Phase transition zones in relation with constitutive equations of elastic solids

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Abstract

The analysis of the conditions on the equilibrium phase boundary in a nonlinear elastic material leads to the concept of phase transition zones (PTZ) which are formed in strain-space by all deformations which can exist on the equilibrium interface. The PTZ boundary acts as a phase diagram or yield surface in strain-space. The PTZ is determined entirely by the strain-energy function and represents some kind of a passport of a material suffering two phase deformations. We consider a number of strain energy functions and categorize the types of phase boundaries which are possible, i.e. determine the relation between the orientation of the phase boundaries and the corresponding jumps in strains, depending on material properties and strain state. We examine compressible and incompressible nonlinear elastic materials as well as materials represented in a case of small strains by piece-wise quadratic strain-energy functions.

1 Introduction

When an elastic solid undergoes phase transformations, the interface between two different phases can be considered as a surface across which the displacement is continuous but the deformation gradient suffers a discontinuity. This kind of interfaces appear, for instance, in martensite transformations. When the interface is in equilibrium, a thermodynamic condition (also known as the Maxwell condition), as well as the conventional conditions of displacement and traction continuity, must be satisfied at the interface [4, 6, 29, 5, 7]. Analysis of these jump conditions leads to the concept of phase transition zones (PTZ) in strain space. Given an elastic material, the PTZ represents all deformations that can exist adjacent to an equilibrium interface.

Reasons to construct PTZs are as follows:

- Deformations outside PTZ cannot exist on any interface, whatever the loading conditions. The PTZ boundary acts as a transformation surface or yield surface or phase diagram in strain-space.
- Different points of the PTZ boundary correspond to different types of interfaces, i.e. different orientations of the normal with respect to strains and different jumps in strains across the interface. Thus, to construct a PTZ is to study how *a strain state* affects the type of strain localization due to phase transformations.
- The PTZ is determined entirely by a strain energy function. If a material can suffer two-phase deformation then the strong ellipticity must be lost at some deformations [22]. But this is only a necessary condition. Namely PTZ construction allows us *to categorize strain energy functions* with respect to existence of two-phase deformations and the types of interfaces in dependence of strain state. Since this can be done, the PTZ can be used as a guide in searching for the appropriate strain energy functions if the interfaces appearing on different deformation paths are known from experiments.
- Although the PTZ itself does not give a solution of a boundary value problem, except in some simple cases, any two-phase deformation can be related with the PTZ. Examples of relations between the PTZ and locally unstable and possibly stable two-phase deformations with smooth interfaces show that in the unstable cases there are points in the elastic body where the deformation is inside the external PTZ boundaries. In the other cases, when instability is not found, deformations throughout the body are outside the external PTZ boundaries except the interface where the deformation belongs to the external PTZ boundary [1, 2, 3, 19].

On the whole, the PTZ can be viewed as a “passport” of a material that can suffer two-phase deformations. We present below the PTZs for a variety of strain energy functions (both finite and small strains) — some kind of the ”PTZs-catalogue”. We demonstrate how the PTZ can be used to characterize materials (the strain energy functions) according to the types of interfaces in dependence on strain state.

2 Conditions on the interface and phase transition zones in finite strains

The static deformation of an elastic body is given by

$$\mathbf{x} = \mathbf{x}(\mathbf{X}), \tag{1}$$

where $\mathbf{x}$ and $\mathbf{X}$ are the positions of the material point in the deformed (current) and undeformed (reference) configurations. Let Γ be an interface between two different phases in the undeformed configuration. Then the deformation must satisfy the jump conditions

$$[\![\mathbf{F}]\!] = \mathbf{f} \otimes \mathbf{m}, \quad [\![\mathbf{S}]\!]\mathbf{m} = 0, \quad [\![W]\!] = \mathbf{f} \cdot \mathbf{S}_\pm \mathbf{m}, \tag{2}$$

which correspond to displacement continuity, traction continuity and thermodynamic equilibrium of the interface (the Maxwell relation), respectively, where $\mathbf{F}$ is the deformation gradient, $\mathbf{f} = [\![\mathbf{F}]\!]\mathbf{m}$ is the amplitude of the jump, W is the strain energy per unit reference volume, $\mathbf{S} = \partial W/\partial \mathbf{F}$ is the first Piola-Kirchhoff stress tensor related to the Cauchy stress tensor by $\mathbf{T} = J^{-1}\mathbf{S}\mathbf{F}^T$, $J = \det \mathbf{F} = \rho_0/\rho > 0$ (ρ and ρ_0 are the mass densities in the deformed and reference configurations), the brackets $[\![\cdot]\!] = (\cdot)_+ - (\cdot)_-$ denote the jump of a function across Γ, super- or subscripts "$-$" and "$+$" signify values on different sides of the interface, and $\mathbf{m}$ is the unit normal to Γ.

We may use $(2)_1$ to rewrite $(2)_{2,3}$ as

$$(\mathbf{S}(\mathbf{F}_- + \mathbf{f} \otimes \mathbf{m}) - \mathbf{S}(\mathbf{F}_-))\,\mathbf{m} = 0,$$
$$W(\mathbf{F}_- + \mathbf{f} \otimes \mathbf{m}) - W(\mathbf{F}_-) = \mathbf{f} \cdot \mathbf{S}(\mathbf{F}_-)\mathbf{m}.$$

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 $\mathbf{m}$. The *phase transition zone* (PTZ) is defined as the union of all those $\mathbf{F}_-$ for which the above system of equations have a solution for $\mathbf{f}$ and $\mathbf{m}$; see [10, 11].

The jump conditions (2) can be rewritten with respect to the deformed (current) configuration:

$$\mathbf{F}_+ = \left(\mathbf{I} + \frac{1}{J_-}\mathbf{c} \otimes \mathbf{n}\right)\mathbf{F}_- \quad \text{or} \quad \mathbf{F}_- = \left(\mathbf{I} - \frac{1}{J_+}\mathbf{c} \otimes \mathbf{n}\right)\mathbf{F}_+, \tag{3}$$

$$[\![\mathbf{T}]\!]\mathbf{n} = 0, \tag{4}$$

$$[\![W]\!] = \mathbf{c} \cdot \mathbf{T}\mathbf{n}, \tag{5}$$

where $\mathbf{n}$ is the normal to the interface in the deformed configuration, $\mathbf{c}$ is the recalculated amplitude, the Cauchy stress $\mathbf{T}$ in (5) is taken at any side of the interface because of the traction continuity.

