Equilibrium cylindrical new phase inclusion

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Abstract

We consider an elastic body undergoing stress-induced phase transformations of martensite type. We examine an existence of cylindrical new phase inclusions. We prove characteristic properties of the equilibrium cylindrical inclusion and construct the existence surfaces in strain space. We relate the surfaces with phase transition zones and new phase nucleation surfaces.

1 Introduction

Description of phase transitions in solids remains the open problem of mechanics. Roughly speaking, there are two approaches. The first one introduces internal parameters, such as a new phase concentration, and describe new phase evolution basing on formulated constitutive equations (see [1] and reference therein). This gives proper tools for quantitative descriptions "on average", but does not consider an interface as it is and remains undetermined the local strains and stresses which are important for example in related fracture problems. The second approach is based on the consideration of the conditions on the interfaces and meet the problem of finding unknown interfaces and stability analysis (see e.g. [9, 10, 11] and reference therein).

The present work represents results obtained within the framework of the second approach. Various two phase structures were described earlier. For example, ellipsoidal new phase inclusions were considered in [2, 12, 14, 5, 7], spherically symmetric two-phase deformations were studied (see [3] and reference therein), heterogeneous deformation due to multiple appearance of new phase domains was presented for laminates and ellipsoidal new pase inclusions [6, 7]. Irrespectively of new phase domain examinations, the concept of phase transition zones (PTZ) formed by of all strains which can coexist on the equilibrium two phase interface was developed (see, e.g., [6, 8]and reference therein).

The PTZ boundary acts as a transformation surface if a new phase nucleates in a form of layers (laminates). In this paper we supplement the PTZ with surfaces of ellipsoidal and cylindrical new phase domains of existence. We use previous results in the case of ellipsoids [14, 5] and we present new results for cylindrical domains, briefly mentioned in [5]. As a result we construct a transformation surfaces and demonstrate that the type of new phase domains on the direct and reverse phase transformations depends on the strain state.

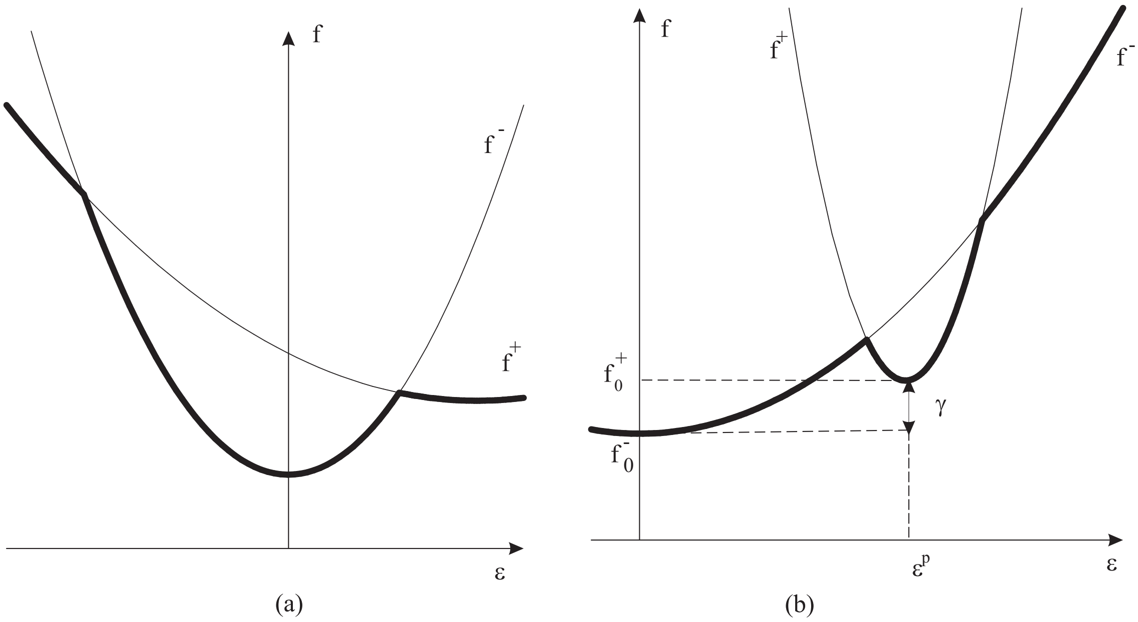

Figure 1: One-dimensional two-well energy. a – the new phase is softer. b – the parent phase is softer.

