



PHASE TRANSITIONS IN ELASTOPLASTIC MATERIALS : CONTINUUM THERMOMECHANICAL THEORY AND EXAMPLES OF CONTROL—PART I†

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ABSTRACT

A general thermomechanical theory of phase transitions (PT) in elastoplastic materials is presented. The PT criterion and extremum principle for the determination of all unknown parameters are derived. We obtain the result that the dissipative threshold in the PT criterion is proportional to yield stress. Two boundary-value problems are solved analytically: PT in a thin layer (horizontally and optimally inclined) in a rigid-plastic half-space under the action of applied pressure and shear stresses and PT under compression and shear of materials in Bridgman anvils. The solutions illustrate the fundamental difference in PT conditions for the homogeneously distributed pressure and shear stresses in the first problem and strongly nonhomogeneous pressure distribution in the second problem. In particular, in the first problem additional shearing significantly improves the condition of appearance of soft materials and does not affect the appearance of strong materials. In the second problem, rotation of an anvil works much more effectively for the synthesis of strong phases than weak ones. A number of experimental results are explained, and some of the interpretations are completely unexpected. It is found that an improvement in PT condition due to a rotation of an anvil is attributed not to the plastic strain, but to the possibility of an additional displacement, compensating a volume decrease because of PT. It is connected with a reduction of frictional shear stress in a radial direction. © 1997 Elsevier Science Ltd

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1. INTRODUCTION

Phase transitions (PT) in elastoplastic materials are phenomena that are very widespread in nature, physical experiments and modern technologies. Practically all PT with volumetric transformation strain exceeding 0.5% are accompanied by plastic strains, e.g. by heat treatment of steels. Thermomechanical treatment of materials involves consecutively or simultaneously occurring PT and plastic straining, which results in the required microstructure and the physical–mechanical properties. Strain-induced PT and transformation-induced plasticity (TRIP) are other important examples. Known experiments exhibit a very strong influence of large shear plastic strains on PT, e.g. a significant reduction in PT pressure and the obtaining of fundamentally new materials which are impossible to produce without additional plastic strains

† Dedicated to Professor Dr.-Ing. Dr.h.c. mult. Erwin Stein on the occasion of his 65th birthday.

(Bridgman, 1952; Alexandrova *et al.*, 1987, 1988; Blank *et al.*, 1994; Serebryanaya *et al.*, 1995; Batsanov *et al.*, 1995).

Most of the above phenomena have purely qualitative explanations and their applications in technologies are based on purely empirical observations. The deeper understanding of the fundamental principles of temperature, stress and strain induced PT in inelastic materials and their quantitative description can yield fundamentally new results in the development of new technologies and materials, as well as the optimization of existing ones.

In order to describe PT in an elastic solid, the principle of a minimum of free energy is usually used. Very impressive physical, mechanical and mathematical results related to the formulation and solution of various problems (e.g. problems of formation of the heterophase structure and elastic domains) are considered in various papers and books [see, e.g. Khachaturyan (1983), Grinfeld (1991), Hornbogen (1991), Ball and James (1992), Gurtin (1993), Roitburd (1993), Wollants *et al.* (1993) and Olson (1996)].

For inelastic materials the corresponding principle was lacking and the theory of PT in inelastic solids is only in its early stages. The first results were related to the solution of some simple problems, e.g. the appearance of the spherical (Lifshitz and Gulida, 1952; Roitburd and Temkin, 1986; Kaganova and Roitburd, 1987), ellipsoidal (Kaganova and Roitburd, 1989) and the plate-like nucleus (Bar'yachtar *et al.*, 1986) and growth of the spherical nucleus (Roitburd and Temkin, 1986; Kaganova and Roitburd, 1987). In most of these papers the PT criterion and extremum principle for the definition of some unknown parameters are the same as for PT in elastic materials, i.e. some thermodynamic potential (Gibbs free energy of the whole system) is minimized. It is known that, in contrast to elastic materials, for elastoplastic ones such an extremum principle could not be proved. It is related to the necessity of considering the plastic dissipation and path-dependency. Consequently, all the above solutions have a preliminary character and should be checked based on more recent approaches. Only in a paper by Roitburd and Temkin (1986) is an alternative description of the appearance of the spherical nucleus used. It is assumed that some mechanical work (not energy!) should be less than the change in chemical free energy, which in some particular cases can be derived from recent considerations. Unfortunately this idea did not receive any further development: the appearance of the ellipsoidal nucleus (Kaganova and Roitburd, 1989) is based on the principle of the minimum of free energy. Numerous investigations of PT in elastoplastic materials (Fischer *et al.*, 1994; Marketz and Fischer, 1994, 1995) are related to the comparison of Gibbs free energy before and after PT. In a paper by Kondaurov and Nikitin (1986) the PT criterion is obtained for the points of a moving interface in viscoplastic material, when the plastic strain increment is equal to zero in the course of PT. An interface propagation condition which takes into account the plastic strain increment is derived by Levitas (1992a, 1995a-c).