For isotropic materials

$$W = W(I_1, I_2, J), \quad \mathbf{T} = \mu_0\mathbf{I} + \mu_1\mathbf{B} + \mu_{-1}\mathbf{B}^{-1}, \tag{6}$$

$$\mu_0 = W_3 + 2J^{-1}I_2W_2,\ \mu_1 = 2J^{-1}W_1,\ \mu_{-1} = -2JW_2, \tag{7}$$

where $\mathbf{B} = \mathbf{F}\mathbf{F}^T$ is the left Cauchy-Green tensor,

$$\begin{aligned} I_1 &= \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = \mathrm{tr}\,\mathbf{B}, \\ I_2 &= \lambda_1^2\lambda_2^2 + \lambda_1^2\lambda_3^2 + \lambda_2^2\lambda_3^2 = J^2 \mathrm{tr}\,\mathbf{B}^{-1}, \\ I_3 &= \lambda_1^2\lambda_2^2\lambda_3^2 = J^2 \end{aligned} \tag{8}$$

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. Since W can be expressed as $W = \widetilde{W}(\lambda_1, \lambda_2, \lambda_3)$, the PTZ can be defined in terms of the three strain invariants or the three principal stretches $\lambda_1, \lambda_2, \lambda_3$. The interface locally is characterized by the direction of the normal $\mathbf{n}$ to the interface in the deformed configuration with respect to axes $\mathbf{e}_i$ $(i = 1, 2, 3)$ of $\mathbf{B}$ on one side of the interface and by the jump in $\mathbf{B}$.

A general procedure for constructing the PTZ for arbitrary isotropic nonlinear elastic materials has been developed earlier; see [10, 11, 14, 15, 17, 20] where examples of the PTZ construction are also given. Below we summarize those results.

By (3), the amplitude $\mathbf{c}$ can be decomposed as

$$\mathbf{c} = [\![J]\!]\mathbf{n} + \mathbf{h}, \quad \mathbf{h} \triangleq \mathbf{P}\mathbf{c}, \tag{9}$$

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

The normal appears in relationships through the orientation invariants

$$G_1 \triangleq \frac{N_1}{J^2}, \quad G_{-1} \triangleq \frac{I_2}{J^2} - N_{-1}, \quad N_{\pm 1} = \mathbf{n} \cdot B^{\pm 1}\mathbf{n}. \tag{10}$$

Given $\mathbf{B}$ every pair $G_1, G_{-1}\mathcal{G}$ determines the unit normal where $\mathcal{G}$ is an admissible values domain for G_1, G_{-1} (see details in [10, 15, 20]).

The tangent component $\mathbf{h}$ of the amplitude $\mathbf{c}$ can be decomposed using the vectors

$$\widetilde{\mathbf{t}}_1 = J^{-1}\mathbf{P}\mathbf{B}\mathbf{n}, \quad \widetilde{\mathbf{t}}_{-1} = J\mathbf{P}\mathbf{B}^{-1}\mathbf{n}. \tag{11}$$

The system of conditions on the equilibrium phase boundary reduces to the following relationships between strain invariants on both sides of the phase boundary and the orientation invariants:

– from the kinematic relationships (3) it follows that

$$[\![I_1]\!] = G_1[\![J^2]\!] + 2\mathbf{h} \cdot \tilde{\mathbf{t}}_1^- + G_1\mathbf{h} \cdot \mathbf{h}, \tag{12}$$

$$[\![I_2]\!] = G_{-1}[\![J^2]\!] - 2\mathbf{h} \cdot \tilde{\mathbf{t}}_{-1}^- + \mathbf{h} \cdot \mathbf{B}^{-1}\mathbf{h}; \tag{13}$$

– continuity of the normal component of traction gives

$$-\left[\!\left[W_3\right]\!\right] = 2\left[\!\left[JW_1\right]\!\right] G_1 + 2\left[\!\left[JW_2\right]\!\right] G_{-1}; \tag{14}$$

– the thermodynamic (Maxwell) relation takes the form

$$\left[\!\left[W\right]\!\right] = \tau_n \left[\!\left[J\right]\!\right] + 2W_1^- \mathbf{h} \cdot \tilde{\mathbf{t}}_1^- - 2W_2^- \mathbf{h} \cdot \tilde{\mathbf{t}}_{-1}^-, \tag{15}$$

where the normal component of the traction

$$\tau_n = \mathbf{n} \cdot \mathbf{T}\mathbf{n} = 2J\left(G_1 W_1 + G_{-1} W_2\right) + W_3 \tag{16}$$

can be calculated at any side of the phase boundary;

– continuity of the tangent component of traction leads to the representation of $\mathbf{h}$ (the tangent component of the amplitude) in a form

$$\mathbf{h} = \alpha \tilde{\mathbf{t}}_1^- + \beta \tilde{\mathbf{t}}_{-1}^-, \tag{17}$$

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

$$\begin{pmatrix} G_1 W_1^+ & W_2^+ \\ -G_1 W_2^+ & G_1 W_1^+ + G_{-1} W_2^+ \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} -\left[\!\left[W_1\right]\!\right] \\ \left[\!\left[W_2\right]\!\right] \end{pmatrix}. \tag{18}$$

In the case of incompressible materials one has to put $J \equiv 1$ and replace (14) by the formula for computing the jump of the incompressibility reaction p

$$\left[\!\left[p\right]\!\right] = 2\left[\!\left[W_1\right]\!\right] N_1 - 2\left[\!\left[W_2 N_{-1}\right]\!\right]. \tag{19}$$

If α and β are given by the system (18), then substituting the representation (17) into (12), (13) and (15) gives three equations for five unknowns I_1^+, I_2^+, J_+, G_1 and G_{-1}. The equation (14) is a fourth one. As a result we obtain a system of four equation that determines a one-parameter family of solutions, i.e. the normals and strain invariants on the other side of the interface, which, at given I_1^-, I_2^-, J_-, satisfy the local phase equilibrium conditions.