2 Cylindrical new phase inclusion

Suppose that a cylindrical inclusion with the ellipse in the base exists in an infinite body made of a material capable of undergoing stress-induced phase transformations. External strain $\boldsymbol{\varepsilon}_0$ (prescribed by conditions at infinity) is uniform. Describing phase transformations, we deal with materials characterized by a multi-well free energy density sketched for a two-well case in Fig. 1 and represented in a case of small deformations by quadratic functions

$$\begin{aligned} f(\boldsymbol{\varepsilon},\theta) &= \min_{-,+}\{f_-(\boldsymbol{\varepsilon},\theta), f_+(\boldsymbol{\varepsilon},\theta)\}, \\ f_\pm(\boldsymbol{\varepsilon},\theta) &= f^0_\pm(\theta) + \frac{1}{2}(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^p_\pm) : \mathbf{C}_\pm : (\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^p_\pm), \end{aligned} \tag{1}$$

where "–" and "+" denote the parent and new phases, $\mathbf{C}_\pm$ is a tensor of the elastic modules of the phases, $\boldsymbol{\varepsilon}$ is a strain tensor, $\boldsymbol{\varepsilon}^p_\pm$ are strains in stress-free states, $[\boldsymbol{\varepsilon}^p] \equiv \boldsymbol{\varepsilon}^p_+ - \boldsymbol{\varepsilon}^p_-$ is a transformation strain tensor, $f_\pm$ are strain energy densities of the stress free phases, θ is the temperature. The problem of the two phase equilibrium of the elastic body is reduced to the problem of equilibrium of the composite material with the unknown interface and to the problem of finding the phase interface Γ and the displacement fields $\mathbf{u}$ which are sufficiently smooth when $\mathbf{x} \notin \Gamma$ and continuous when $\mathbf{x} \in \Gamma$:

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

$$\mathbf{x} \in \Gamma \ : \ [\mathbf{u}] = 0, \tag{3}$$

$$[\boldsymbol{\sigma}] \cdot \mathbf{n} = 0, \tag{4}$$

$$[f] - \boldsymbol{\sigma} : [\boldsymbol{\varepsilon}] = 0 \tag{5}$$

Traction and displacement continuity across the interface is reduced to [14, 5]

$$[\boldsymbol{\varepsilon}] = \mathbf{K}_{\mp}(\mathbf{n}) : \mathbf{q}_{\pm}, \mathbf{q}_{\pm} = -\mathbf{C}_1 : \boldsymbol{\varepsilon}_{\pm} + [\mathbf{C} : \boldsymbol{\varepsilon}^p], \\ \mathbf{K}_{\pm}(\mathbf{n}) = \{\mathbf{n} \otimes \mathbf{G}_{\pm} \otimes \mathbf{n}\}^s, \mathbf{G}_{\pm} = (\mathbf{n} \cdot \mathbf{C}_{\pm} \cdot \mathbf{n})^{-1}, \mathbf{C}_1 = \mathbf{C}_+ - \mathbf{C}_- \tag{6}$$

where the jump in trains is determined by the normal to the interface, the strains on one side of the interface and the elastic modules on the other one.
In the case of isotropic phases

$$\mathbf{K}_{\pm} = \frac{1}{\mu_{\pm}} \left((\mathbf{nEn})^s - \frac{1}{2(1+\nu_{\pm})} \mathbf{nnnn} \right), \tag{7}$$

where $\nu_{\pm}$ and $\mu_{\pm}$ are Poisson's coefficients and the shear modules of the phases.
Using (1) and (6) one can reduce the thermodynamic equilibrium equation (5) to the equation