An averaged description of PT in terms of the volume fraction of martensite is presented by Levitas (1990, 1992b, 1995b), Raniecki and Bruhns (1991), Bhattacharyya and Weng (1994) at small strain and by Levitas (1992b, 1996c) at large strain. Numerical averaging using the thermodynamic description is presented by Marketz and Fischer (1994, 1995) and Levitas *et al.* (1995, 1996); Leblond *et al.*

(1989) considered PT without regard for thermodynamics. A self-consistent approach to TRIP (without any thermodynamic criterion) is developed by Diani *et al.* (1995). Phase transitions from the point of view of instability and post-bifurcation phenomena were investigated by Levitas (1992a, 1995a). It was shown that the fulfilment of the local PT criterion (e.g. for propagation of an interface) is not sufficient for the occurrence of PT. Only the choice of the stable post-bifurcation solution for the whole body gives a final result and represents the global PT criterion. The statistical model (Olson and Cohen, 1975) is based on the observation that strain-induced nucleation occurs predominantly at intersections of shear-bands. The development of the model and its numerical implementation is presented in Stringfellow *et al.* (1992).

In this paper we will use a general thermomechanical approach for the description of coherent and noncoherent PT in dissipative materials developed by Levitas (1992a, 1995a–d, 1996a, d). We consider not the whole body, but *material points* only in which the PT occurs at the current time, e.g. the point of the new nucleus or a moving interface. Phase transitions are considered as a *thermomechanical process* of growth of transformation (Bain) strain from the initial to the final value, which is accompanied by a change in all the material's properties. Using the second law of thermodynamics we determine a *dissipation increment* during the PT X , related to the PT only (excluding plastic dissipation and dissipation due to other processes). For $X < 0$ PT is thermodynamically impossible, for $X = 0$ PT is possible but without dissipation. Consequently the criterion of PT without dissipation due to PT is obtained without any additional assumptions, using the second law of thermodynamics only. For PT with dissipation it is accepted that $X = k$, where k is an experimentally determined value of dissipation due to PT. After the integration over the transforming volume the nucleation and interface propagation criteria are derived both for coherent and noncoherent PT. For points without PT evidently $X = 0$; that is why it is senseless to study them. They affect the PT through the stress field, because the stress variation in the transforming region in the course of PT is determined by the solution of the boundary-value problem for the whole body.

The PT criterion is only one scalar equation which is not sufficient for the determination of all unknown parameters such as position, shape and orientation of nuclei, transformation strain and so on. For these purposes a new thermomechanical postulate, named the *postulate of realizability*, is formulated (Levitas, 1992a, 1995a). It is shown (Levitas, 1992a, 1995a, e) that the postulate of realizability gives some known and some completely new results for various dissipative systems. Using it, the extremum principle for the determination of all unknown parameters is derived.

The advantages of the proposed approach are the following. The PT criterion is derived practically using the second law of thermodynamics only. It is valid for an arbitrary dissipative material, because the material's constitutive equations are not used in the derivation. Derivation of the extremum principle is based on the postulate of realizability, which is checked for various thermodynamic systems. It is easy to extend the approach to new situations, using the second law of thermodynamics. For example in papers by Levitas (1995c, 1996a, d) the results are generalized with a consistent account of the temperature variation in transforming particles in the course of PT and for media with internal variables. The aims of the present paper are:

- Using the theory developed to formulate and solve analytically a number of

model problems which can be applied to the interpretation of typical experimental results.

