & I_1 \in (I_c, \infty) \end{cases}, \quad c_1 > c_2, \tag{32}$$
$$\Phi(J) = aJ^2 + bJ + c$$

where the coefficient $a > 0$ characterizes the reaction of a 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 (26), (28) and (29) take the form

$$[I_1] = (\gamma^2 - 1)G_1 J_-^2 + (k^2 - 1)L_1^- \tag{33}$$

$$-A(\gamma - 1) = (\gamma - k)G_1 \tag{34}$$

$$[I_1] = (k + 1)(I_c - I_1^-) - AJ_-^2(\gamma - 1)^2 \tag{35}$$

where $\gamma = J_+/J_-$, $k = c_1/c_2$, $A = a/c_2$ and L_1 is determined by (27).

The equation (34) can be solved for $\gamma = \gamma(G_1)$. Then substituting (33) into (35) leads to the following relationship for the orientation invariants

$$\frac{J_-^2 G_1^2}{A + G_1} + L_1^- = \frac{I_c - I_1^-}{k - 1} \tag{36}$$

The "$-$"– PTZ subzone is determined by the inequalities

$$\min_{G_1, G_{-1}\in\mathcal{G}} \left(\frac{J_-^2 G_1^2}{A + G_1} + L_1^-\right) \le \frac{I_c - I_1^-}{k - 1} \le \max_{G_1, G_{-1}\in\mathcal{G}} \left(\frac{J_-^2 G_1^2}{A + G_1} + L_1^-\right) \tag{37}$$

and restricted by external and internal boundaries.

Let $\lambda_1 \le \lambda_2 \le \lambda_3$. Then the PTZ boundaries equations are given by the following relations:

i) a part of the external boundary with the normal $\mathbf{n} = \mathbf{n}_*$ laying in the 1–3 principal plane:

$$\left(\frac{\lambda_1 + \lambda_3}{\sqrt{2}}\right)^2 + (2k - 1)\left(\frac{\lambda_3 - \lambda_1}{\sqrt{2}}\right)^2 = I_c - \lambda_2^2 - \frac{k - 1}{A\lambda_2^2} \tag{38}$$

$$\lambda_3 > k\left(A\lambda_2^2\right)^{-1}\lambda_1^{-1} + \lambda_1 \tag{39}$$

ii) a part of the external boundary with the normal $\mathbf{n} = \mathbf{e}_3$:

$$\lambda_3^2 = (I_c - \lambda_2^2 - \lambda_1^2)\frac{1 + A\lambda_2^2\lambda_1^2}{k + A\lambda_2^2\lambda_1^2}. \tag{40}$$

$$\lambda_3 \le k\left(A\lambda_2^2\right)^{-1}\lambda_1^{-1} + \lambda_1 \tag{41}$$