$$\gamma + \frac{1}{2}[\boldsymbol{\varepsilon}^p : \mathbf{C} : \boldsymbol{\varepsilon}^p] + \frac{1}{2}\boldsymbol{\varepsilon}_{\pm} : \mathbf{C}_1 : \boldsymbol{\varepsilon}_{\pm} - \boldsymbol{\varepsilon}_{\pm} : [\mathbf{C} : \boldsymbol{\varepsilon}^p] \pm \frac{1}{2}\mathbf{q}_{\pm} : \mathbf{K}_{\mp}(\mathbf{n}) : \mathbf{q}_{\pm} = 0, \tag{8}$$

(see, e.g., [5]) that can be rewritten as

$$\varphi(\boldsymbol{\varepsilon}_{\pm}) = \mp\frac{1}{2}\mathbf{q}_{\pm} : \mathbf{K}_{\mp}(\mathbf{n}) : \mathbf{q}_{\pm}, \tag{9}$$

where

$$\varphi(\boldsymbol{\varepsilon}_{\pm}) = \gamma + \frac{1}{2}[\boldsymbol{\varepsilon}^p : \mathbf{C} : \boldsymbol{\varepsilon}^p] + \frac{1}{2}\boldsymbol{\varepsilon}_{\pm} : \mathbf{C}_1 : \boldsymbol{\varepsilon}_{\pm} - \boldsymbol{\varepsilon}_{\pm} : [\mathbf{C} : \boldsymbol{\varepsilon}^p] \tag{10}$$

Since external strains are uniform, strains inside the elliptical cylinder are also uniform [4]. Then the function $\varphi(\boldsymbol{\varepsilon}_{\pm})$ is uniform inside the cylinder. Thus, the thermodynamic condition (9) can be satisfied only if the strains $\boldsymbol{\varepsilon}_+$ are such that $\mathbf{q}_+ : \mathbf{K}_- : \mathbf{q}_+$ does not depend on the normal $\mathbf{n}$. This fact leads to the following theorem.
Theorem. *If an equilibrium new phase domain is an elliptical cylinder in an isotropic homogeneous parent phase "–", and the tensors $\boldsymbol{\varepsilon}^p_+$ and $\mathbf{C}_+$ are constant inside the cylindrical inclusion and the tensor $\mathbf{C}_1$ exists, and the strain $\boldsymbol{\varepsilon}_+$ is uniform inside the inclusion, then the tensor $\mathbf{q}_+$ is axially-symmetric,*

$$\mathbf{q}_+ = q_1\mathbf{kk} + q_*(\mathbf{E} - \mathbf{kk}), \tag{11}$$

where $\mathbf{k}$ is the axe of the cylinder. The jump in strains on the phase interface is

$$[\boldsymbol{\varepsilon}] = \frac{1-2\nu_-}{2\mu_-(1-\nu_-)} q_*\mathbf{nn}. \tag{12}$$

In the case of isotropic parent phase "–" the thermodynamic equilibrium equation (8) is reduced to

$$2\gamma_* + \frac{(q_1+2q_*)^2}{9k_1} + \frac{(q_1-q_*)^2}{3\mu_1} + \frac{1-2\nu_-}{2\mu_-(1-\nu_-)} q_*^2 = 0, \tag{13}$$

where $\gamma_* = \gamma + \frac{1}{2}[\varepsilon^p] : \boldsymbol{B}_1^{-1} : [\varepsilon^p]$, $\boldsymbol{B}_\pm = \boldsymbol{C}_\pm^{-1}$, $\boldsymbol{B}_1 = \boldsymbol{B}_+ - \boldsymbol{B}_-$, μ_1 *and* k_1 *are the differences between the share and volume elastic modules of the new phase and the parent one.*

Proof. By (7),

$$\mathcal{K}(\mathbf{q},\mathbf{n}) \equiv \mathbf{q} : \mathbf{K}(\mathbf{n}) : \mathbf{q} = \frac{1}{\mu}(\mathbf{n}\cdot\mathbf{q}^2\cdot\mathbf{n} - a(\mathbf{n}\cdot\mathbf{q}\cdot\mathbf{n})^2) \tag{14}$$

where $a = \dfrac{1}{2(1-\nu)}$.