- To show that in the first approximation plastic strains affect a stress variation in transforming particles in the course of PT and a value k only. But this is sufficient for the description of the majority of experimental results, without additional physical mechanisms and hypotheses, using a suggested thermomechanical theory and classical elastoplasticity.
- To analyze and classify the various useful examples of stress field variation during PT.
- To suggest the methods of control of PT by the purposeful control of stress-strain fields.

In Section 2 the PT criterion and extremum principle for the determination of all unknown parameters are derived. Two boundary-value problems are formulated and solved analytically in Sections 3 and 4: PT in a thin layer (horizontal and optimally inclined) in a rigid-plastic half-space under the action of applied pressure and shear stresses; PT under compression and shear of materials in Bridgman anvils. The solutions illustrate the fundamental difference in PT conditions for the homogeneously distributed pressure and shear stresses in the first problem and strongly non-homogeneous pressure distribution in the second problem. In particular, in the first problem additional shearing significantly improves the condition of appearance of soft materials and does not affect the appearance of strong materials. In the second problem, rotation of an anvil works much more effectively for the synthesis of strong phases than weak ones. A number of experimental results are explained, and some of the interpretations are completely unexpected. It is found that an improvement in PT condition due to a rotation of an anvil is attributed not to the plastic strain, but to the possibility of an additional displacement, compensating a volume decrease because of PT. It is connected with a reduction of frictional shear stress in a radial direction due to the rotation of an anvil. A new explanation of the pressure self-multiplication effect is obtained based on the higher yield stress of the new phase.

These solutions together with the solutions obtained in Part II of this paper are used for the formulation of methods of control of PT by means of the purposeful control of stress-strain fields.

2. THERMOMECHANICAL THEORY

2.1. Phase transition criterion

Consider a volume V of a multiphase material with prescribed boundary data on a surface S . Assume that in small volume $V_n \in V$ with the boundary Σ_n a PT occurs in time Δt . We will consider simple materials only, i.e. material's behaviour at the given point is independent of thermomechanical processes at other points. We admit the second law of thermodynamics for each point of a volume V_n in the form of the Planck inequality

$$\mathcal{D} = \sigma : \dot{\epsilon} - \rho \dot{\psi} - \rho s \dot{\theta} \geq 0. \quad (1)$$

Here \mathcal{D} is the rate of dissipation per unit volume, ρ is the mass density, s is the entropy, ψ is the specific Helmholtz free energy, σ and ε are the stress and strain tensors, θ is the temperature. PT is considered as a thermomechanical process of growth of transformation (Bain) strain from the initial to the final value, which is accompanied by change in all the material's properties. The total dissipation increment during the PT at each transforming material point is defined as follows

$$N := \int_t^{t+\Delta t} \mathcal{D} dt = \int_{\varepsilon_1}^{\varepsilon_2} \sigma : d\varepsilon - \Delta\psi - \int_{\theta_1}^{\theta_2} \rho s d\theta, \quad (2)$$

where $\Delta\psi = \rho(\psi_2 - \psi_1)$. Assume that during PT three dissipative processes occur: PT itself, plastic flow and the process of variation of a certain unspecified internal variable \mathbf{g} . As an example of an internal variable a dislocation density tensor or tensor of internal stresses can be considered. The dissipation increment in the course of PT due to plastic flow and variation of the internal variable can be given as

$$N_{pg} = \int_t^{t+\Delta t} (\mathbf{X}_p : \dot{\varepsilon}^p + \mathbf{X}_g : \dot{\mathbf{g}}) dt, \quad \mathbf{X}_p := \sigma - \rho \frac{\partial \psi}{\partial \varepsilon^p}, \quad \mathbf{X}_g := -\rho \frac{\partial \psi}{\partial \mathbf{g}}, \quad (3)$$

where \mathbf{X}_p and \mathbf{X}_g are the generalized dissipative forces, conjugated with plastic strain rates $\dot{\varepsilon}^p$ and $\dot{\mathbf{g}}$, respectively. The expression for \mathbf{X}_p and \mathbf{X}_g is defined using the standard thermodynamic procedure for materials without a PT (Levitas, 1992b, 1996a). The dissipation increment X due to a PT itself (the driving force for the PT) is the difference between N and the N_{pg} , i.e.

$$X = \int_{\varepsilon_1}^{\varepsilon_2} \sigma : d\varepsilon - \Delta\psi - \int_{\theta_1}^{\theta_2} \rho s d\theta - \int_t^{t+\Delta t} (\mathbf{X}_p : \dot{\varepsilon}^p + \mathbf{X}_g : \dot{\mathbf{g}}) dt. \quad (4)$$