If we solve three of the equations for I_1^+, I_2^+ and J_+ as functions of $G_1, G_{-1}, I_1^-, I_2^-, J_-$, then the forth equation takes the form of an equation for the one-parameter family of the orientation invariants:

$$\Psi(G_1, G_{-1} \mid I_1^-, I_2^-, J_-) = 0. \tag{20}$$

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

$$\begin{gathered} \Psi_{min}(J_-, I_1^-, I_2^-) \le 0 \le \Psi_{max}(J_-, I_1^-, I_2^-), \\ \Psi_{min}(J_-, I_1^-, I_2^-) = \min_{G_1, G_{-1} \in \mathcal{G}_-} \Psi(G_1, G_{-1}, J_-, I_1^-, I_2^-), \\ \Psi_{max}(J_-, I_1^-, I_2^-) = \max_{G_1, G_{-1} \in \mathcal{G}_-} \Psi(G_1, G_{-1}, J_-, I_1^-, I_2^-). \end{gathered} \tag{21}$$

Note that we assume that a material is strongly elliptic on both sides of the interface, and the non-ellipticity sub-zone is placed inside the PTZ in the case.

3 Hadamard material

The PTZ construction for the Hadamard material, relations of various two-phase deformations with PTZs and stability were considered in [10, 15, 21, 19]. The strain energy function is given by

$$W = \frac{c}{2} I_1 + \frac{d}{2} I_2 + \phi(J) \quad (c,\, d \ge 0,\, c + d \ne 0),$$

where $\phi(J)$ is specified as

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

The material parameters c, d, J_c, A and a are chosen such that (i) the material is strongly elliptic at the interface, (ii) the stress-free state $\lambda_1 = \lambda_2 = \lambda_3 = 1$ is outside the PTZ, and (iii) stress is zero and the volume modulus is positive at $\lambda_1 = \lambda_2 = \lambda_3 = 1$.

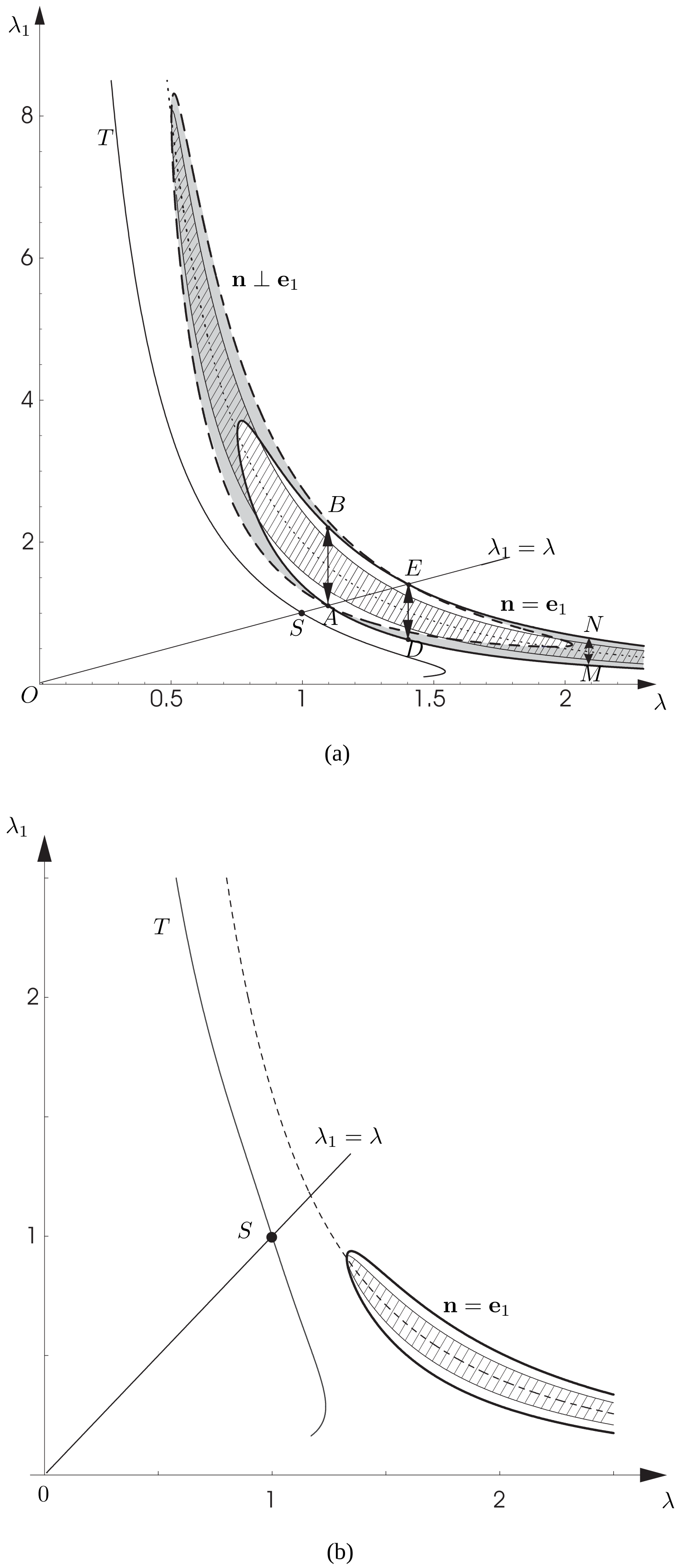
The Figure 1 represents examples the PTZ cross-section by the plane $\lambda_2 = \lambda_3 = \lambda$ at different material parameters. The PTZ is bounded by the two curves on the (λ, λ_1)-plane:

$$u(J) = h(\lambda, \lambda), \quad \text{corresponding to } \mathbf{n} = \mathbf{e}_1 \tag{22}$$

$$u(J) = h(\lambda, \lambda_1), \quad \text{corresponding to } \mathbf{n} \perp \mathbf{e}_1. \tag{23}$$

where $u(J) = A - (J - J_c)^2$,

$$h(\lambda_i, \lambda_j) = \frac{c}{\lambda_i \lambda_j} + d\left(\frac{1}{\lambda_i} + \frac{1}{\lambda_j}\right).$$



(a)

(b)

Figure 1: Hadamard material. PTZ at $\lambda_2 = \lambda_3 \equiv \lambda$; ST – the line of the uniaxial stretching; (a) $c = 0.032$, $d = 0.2$, $J_c = 2$, $A = 0.8$, $a = -0.23$ (b) $J_c = 1.6$, $d = 0.3$, $A = 0.35$, $c = 0.03$, $a = -0.62$)