First, we prove that the quadratic form $\mathcal{K}(\mathbf{q},\mathbf{n})$ does not depend on the normal $\mathbf{n}$ to cylindrical interface if and only if the tensor $\mathbf{q}$ is axially-symmetric,

$$\mathbf{q} = q_1\mathbf{kk} + q_*(\mathbf{E} - \mathbf{kk}) \tag{15}$$

where $\mathbf{k}$ is the cylinder axe.

To prove the sufficiency we substitute (15) into (14) and obtain the expression independent on the normal to the interface,

$$\mathbf{q} : \mathbf{K} : \mathbf{q} = \frac{1}{\mu}q_*^2(1-a). \tag{16}$$

To prove the necessity we note that $\mathbf{n} = \mathbf{P}\cdot\mathbf{n}$ where $\mathbf{P} = \mathbf{E} - \mathbf{kk}$ is a projector onto the plane of the base of the cylinder. Then

$$\mathcal{K}(\mathbf{n}) = \mathbf{n}\cdot\widetilde{\mathbf{q}}^2\cdot\mathbf{n} + (\mathbf{n}\cdot\mathbf{q}\cdot\mathbf{k})^2 - a(\mathbf{n}\cdot\widetilde{\mathbf{q}}\cdot\mathbf{n})^2 \tag{17}$$

where $\widetilde{\mathbf{q}}^2 = \mathbf{P}\cdot\mathbf{q}\cdot\mathbf{P}$. The necessity condition takes the form

$$\frac{d\Phi(\mathbf{n})}{d\mathbf{n}} = 0 \tag{18}$$

where the Lagrange function

$$\Phi(\mathbf{n}) = \mathcal{K}(\mathbf{n}) + \mathcal{A}(\mathbf{n}\cdot\mathbf{n} - 1) + \mathcal{B}\mathbf{n}\cdot\mathbf{k}, \tag{19}$$

$\mathcal{A}$ and $\mathcal{B}$ are the Lagrange multipliers. By (18) and (19),

$$2\widetilde{\mathbf{q}}^2\cdot\mathbf{n} + 2(\mathbf{q}\cdot\mathbf{k})(\mathbf{n}\cdot\mathbf{q}\cdot\mathbf{k}) - 4a(\widetilde{\mathbf{q}}\cdot\mathbf{n})(\mathbf{n}\cdot\widetilde{\mathbf{q}}\cdot\mathbf{n}) + 2\mathcal{A}\mathbf{n} + \mathcal{B}\mathbf{k} = 0. \tag{20}$$

Multiplying (20) by $\mathbf{t} = \mathbf{k}\times\mathbf{n}$ we obtain

$$\mathbf{t}\cdot\widetilde{\mathbf{q}}^2\cdot\mathbf{n} + (\mathbf{t}\cdot\mathbf{q}\cdot\mathbf{k})(\mathbf{n}\cdot\mathbf{q}\cdot\mathbf{k}) - 2a(\mathbf{t}\cdot\widetilde{\mathbf{q}}\cdot\mathbf{n})(\mathbf{n}\cdot\widetilde{\mathbf{q}}\cdot\mathbf{n}) = 0. \tag{21}$$

Since the ellipse is a closed figure, $\mathbf{n}$ is an arbitrary unit vector perpendicular to the vector $\mathbf{k}$, and vectors $\mathbf{n},\mathbf{t}$ represent an arbitrary pair of orthogonal unit vectors lying in the plane of the cylinder base. Let $\mathbf{i}_1$, $\mathbf{i}_2$ in a pair of arbitrary orthogonal unit vectors in the base plane. Let take $\mathbf{n} = \mathbf{i}_1, \mathbf{t} = \mathbf{i}_2$ and then take $\mathbf{n} = \mathbf{i}_2$, $\mathbf{t} = -\mathbf{i}_1$. By (21), the following equalities must hold