The simplest assumption that all the three dissipative processes are mutually independent results in conditions that dissipation increments due to each dissipative process should be nonnegative, in particular $X \geq 0$. Consequently, at $X < 0$ PT is impossible. The condition $X = 0$ is the criterion of PT without dissipation due to PT, because PT is possible (no conflict with the second law of thermodynamics) and dissipation increment due to PT is zero. Since practically all martensitic transformations, even in elastic materials, are accompanied with dissipation and hysteresis, the PT criterion has the form

$$X = k. \quad (5)$$

Here k is an experimentally determined value of dissipation due to PT, which can depend on parameters θ , ε^p , \mathbf{g} , ... At $X < k$ PT is impossible.

It looks unusual that the PT criterion is formulated for the dissipation increment and not for the generalized dissipative force like \mathbf{X}_p or \mathbf{X}_g . The strict thermomechanical derivation of necessity to use the dissipation increment X is given by Levitas (1996a, d).

For each point of nuclei V_n , PT criterion (5) should be met. Integrating this criterion over the volume V_n we obtain the necessary condition of *nucleation*

$$\int_{V_n} X dV_n = \int_{V_n} k dV_n, \quad (6)$$

or taking into account (4) for X we have

$$\begin{aligned} \int_{V_n} \int_{\varepsilon_1}^{\varepsilon_2} \boldsymbol{\sigma} : d\varepsilon dV_n &= \int_t^{t+\Delta t} \int_{\Sigma_n} \mathbf{p} \cdot \mathbf{v} d\Sigma_n dt = \int_{V_n} \Delta\psi dV_n + \int_{V_n} \int_{\theta_1}^{\theta_2} \rho s d\theta dV_n \\ &+ \int_{V_n} \int_t^{t+\Delta t} (\mathbf{X}_p : \dot{\boldsymbol{\varepsilon}}^p + \mathbf{X}_g : \dot{\mathbf{g}}) dt dV_n + \int_{V_n} k dV_n, \quad (7) \end{aligned}$$

where \mathbf{v} is the velocity on Σ_n from the side of the nucleus, $\mathbf{p} = \boldsymbol{\sigma} \cdot \mathbf{n}$ is the stress vector, \mathbf{n} is the unit normal to Σ_n . Note that Gauss' theorem was used in this case. In the given work we neglect the surface energy in comparison with other terms in (7). Equation (5) is valid for the points of an interface; in this case some additional transformations are useful (Levitas, 1995c, 1996a).

Temperature variation in the course of PT can be determined using the first law of thermodynamics or entropy balance equation, in particular, under assumption that the process is adiabatic (Levitas, 1996a, d). Here we assume the isothermal process and $\mathbf{X}_g = 0$.

If we decompose

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p + \boldsymbol{\varepsilon}^t, \quad (8)$$

where $\boldsymbol{\varepsilon}^e$ and $\boldsymbol{\varepsilon}^t$ are elastic and transformation strains, then terms $\boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^p$ in the left and right parts of (7) eliminate each other:

$$\int_{\varepsilon_1}^{\varepsilon_2} \int_{V_n} \left(\boldsymbol{\sigma} : d(\boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^t) + \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^p} : d\boldsymbol{\varepsilon}^p \right) dV_n - \int_{V_n} \Delta\psi dV_n - \int_{V_n} k dV_n = 0. \quad (9)$$

At $(\partial\psi)/(\partial\boldsymbol{\varepsilon}^p) = 0$, (9) has the same form as for PT in elastic materials; plasticity affects a variation of $\boldsymbol{\sigma}$ in the course of PT and the value k . If

$$\rho\psi_i = 0.5\boldsymbol{\varepsilon}_i^e : \mathbf{E}_i : \boldsymbol{\varepsilon}_i^e + \rho\psi_i^\theta, \quad i = 1, 2 \quad \text{and} \quad \mathbf{E}_1 = \mathbf{E}_2, \quad (10)$$

where \mathbf{E}_i are the tensors of elastic moduli of i -phase, ψ_i^θ is the thermal part of the free energy, then