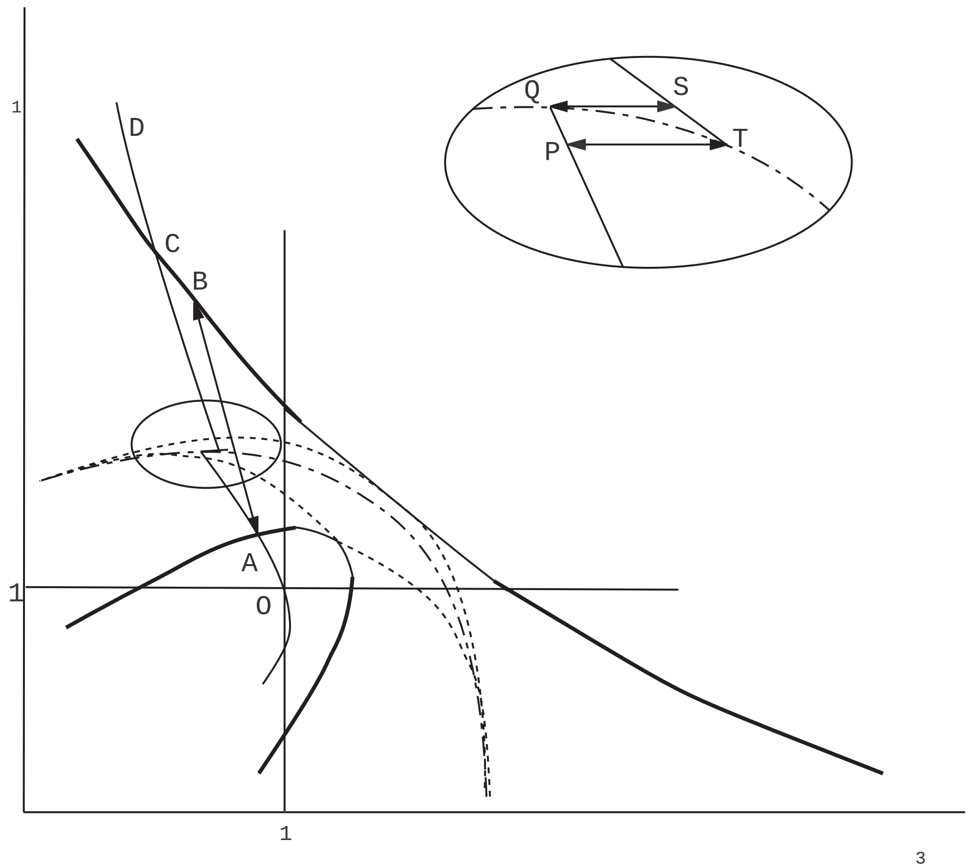

Figure 2: PTZ for the model material in a plane case.

iii) the internal boundary with the normal $\mathbf{n} = \mathbf{e}_1$:

$$\lambda_1^2 = (I_c - \lambda_2^2 - \lambda_3^2)\frac{1 + A\lambda_2^2\lambda_3^2}{k + A\lambda_2^2\lambda_3^2}. \tag{42}$$

The boundary (38) corresponds to the line of solution tangent to the stright line passing through the vertexes 1 and 3. Inequality (39) provides the tangent point to be on the corresponding side of the triangle between the vertexes.

The "+"– subzone is constructed analogously.

On the interfaces with $\mathbf{n} = \mathbf{n}_\alpha$ only λ_α ($\alpha = 1, 2$) suffer a jump. On the interfaces with $\mathbf{n} = \mathbf{n}_*$ plane jump takes place ($[\![\lambda_2]\!] = 0$). Thus, three types of strain localization due to phase transitions can be expected if the interface corresponds to the PTZ boundary: (1) the interface perpendicular to the direction of the maximal stretch; only the maximal stretch suffers a jump on the phase boundary; (2) the interface oriented analogously to the shear band with a jump of a shear parameter; (3) the interface perpendicular to the direction of the minimal stretch that suffers a jump.

The PTZ cross-section for the material (31) at $A > k$ is shown at Fig. 2. 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 corresponding to the external PTZ boundary also depends on the material parameters. If $A \gg k$ then interfaces of shear band type are preferential. The interface perpendicular to the direction of maximal stretching is possible only in a case of hydrostatic deformation. If the parameter A decreases then the interface perpendicular to the direction of maximal stretching can also appear on other loading pathes. 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. In this case

$$\lambda_2 = 1, \quad \lambda_1 = \Lambda(\lambda_3)\lambda_3, \quad \tau_1(\lambda_1, \lambda_3) = 0 \tag{43}$$

where τ_1 is the principal Cauchy stress and the function $\Lambda(\lambda_3)$ is found from the condition $(43)_3$.

Note that in the vicinity of the line $I_1 = I_c$ the behavior at loading and unloading includes hysteresis $PQST$.

One can see that the sample can be divided into two phases before the kink point I_c (which replace the non-ellipticity zone) 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 loading 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 $(43)_3$ fails. That is why the point B does not belong to the curve DCS. Analogously, if the point C is reached on the path DCS, appearance of the layer of the phase "$-$" surrounded by the phase "$+$" can be expected.

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.

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