$$\mathbf{i}_2\cdot\widetilde{\mathbf{q}}^2\cdot\mathbf{i}_1 + (\mathbf{i}_2\cdot\mathbf{q}\cdot\mathbf{k})(\mathbf{i}_1\cdot\mathbf{q}\cdot\mathbf{k}) - 4a(\mathbf{i}_2\cdot\widetilde{\mathbf{q}}\cdot\mathbf{i}_1)(\mathbf{i}_1\cdot\widetilde{\mathbf{q}}\cdot\mathbf{i}_1) = 0, \tag{22}$$

$$\mathbf{i}_1\cdot\widetilde{\mathbf{q}}^2\cdot\mathbf{i}_2 + (\mathbf{i}_1\cdot\mathbf{q}\cdot\mathbf{k})(\mathbf{i}_2\cdot\mathbf{q}\cdot\mathbf{k}) - 4a(\mathbf{i}_1\cdot\widetilde{\mathbf{q}}\cdot\mathbf{i}_2)(\mathbf{i}_2\cdot\widetilde{\mathbf{q}}\cdot\mathbf{i}_2) = 0. \tag{23}$$

From (22) and (23) it follows that

$$\mathbf{i}_1 \cdot \widetilde{\mathbf{q}} \cdot \mathbf{i}_1 = \mathbf{i}_2 \cdot \widetilde{\mathbf{q}} \cdot \mathbf{i}_2 \quad \text{or/and} \quad \mathbf{i}_1 \cdot \widetilde{\mathbf{q}} \cdot \mathbf{i}_2 = 0 \quad \forall \mathbf{i}_1, \mathbf{i}_2 : \ \mathbf{i}_1 \perp \mathbf{i}_2, \mathbf{i}_1 \perp \mathbf{k}, \mathbf{i}_2 \perp \mathbf{k}.$$

Thus,

$$\widetilde{\mathbf{q}} = q_* \mathbf{P}. \tag{24}$$

Then, by (22),

$$(\mathbf{i}_2 \cdot \mathbf{q} \cdot \mathbf{k})(\mathbf{i}_1 \cdot \mathbf{q} \cdot \mathbf{k}) = 0 \quad \forall \mathbf{i}_1, \mathbf{i}_2 : \ \mathbf{i}_1 \perp \mathbf{i}_2, \mathbf{i}_1 \perp \mathbf{k}, \mathbf{i}_2 \perp \mathbf{k}. \tag{25}$$

Thus, the vector $\mathbf{k}$ is a eigenvector of the tensor $\mathbf{q}$ and the tensor $\mathbf{q}$ is axially-symmetric.
Formula (12) for the jump in strain immediately follows from (15) and (6). Finally, substituting (11) into (8) we obtain (13). □
Strain tensor $\boldsymbol{\varepsilon}_+$ inside the cylinder is related with the external strain $\boldsymbol{\varepsilon}_0$ as [4, 13]

$$\boldsymbol{\varepsilon}_+ = \boldsymbol{\varepsilon}_0 + \mathbf{A} : \mathbf{q}_+, \tag{26}$$

where $\mathbf{A}$ is the Eshelby tensor which characterizes the geometrical parameters of the ellipsoidal inclusions. Its components are given by the integrals (see [13])

$$\begin{aligned}
A_{pppp} &= \frac{\chi_-}{8\pi\mu_-}(3J_{pp} + (1-4\nu_-)J_p),\\
A_{ppqq} &= \frac{\chi_-}{8\pi\mu_-}(J_{qp} - J_p),\\
J_p &= \frac{3}{2}\upsilon a_p^2 \int_0^\infty \frac{du}{(a_p^2+u)(a_q^2+u)\Delta(u)},\\
\Delta(u) &= \sqrt{(a_1^2+u)(a_2^2+u)(a_3^2+u)},\\
\upsilon &= \frac{4}{3}\pi a_1 a_2 a_3, \ \ \chi_- = \frac{1}{2(1-\nu_-)}, \ \ p, q = 1, 2, 3.
\end{aligned} \tag{27}$$