$$\begin{aligned} \int_{\varepsilon_1^e}^{\varepsilon_2^e} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^e &= \int_{\varepsilon_1^e}^{\varepsilon_2^e} \boldsymbol{\varepsilon}^e : \mathbf{E} : d\boldsymbol{\varepsilon}^e = 0.5(\boldsymbol{\varepsilon}_2^e : \mathbf{E} : \boldsymbol{\varepsilon}_2^e - \boldsymbol{\varepsilon}_1^e : \mathbf{E} : \boldsymbol{\varepsilon}_1^e) \quad \text{and} \\ \int_{V_n} \int_{\varepsilon_1^t}^{\varepsilon_2^t} \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^t dV_n &- \int_{V_n} \Delta\psi^\theta dV_n - \int_{V_n} k dV_n = 0, \quad (11) \end{aligned}$$

i.e. the elastic strains also disappear. In the quasi-static formulation the equilibrium equations should be fulfilled for each intermediate value of transformation strain $\boldsymbol{\varepsilon}^t$. The constitutive equations should be given for each $\boldsymbol{\varepsilon}^t$ (i.e. for the whole transformation process) as well.

2.2. The postulate of realizability

To determine all unknown parameters \mathbf{b} (position, shape and orientation of nucleus, ε^t , ε_2 and ε_1 and so on) let us use the postulate of realizability (Levitas, 1992a, 1995a).

If starting from the state with

$$\int_{V_n^*} (X(\mathbf{b}^*) - k(\mathbf{b}^*)) dV_n < 0 \quad (12)$$

for all possible PT parameters \mathbf{b}^* (i.e. PT does not occur) in the course of variation of boundary data the condition (6) is fulfilled the first time for some of the parameters \mathbf{b} , then nucleation will occur with this \mathbf{b} .

If, in the course of variation of boundary data the criterion (6) is met for one or several \mathbf{b} , then for other arbitrary \mathbf{b}^* inequality (12) should hold, as in the opposite case for this \mathbf{b}^* condition (6) had to be met before it was satisfied for \mathbf{b} . Consequently, we obtain the extremum principle

$$\int_{V_n^*} (X(\mathbf{b}^*) - k(\mathbf{b}^*)) dV_n < 0 = \int_{V_n} (X(\mathbf{b}) - k(\mathbf{b})) dV_n \quad (13)$$

for determination of all unknown parameters \mathbf{b} . From principle (13) using (9) we obtain

$$\begin{aligned} \int_{\varepsilon_1^*}^{\varepsilon_2^*} \int_{V_n^*} \boldsymbol{\sigma}^* : d(\boldsymbol{\varepsilon}^{e*} + \boldsymbol{\varepsilon}^{t*}) dV_n - \int_{V_n^*} \Delta\psi^* dV_n - \int_{V_n^*} k^* dV_n < 0 \\ = \int_{\varepsilon_1}^{\varepsilon_2} \int_{V_n} \boldsymbol{\sigma} : d(\boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^t) dV_n - \int_{V_n} \Delta\psi dV_n - \int_{V_n} k dV_n. \end{aligned} \quad (14)$$

Corresponding principles for points of coherent and noncoherent interfaces, based on the principle (13), are given in detail in papers by Levitas (1992a, 1995a, b). The main essence of the postulate of realizability is: if only some dissipative process (plastic flow, PT) can occur, it will occur, i.e. the first fulfilment of the necessary energetic condition is sufficient for the beginning of a dissipative process.

3. PHASE TRANSITION IN A THIN LAYER

3.1. Phase transition in a thin horizontal layer

Consider an infinite rigid-plastic half-space with prescribed normal σ_n and shear τ stresses on the whole surface (Fig. 1) under plane strain condition. Assume that a coherent PT occurs in the layer along the whole surface and the solution does not depend on the x coordinate. The same solution is valid, if PT occurs in a parallel layer inside of the half-space. Material outside of the layer is rigid. Let

$$\boldsymbol{\varepsilon}^t = (0.5\varepsilon_0 \mathbf{i} + \gamma^t(\mathbf{tn})_s) \boldsymbol{\xi} = 0.5\boldsymbol{\xi} \begin{pmatrix} \varepsilon_0 & \gamma^t \\ \gamma^t & \varepsilon_0 \end{pmatrix}, \quad (15)$$