A non-ellipticity sub-zone is embedded in the PTZ and is described by

$$h(\lambda, \lambda_1) + \ddot{\phi} < 0 \ \text{ if } \ \lambda < \lambda_1, \tag{24}$$

$$h(\lambda, \lambda) + \ddot{\phi} < 0 \ \text{ if } \ \lambda > \lambda_1, \tag{25}$$

where the dot denotes differentiation with respect to J (see [28, 10]). The shaded area in the figures represents the interior of the PTZ, and the hashed area denotes the non-ellipticity zone. The thick line denotes the PTZ boundary corresponding to $\mathbf{n} = \mathbf{e}_1$ and is given by the equation (22). Only λ_1 may suffer a jump if the PTZ is reached for example at point M or N. The thick dotted line denotes the PTZ boundary corresponding to the normal $\mathbf{n} \perp \mathbf{e}_1$. The thin dotted line corresponds to $J = J_c : \lambda_1 = J_c/\lambda^2$. The point S denotes the undeformed state. The arrows in the figures denote the jumps in strains across the interface.

The line ST is the path of uniaxial tension in the "1" - direction:

$$\lambda_2 = \lambda_3 = \Lambda(\lambda_1), \quad \tau_2 = \tau_3 = 0$$

(τ_i are the principal Cauchy stresses ($i = 1, 2, 3$)). In Figure 1 the line of uniaxial stretching does not cross the PTZ boundary. This means that piecewise-homogeneous two-phase deformations cannot appear under uniaxial tension at this material parameters.

Other paths may lead to forming two-phase states. For example, two points A and E in Fig. 1 a correspond to two spherical deformations in the core of the equilibrium two-phase sphere. The arrays AB and ED denote the corresponding jumps in strains across the interface (see details in [19]).

We emphasize that an opportunity of spherically-symmetric deformations and the number of the solutions can be predicted *a priory* if the PTZ is constructed. In a case of Figure 1 b one can see that two-phase spherical deformations are impossible because the PTZ does not contain a point at which $\lambda_1 = \lambda$ at that set of material parameters. Note also that a phase transformation may not take place even if strain energy is a non-convex function of all-round stretch. One can check that this is the case of material parameters for Figure 1 (b).

4 Treloar material with a "kink"

Now we consider an incompressible material. The strain energy function is given by

$$W(I_1) = \begin{cases} c_1 I_1, & I_1 \in (0, I_c) \\ c_2(I_1 - I_c) + c_1 I_c, & I_1 \in (I_c, \infty) \end{cases}, \quad c_1 > c_2, \quad J \equiv 1.$$

This material can be called the Treloar material "with a kink". (Figure 2). It has been considered in [11] as the simplest incompressible material model that allows two-phase deformations. The "kink" point $I = I_c$ replaces the nonellipticity sub-zone. The PTZ on the $\lambda_1\lambda_3-$ is shown it the Figure 3. Note that $\lambda_2 = (\lambda_1\lambda_3)^{-1}$ because of the incompressibility restriction.

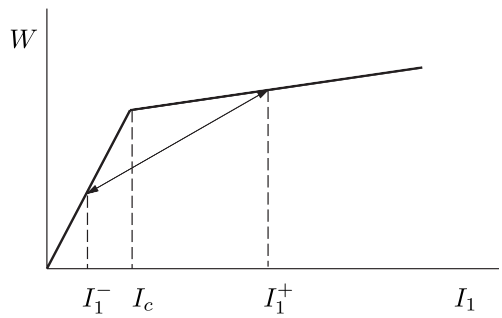


Figure 2: Strain energy function for the Treloar material "with a kink"

For such a material interfaces, corresponding to the PTZ boundary, are given by

$$n_1^2 = \lambda_1/(\lambda_1 + \lambda_3), \ n_2 = 0, \ n_3^2 = 1 - n_1^2$$

(assuming $\lambda_1 > \lambda_2 > \lambda_3$), and across the interface a shear strain suffers a jump. Since λ_2 does not suffer a jump in the case, we have on the interface $\lambda_1^-\lambda_3^- = \lambda_1^+\lambda_3^+$. The dotted line denotes $I = I_c$. The small dotted lines are $\lambda_3 = 1/\lambda_A\lambda_1$ and $\lambda_3 = 1/\lambda_B\lambda_1$, correspondingly. The jumps are denoted by arrays. The interface represents some kind of a shear band. The lines SA and BT correspond to the path of uniaxial tension in the "3" - direction under the loading and unloading, respectively. If the point A is reached on the loading path, one can suppose that a thin layer of the phase "+" appears in an unbounded media and the point A' corresponds to the deformation inside the layer. Because of internal stresses acting in the "1" - direction inside the layer, the principal Cauchy stress in this direction doesn't equal to zero any more. That is why the point A' does not coincide with point the B. Analogously, the points A and B' are also different.

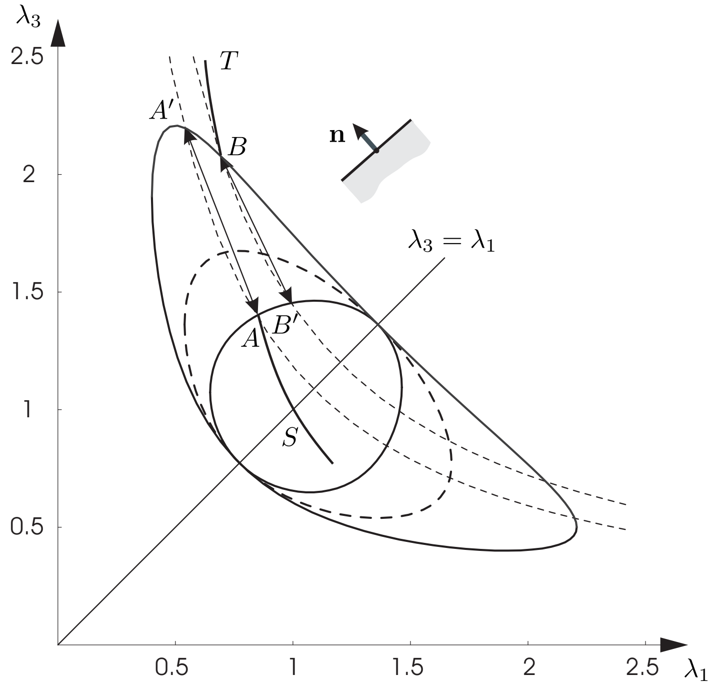


Figure 3: The PTZ for the Treloar material "with a kink" ($I_c = 4$, $c1/c2 = 3$).