where a_1, a_2 and a_3 are the semiaxises of the ellipsoid. In the case of a cylindrical inclusion $a_1 \to \infty$ and we obtain

$$\begin{aligned}
A_{1111} &= A_{1122} = A_{1133} = A_{2211} = A_{3311} = 0,\\
A_{2222} &= \frac{\chi_-}{2\mu_-(1+\xi)^2}(3\xi + 2 - 4\nu_-(1+\xi)),\\
A_{2233} &= A_{3322} = -\frac{\chi_-\xi}{2\mu_-(1+\xi)^2},\\
A_{3333} &= \frac{\chi_-\xi}{2\mu_-(1+\xi)^2}(3\xi + 2 - 4\nu_-(1+\xi)),
\end{aligned} \tag{28}$$

where $\xi = \dfrac{a_2}{a_3}$ is the ratio of the semiaxes of the elliptical base of the cylinder. Substituting (28) into (26) and using the fact that $\boldsymbol{\varepsilon}_+ = \varepsilon_1^+ \mathbf{e}_1\mathbf{e}_1 + \varepsilon_*^+(\mathbf{e}_2\mathbf{e}_2 + \mathbf{e}_3\mathbf{e}_3)$ we obtain that

$$\begin{aligned} \varepsilon_1^0 &= \varepsilon_1^+, \\ \varepsilon_2^0 &= \varepsilon_*^+ - \frac{\chi_-}{2\mu_-(1+\xi)}(3k_+\varepsilon_p - \lambda_1(2\varepsilon_*^+ + \varepsilon_1^+) - \mu_1\varepsilon_*^+), \\ \varepsilon_3^0 &= \varepsilon_*^+ - \frac{\chi_-\xi}{2\mu_-(1+\xi)}(3k_+\varepsilon_p - \lambda_1(2\varepsilon_*^+ + \varepsilon_1^+) - \mu_1\varepsilon_*^+). \end{aligned} \tag{29}$$

The domains of existence of the cylindrical new phase inclusions can be constructed in the external strains space if we substitute (29) into (13) taking into account that

$$\mathbf{q}_+ = -\mathbf{C}_1 : \boldsymbol{\varepsilon}_+ + [\mathbf{C} : \boldsymbol{\varepsilon}^p]. \tag{30}$$

Substituting (15) into (26) we obtain

$$\boldsymbol{\varepsilon}_+ = \boldsymbol{\varepsilon}_0 + q_*\boldsymbol{\omega}, \tag{31}$$

where $\boldsymbol{\omega} = \mathbf{A} : \mathbf{E}$. The eigenvectors of $\boldsymbol{\omega}$ coincide with the cylinder axes and its eigenvalues are positive. Then

$$\frac{1}{q_*}(\varepsilon_*^+ - \mathbf{n}\cdot\boldsymbol{\varepsilon}_0\cdot\mathbf{n}) \geqslant 0, \tag{32}$$

where $\mathbf{n}$ is a arbitrary normal to the cylinder surface. The inequality (32) is a restriction on the domain of existence of equilibrium new phase cylinders.

From (31) it also follows that, since tensors $\boldsymbol{\omega}$ and $\boldsymbol{\varepsilon}_+$ are coaxial to the new phase cylinder, the external strain tensor $\boldsymbol{\varepsilon}_0$ is coaxial to the cylinder too. It means that in the media loaded by external strains coaxial to the external strains cylinder appears.

In Fig.2 axisymmetric sections of phase transition zones and domains of new phase ellipsoids and cylinders existence are presented. Filled areas are the phase transition zones (see, e.g., [8, 6]). PTZ boundaries correspond to the laminates of infinitesimal concentration of the new phase. Dotted lines correspond to the appearance of cylindrical inclusion, dashed lines a constructed according to [14] and correspond to the appearance of ellipsoidal inclusions.