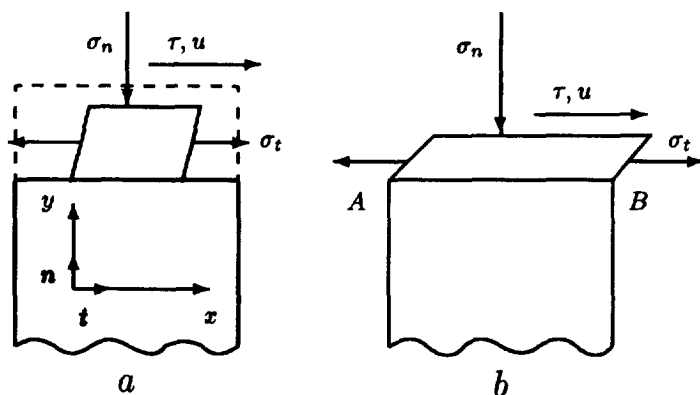


Fig. 1. Coherent PT in thin layer.

where ε_o and γ^t are the volumetric and shear transformation strains, \mathbf{i} the two dimensional unit tensor, ξ is a parameter, growing from 0 to 1 during the PT; the subscript s means symmetrization. It is assumed for convenience that compressive strains and stresses are positive. The Tresca yield condition results in

$$f(\sigma) = (\sigma_n - \sigma_t)^2 + 4\tau^2 = \sigma_y^2 \quad (16)$$

(Hill, 1950), where σ_t is the tangential stress and σ_y the yield limit in simple compression (tension).

For the complete solution of a problem it is necessary to know how the yield stress in the transforming particle varies during the PT, i.e. a function $\sigma_y(\xi)$ with $\sigma_y(0) = \sigma_{y1}$ and $\sigma_y(1) = \sigma_{y2}$. For simplicity we assume that at the beginning of the PT the yield stress makes an instantaneous jump to the value in the new phase. Various alternative assumptions are possible, e.g. $\sigma_y(\xi) = (1 - \xi)\sigma_{y1} + \xi\sigma_{y2}$.

In Fig. 1(a) a transformed particle is shown after transformation strain, but to satisfy displacement continuity across the interface AB and independence of solution of x , additional plastic strain is needed [Fig. 1(b)]. We assume that transformation and plastic strains are homogeneous in a layer and that the stress field is homogeneous and time independent. The nucleation criterion (11) gives

$$X = 0.5(\sigma_n \varepsilon_o + \sigma_t \varepsilon_o) + \tau \gamma^t - \Delta\psi^\theta = k_{1 \rightarrow 2}, \quad (17)$$

with $\tau \gamma^t \geq 0$. The yield condition (16) gives $\sigma_t = \sigma_n - \sqrt{\sigma_{y2}^2 - 4\tau^2}$, because plastic compression in direction \mathbf{n} is possible for $\sigma_n > \sigma_t$ only. Substituting σ_t in (17) we obtain the PT pressure

$$\sigma_n^{1 \rightarrow 2} = \frac{\Delta\psi^\theta}{\varepsilon_o} + \frac{k_{1 \rightarrow 2}}{\varepsilon_o} + \frac{\sqrt{\sigma_{y2}^2 - 4\tau^2}}{2} - \frac{\tau \gamma^t}{\varepsilon_o}. \quad (18)$$

For reverse PT we have

$$X = -0.5(\sigma_n \varepsilon_o - \sigma_t \varepsilon_o) - \tau \gamma^t + \Delta\psi^\theta = k_{2 \rightarrow 1} > 0. \quad (19)$$

It follows from the yield condition in this case that $\sigma_t = \sigma_n + \sqrt{\sigma_{y1}^2 - 4\tau^2}$, because

plastic compression in direction \mathbf{t} is possible for $\sigma_t > \sigma_n$ only. Substituting σ_t in the expression for X we obtain the reverse PT pressure

$$\sigma_n^{2 \rightarrow 1} = \frac{\Delta\psi^\theta}{\varepsilon_o} - \frac{k_{2 \rightarrow 1}}{\varepsilon_o} - \frac{\sqrt{\sigma_{y1}^2 - 4\tau^2}}{2} - \frac{\tau\gamma^t}{\varepsilon_o}. \quad (20)$$