5 Model material

Another example is a model material with a strain energy function given by

$$W(I_1, J) = V(I_1) + \Phi(J) \tag{26}$$

$$V(I_1) = \begin{cases} c_1 I_1, & I_1 \in (0, I_c) \\ c_2(I_1 - I_c) + c_1 I_c, & I_1 \in (I_c, \infty) \end{cases}, \quad c_1 > c_2, \tag{27}$$

$$\Phi(J) = aJ^2 + bJ + c. \tag{28}$$

The material (26) was proposed in [9] and studied in the PTZ construction in papers [15, 16, 19]. Note that the strain-energy function only depends on the first and third strain invariants. Such materials in the context of PTZ construction was analyzed in [10, 15, 16, 20].

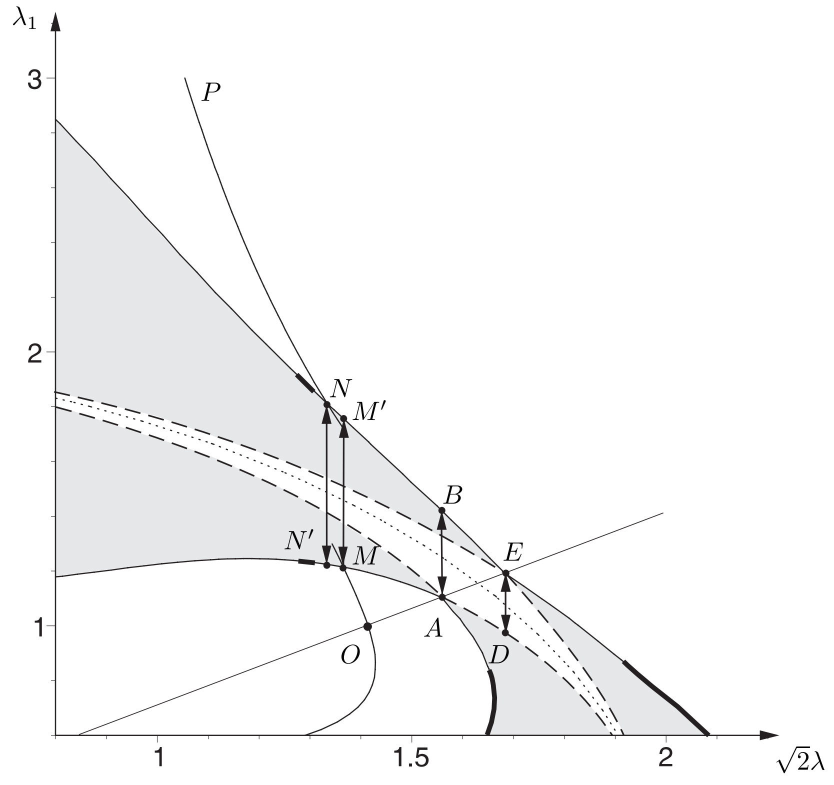
If $W \equiv V$, and $J \equiv 1$ then (27) describes the incompressible Treloar material with a kink (see the previous section). On the other hand, the material (26)–(28) can be considered as a composite of two Hadamard materials which are identified with different phase states. But in contrast to the Hadamard material, where the function $\Phi(J)$ provided an opportunity of phase transformations, in the current model $\Phi(J)$ itself does not give rise to loss of ellipticity and to suffer two-phase deformations. Namely the "kink" point $I = I_c$ in the dependence W on I_1 and the choice $c_1 > c_2$ provide the permissibility of two-phase deformations.

In the case of the Hadamard material the normal to the interface coincides with the eigenvector of the strain tensor corresponding to *the minimal* principal stretch if the interface corresponds to the external PTZ boundary, and across the interface only this stretch suffers a jump.

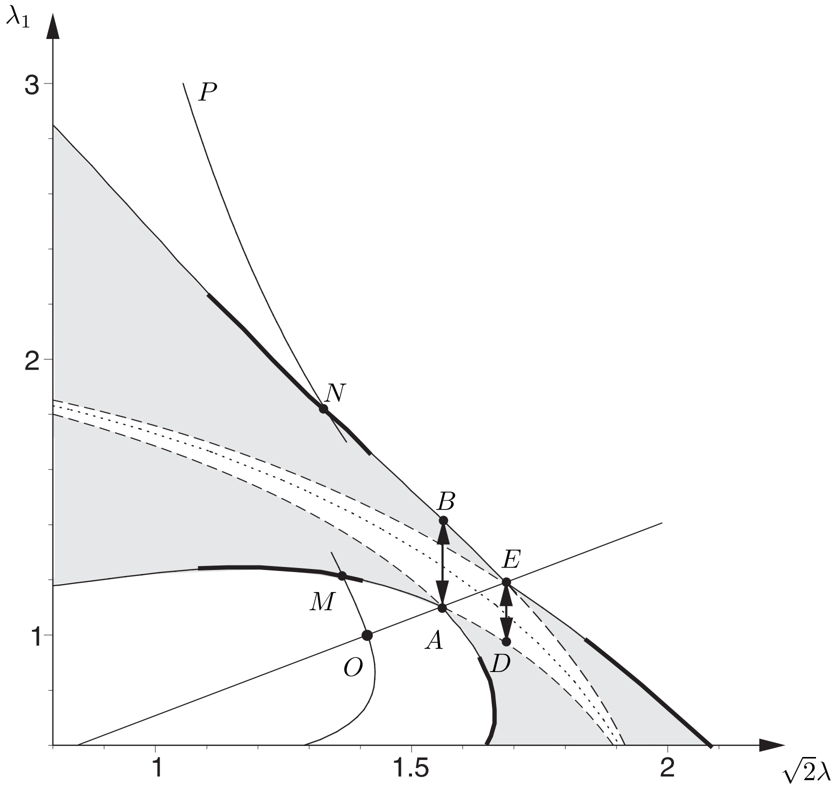
It can be shown that two types of interfaces may correspond to the PTZ boundary in the case of the model material. In the first case, the normal coincides with the eigenvector of the strain tensor corresponding to *the maximal* stretch – contrary to the Hadamard material, and only this stretch suffers a jump. In the other case, the situation is similar the incompressible Treloar material except that the jump is not volume-preserving. These two types of interfaces can be called as the normal-type and shear-type interfaces, respectively.