At the points where dashed lines touch the dotted lines one of the axes of the ellipsoidal inclusion tend to infinity and the ellipsoid becomes the cylinder. At the points where dashed and dotted lines touch the solid lines two axes of the ellipsoids and one of the axes of the ellipse in the base of the cylinder tends to infinity and both the ellipsoid and the cylinder become simple laminates. At the points where dotted lines touch the solid lines one of the axes of the ellipse in the base of the cylinder tends to infinity and the cylinder becomes the simple laminates.

The limit transformation surface is an envelope of all existence domains. Various parts of the transformation surface on the one hand correspond to various two-phase structures and on the other hand correspond to various strain states. Thus, on the different straining paths one can expect the appearance of the different equilibrium two phase structures.

Note that the PTZ boundaries are not convex everywhere. Cylinders and ellipsoids allowed us to construct the convex envelope almost everywhere. We expect that the remained nonconvex part will be covered after examinations of high-order laminates.

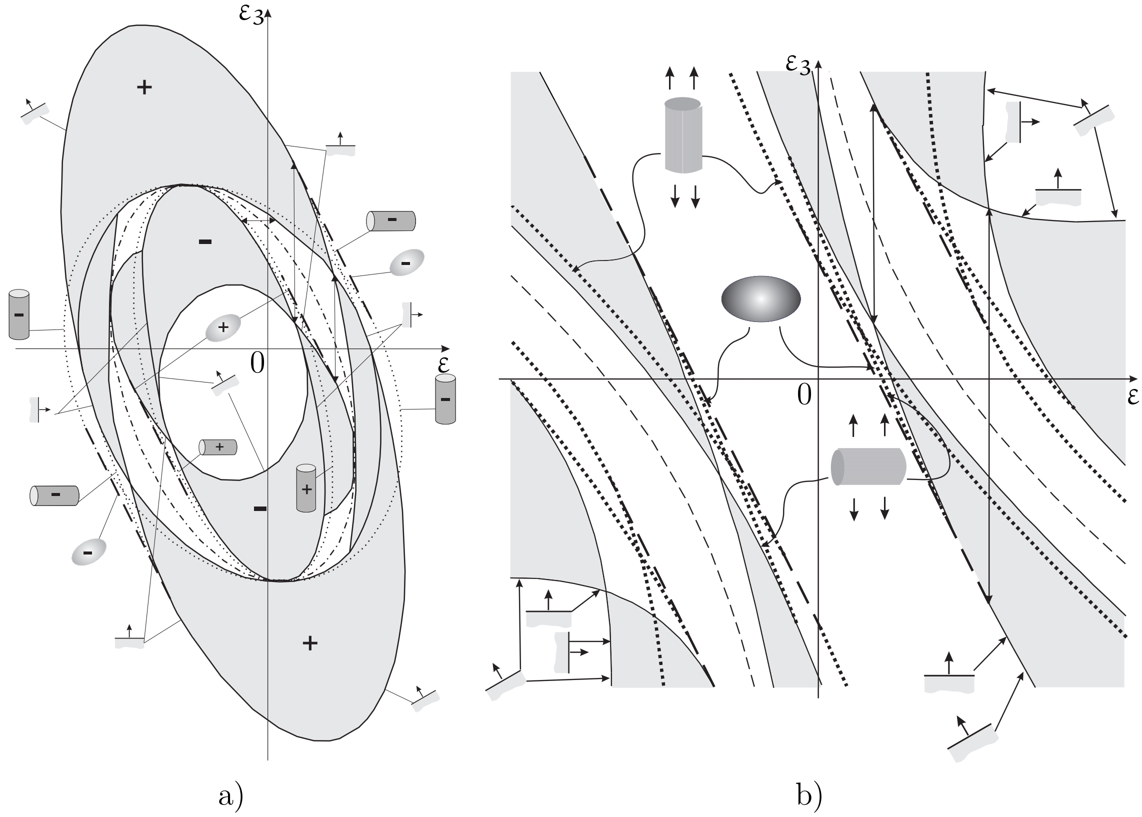

Figure 2: Axisymmetric section of the external strain space, ε_1=ε_2=ε. a) is a case when $\mu_1 < 0$, b) is a case when $\mu_1 > 0$.

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