Figure 4 represents the PTZ for the model material at $\lambda_2 = \lambda_3 = \lambda$. The shaded areas are the interior of the PTZ. The thick lines correspond to the shear-type interfaces. The normal to the interface lies in in the principal plane of the maximal and minimal stretches. The thin lines correspond to the normal-type interfaces. The normal coincides with the direction of the maximal stretching: $\mathbf{n} = \mathbf{e}_1$, and only maximal principal stretch (here λ_1) suffers a jump. The internal PTZ boundaries (the dotted lines) correspond to $\mathbf{n} = \mathbf{e}_3$. The small dotted line is the "switch" surface $I = I_c$. Point O denotes the undeformed state.

The lines OM and PN correspond to the uniaxial tension in "1"-direction. Depending on the material parameters, uniaxial tension may lead to the appearance of an interface perpendicular to the direction of stretching (Figure 4 a) or shear-type interfaces (Figure 4 b). Arrows denote jumps across the interfaces. Spherically-symmetric two-phase deformations are represented by the jumps AB and ED.



(a)



(b)

Figure 4: The model material. The PTZ at $\lambda_2 = \lambda_3 \equiv \lambda$; ST – the line of the uniaxial stretching. (a) $a = 4.09$, $c_1 = 3$, $c_2 = 1$, $I_c = 4$; (b) $a = 4.4$, $c_1 = 3$, $c_2 = 1$, $I_c = 4$. The lines OM and NP correspond to the path of uniaxial stretching, and the points A, B, D, E refer to spherically symmetric deformations.

6 PTZs in the case of small strains

In the case of small strains a problem on the equilibrium two-phase configurations of an elastic body is reduced to the determination of a phase boundary Γ and displacement $\mathbf{u}(\mathbf{x})$ sufficiently smooth at material points $\mathbf{x} \notin \Gamma$, continuous across Γ, and satisfying the boundary and equilibrium conditions [23, 27, 26, 13]:

$$\mathbf{x} \notin \Gamma \quad : \qquad \nabla \cdot \boldsymbol{\sigma} = 0, \quad \theta = \text{const}, \tag{29}$$

$$\mathbf{x} \in \Gamma \quad : \qquad [\![\mathbf{u}]\!] = 0, \quad [\![\boldsymbol{\sigma}]\!] \cdot \mathbf{n} = 0, \quad [\![f]\!] - \boldsymbol{\sigma} : [\![\varepsilon]\!] = 0, \tag{30}$$

where ε and σ are the strain and stress tensors, θ is the temperature.

The free energy volume density f is to be modelled by a number of quadratic functions (see [13, 26]). In the simplest case

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

where $\mathbf{C}_\pm$, $f_0^\pm$ and $\varepsilon_\pm^p$ are positive definite elasticity tensors, free energy densities and strain tensors in unstressed phases "$\pm$",

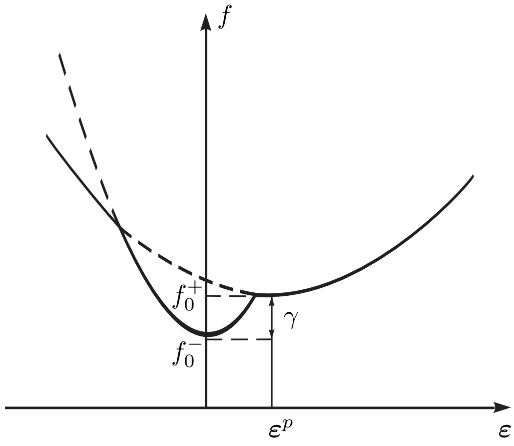


Figure 5: Free energy.

respectively (Figure 5). If $\varepsilon_+^p = 0$, then $[\varepsilon^p] \equiv \varepsilon^p$ is the self–strain tensor of the transformation. If $\mathbf{C}_\pm$ and $\varepsilon_\pm^p$ do not depend on the temperature, then the parameter $\gamma(\theta) = [f_0]$ plays the role of the temperature.

Using $(30)_{1,2}$ one can express the jump in strains or in stresses across the interface through the strains on one side of the interface [24, 13]:

$$[\![\varepsilon]\!] = \mathbf{K}_\mp(\mathbf{n}) : \mathbf{q}_\pm, \quad \mathbf{q}_\pm = -\mathbf{C}_1 : \varepsilon_\pm + [\![\mathbf{C} : \varepsilon^p]\!], \tag{31}$$

$$\mathbf{K}_\pm(\mathbf{n}) = \{\mathbf{n} \otimes \mathbf{G}_\pm \otimes \mathbf{n}\}^s, \quad \mathbf{G}_\pm = (\mathbf{n} \cdot \mathbf{C}_\pm \cdot \mathbf{n})^{-1}, \quad \mathbf{C}_1 = \mathbf{C}_+ - \mathbf{C}_-,$$

s means the symmetrization: $K_{ijkl} = n_{(i}G_{j)(k}n_{l)}$. If the tensor C_1 is nonsingular then the thermodynamic condition $(30)_3$ can be written in q-space [23, 13, 25, 26]:

$$\gamma_* + \frac{1}{2}\mathbf{q}_\pm : \left(\mathbf{C}_1^{-1} \pm \mathbf{K}_\mp(\mathbf{n})\right) : \mathbf{q}_\pm = 0, \quad \gamma_* = \gamma + \frac{1}{2}[\![\varepsilon^p]\!] : \mathbf{B}_1^{-1} : [\![\varepsilon^p]\!]. \tag{32}$$

Tensors $\mathbf{q}$ for which the equation (32) can be solved for a unit normal $\mathbf{n}$ form the phase transition zone in q–space. The PTZ consists of two sub–zones $\mathcal{Q}_-$ and $\mathcal{Q}_+$ formed by the tensors $\mathbf{q}_\pm \in \mathcal{Q}_\pm$ satisfying the inequalities [26, 13]

$$\mathcal{K}_{\min}^\mp(\mathbf{q}_\pm) \leq \mp\varphi(\mathbf{q}_\pm) \leq \mathcal{K}_{\max}^\mp(\mathbf{q}_\pm), \tag{33}$$

$$\mathcal{K}_{\max}^\mp(\mathbf{q}_\pm) = \max_{\mathbf{n}} \mathcal{K}_\mp(\mathbf{q}, \mathbf{n}), \quad \mathcal{K}_{\min}^\mp(\mathbf{q}_\pm) = \min_{\mathbf{n}} \mathcal{K}_\mp(\mathbf{q}_\pm, \mathbf{n}),$$

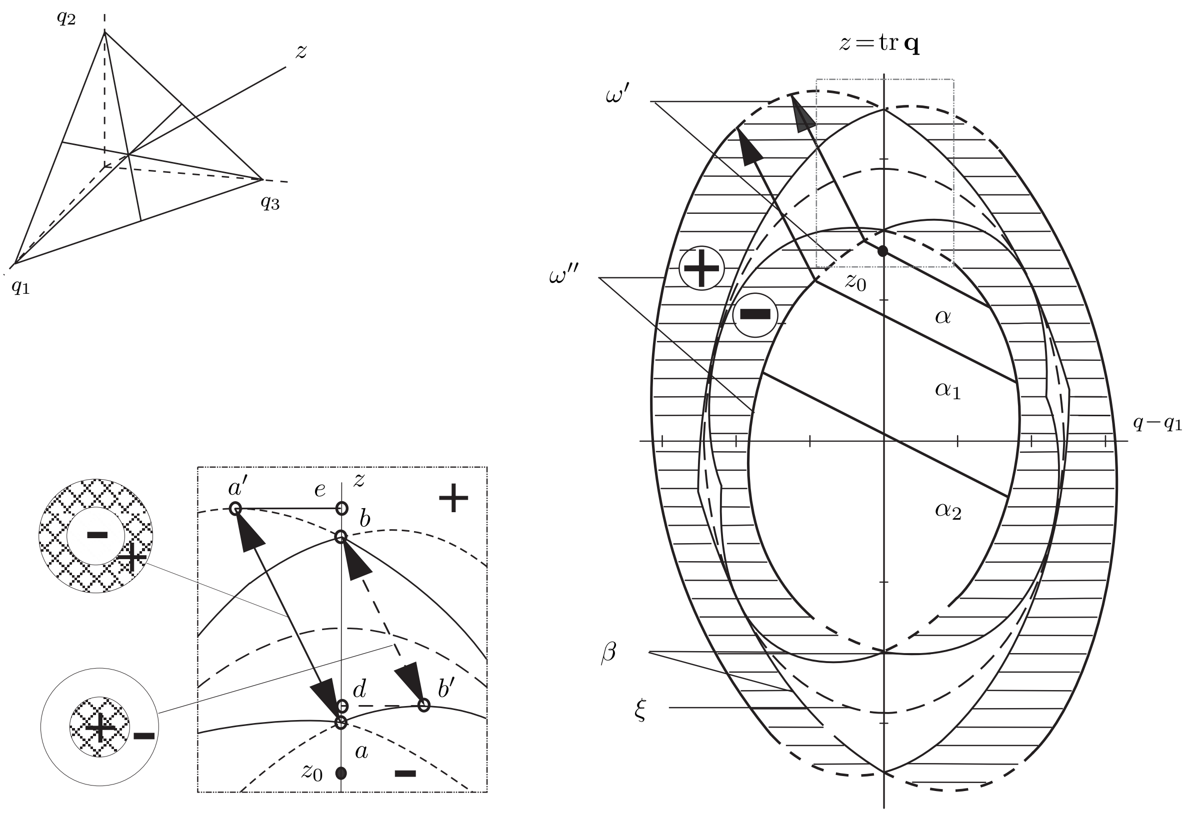
$$\mathcal{K}_\pm(\mathbf{q}, \mathbf{n}) = \mathbf{q} : \mathbf{K}_\pm(\mathbf{n}) : \mathbf{q}, \quad \varphi(\mathbf{q}) = 2\gamma_* + \mathbf{q} : \mathbf{C}_1^{-1} : \mathbf{q}.$$

The equation $\varphi(\mathbf{q}) = 0$ corresponds to the surface of discontinuity in the derivative of $f(\varepsilon)$, i.e. the surface where $f^+(\varepsilon) = f^-(\varepsilon)$. The surface divides the domains of definition of the phases "$-$" and "$+$", and passes between $\mathcal{Q}_-$ and $\mathcal{Q}_+$. For simplicity sake we do not consider twinning in the present paper.

6.1 Isotropic materials

Let the phases "$-$" and "$+$" be isotropic, i.e.

$$\mathbf{C}_\pm = \lambda_\pm \mathbf{I} \otimes \mathbf{I} + 2\mu_\pm {}^4\mathbf{I}, \quad \varepsilon_+^p = (\vartheta^p/3)\mathbf{I}, \quad \varepsilon_-^p = 0,$$



(a) (b)

Figure 6: The PTZ cross-section by the plane $q_2 = q_3 = q$ ($\mu_+ < \mu_-$, $K_+ < K_-$) and spherically-symmetric two-phase deformations [2].

where ${}^4\mathbf{I}$ is the fourth rank identity tensor; $\lambda_\pm$ and $\mu_\pm$ are the Lame constants, $K_\pm = \lambda_\pm + 2/3\mu_\pm$ are the bulk moduli.

Crosshatched regions in Figure 6 represent the PTZ cross-sections by the plane $q_2 = q_3 = q$ in the case $\mu_+ < \mu_-$, $K_+ < K_-$. Let $|q|_{\min}$ and $|q|_{\max}$ are the minimal and maximal absolute values of the eigenvalues of $\mathbf{q}_-$, $\mathbf{e}_{|q|\min}$ and $\mathbf{e}_{|q|\max}$ are the corresponding eigenvectors. Then the PTZ boundaries correspond to the interfaces with

- normals $\mathbf{n}$ lying in the principal plane of the tensor $\mathbf{q}$ (solid lines ω''); plane jumps of strains similar to shearing take place across the interface.
- the normal $\mathbf{n} = \mathbf{e}_{|q|\,\max}$, for example, if $|q_1| > |q_2| > |q_3|$, then $\mathbf{n} = \mathbf{e}_1$ (dotted lines ω'); only the maximal eigenvalue of the strain tensor jumps.
- the normal $\mathbf{n} = \mathbf{e}_{|q|\,\min}$; if $|q_1| > |q_2| > |q_3|$, then $\mathbf{n} = \mathbf{e}_3$ (the lines β –the internal PTZ boundary)

The arrows depict the jump in strains across the interface. The dotted line ξ separates the domains of the phases "$-$" and "$+$". The point z_0 indicates the undeformed state.

If C_1 is sign-definite, then the PTZ are restricted by the closed boundaries as shown in Fig. 6 b. If C_1 is sign-indefinite then the PTZ is unclosed. In this case there are such deformation paths on which an interface never occurs, whatever the values of strains. There are also material parameters at which the PTZ boundaries correspond only to the shear-type interfaces.

The deformation paths α, α_1 and α_2 in Figure 6 b correspond to uniaxial stretching/compression under the action of external pressure $p = 0$, $p = p_1 > 0$ and $p = p_2 > p_1$, respectively. If $p = 0$ then we obtain a normal-type interface at stretching and shear-type interface at compression when the PTZ boundary is reached. There is a critical pressure p_1 at which the normal-type interface is changed by the shear-type interface at stretching, i.e. the type of strain localization due to phase transformation at stretching is changed. Only shear type interface appear both at stretching and compression at $p > p_1$.

Spherically-symmetric two-phase deformations are shown in Figure 6 a. One can see that two solutions are possible. First solution corresponds to the point a (the "$+$" phase is in the hydrostatic state), the jump aa' across the interface and the segment $a'e$ (strains in the shell "made" of the "$-$" phase). Second solution is represented by the point b (the "$-$" phase is in the hydrostatic state), the jump bb' and the segment $b'd$. For the first solution, when the point a is reached, the "$+$" phase begins to spread from the outer surface of the sphere. The strain in the core of sphere remains unchanged (point a) during phase transformation, strains in the shell are represented by parts of the segment $a'e$, the point e shifts to a' as the interface moves to the center. Note that the second solution for which the deformations are inside the external PTZ boundaries is unstable. More detailed description of spherically-symmetric deformations is given in [1, 2, 3].

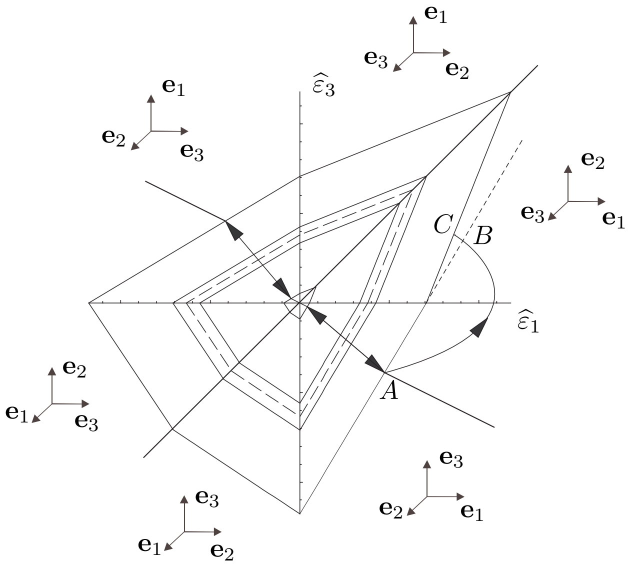


Figure 7: Plane cross-sections of the PTZ: $\varepsilon_1^p > 0$, $\varepsilon_2^p = 0$, $\varepsilon_3^p < 0$.

6.2 Deformation phase transformation

Suppose that $\mathbf{C}_+ = \mathbf{C}_- = \mathbf{C}$ is an isotropic tensor, and the self-strain tensor $\boldsymbol{\varepsilon}^p$ is not spherical. Such phase transformations we call *deformation phase transformations*. The principal axes of the tensor $\boldsymbol{\varepsilon}^p$ are anisotropy axes which are to determined as well as the normal to the interface.

The external boundary of the PTZ sub-zone "$-$" in strain space is given by [8, 12, 18]

$$\sum q_k \varepsilon_k = \gamma + \frac{1}{2}\boldsymbol{\varepsilon}^p : \mathbf{C} : \boldsymbol{\varepsilon}^p - \frac{1}{2}\mathcal{K}_*. \tag{34}$$

The external boundary of the sub-zone "$+$" is given by

$$\sum q_k \varepsilon_k = \gamma + \frac{1}{2}\boldsymbol{\varepsilon}^p : \mathbf{C} : \boldsymbol{\varepsilon}^p + \frac{1}{2}\mathcal{K}_*, \tag{35}$$

where q_k are the material parameters in the case under consideration ($\mathbf{q} = \mathbf{C} : \boldsymbol{\varepsilon}^p$), $\mathcal{K}_*$ is determined by values q_k and the type of the interface, ε_k are the eigenvalues of $\boldsymbol{\varepsilon}$. The values are put in order such that $q_1 > q_2 > q_3$ if $\varepsilon_1 > \varepsilon_2 > \varepsilon_3$.

Depending on relation between the eigenvalues ε_i^p $(i = 1, 2, 3)$ of $\boldsymbol{\varepsilon}^p$ the PTZ-boundaries may be closed (similarly to the Tresca yield surface) or unclosed. In the latter case the phase transformation is impossible on some deformation paths. An example of the PTZ cross-sections by the plane $\varepsilon_2 = 0$ is given in Figure 7. At this choice of $\boldsymbol{\varepsilon}^p$ the shear-type interfaces appear. At other relations between ε_i^p $(i = 1, 2, 3)$ the normal-type interfaces may appear. The directions of $\boldsymbol{\varepsilon}^p-$ axes are shown for different areas of strain space (we assume that $\varepsilon_1^p \geq \varepsilon_2^p \geq \varepsilon_3^p$). The deformation paths of plane stretching/compression in "1" direction and corresponding jumps of strains across the phase boundary are also drawn. Note that if in the forward phase transformation the material transforms into the deformed state A with the corresponding orientation of the axes of $\boldsymbol{\varepsilon}^p$, then during deformation along the path ABC the first appearance of the equilibrium phase boundary may occur in point B, before point C is reached. A material "remembers" the history of the transformation.

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