The pressure hysteresis is

$$H := \sigma_n^{1 \rightarrow 2} - \sigma_n^{2 \rightarrow 1} = \frac{\sqrt{\sigma_{y2}^2 - 4\tau^2}}{2} - \frac{\sqrt{\sigma_{y1}^2 - 4\tau^2}}{2} + \frac{k_{1 \rightarrow 2} + k_{2 \rightarrow 1}}{\varepsilon_o}. \quad (21)$$

At $\tau = 0$,

$$\sigma_n^{1 \rightarrow 2} = \frac{\Delta\psi^\theta}{\varepsilon_o} + \frac{k_{1 \rightarrow 2}}{\varepsilon_o} + 0.5\sigma_{y2}, \quad \sigma_n^{2 \rightarrow 1} = \frac{\Delta\psi^\theta}{\varepsilon_o} - \frac{k_{2 \rightarrow 1}}{\varepsilon_o} - 0.5\sigma_{y1},$$

$$H = 0.5(\sigma_{y1} + \sigma_{y2}) + \frac{k_{1 \rightarrow 2} + k_{2 \rightarrow 1}}{\varepsilon_o}. \quad (22)$$

At $k_{1 \rightarrow 2} = k_{2 \rightarrow 1} = \sigma_{y1} = \sigma_{y2} = \tau = 0$ we will get the result of equilibrium thermodynamics

$$\sigma_{n,eq}^{1 \rightarrow 2} = \sigma_{n,eq}^{2 \rightarrow 1} = \frac{\Delta\psi^\theta}{\varepsilon_o}, \quad H = 0, \quad (23)$$

which neglects all the types of dissipation. Equation (23) defines the pressure of thermodynamic equilibrium. Let us analyze the result. At $\gamma^t = 0$, despite the fact that τ does not contribute to X , due to appearance of τ in the yield condition, it can significantly reduce $\sigma_n^{1 \rightarrow 2}$ and H , which is in agreement with experiments (Bokarev *et al.*, 1986; Alexandrova *et al.*, 1987, 1988; Tang *et al.*, 1993). At $\tau = \tau_{\max} = 0.5\sigma_{y2}$ ($\sigma_{y1} > \sigma_{y2}$) the terms with σ_{y1} disappear in the expressions for $\sigma_n^{1 \rightarrow 2}$. At $\gamma^t \neq 0$ $\sigma_n^{1 \rightarrow 2}$ receives an additional reduction and at large τ and γ^t it is possible that $\sigma_n^{1 \rightarrow 2} < \sigma_{n,eq}^{1 \rightarrow 2}$. This result is in agreement with experiments by Alexandrova *et al.* (1988), in which applied τ or shear plastic strain reduce the PT pressure, up to a value which is less than thermodynamical equilibrium.

Let us consider the influence of plastic shear on PT. We assume that the plastic strain tensor is proportional to the parameter ξ

$$\varepsilon^p = (\varepsilon^p(\mathbf{nn} - \mathbf{tt}) + \gamma^p(\mathbf{tn})_s)\xi = \begin{pmatrix} \varepsilon^p & 0.5\gamma^p \\ 0.5\gamma^p & -\varepsilon^p \end{pmatrix} \xi, \quad \dot{\varepsilon}^p = (\dot{\varepsilon}^p(\mathbf{nn} - \mathbf{tt}) + \gamma^p(\mathbf{tn})_s)\dot{\xi} = \dot{\varepsilon}^p \dot{\xi} / \xi, \quad (24)$$

where ε^p and γ^p are the normal (along \mathbf{n}) and the shear plastic strain, and plastic incompressibility is taken into account. Only in this case can the condition of the displacement continuity across the interface be satisfied. The associated flow rule (Hill, 1950) reads

$$\dot{\varepsilon}^p = \dot{\varepsilon}^p \dot{\xi} / \xi = h \frac{\partial f}{\partial \sigma}, \quad \varepsilon^p \dot{\xi} / \xi = h(\sigma_n - \sigma_t), \quad \gamma^p \dot{\xi} / \xi = 4h\tau, \quad \frac{\gamma^p}{\varepsilon^p} = \frac{4\tau}{\sigma_n - \sigma_t}, \quad (25)$$

where h is a scalar. The displacement continuity across the interface $\mathbf{AB} \varepsilon_{tt} = \mathbf{t} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{t} = 0$ (displacement and consequently normal strain in \mathbf{t} direction are zero) leads to

$$\mathbf{t} \cdot (\boldsymbol{\varepsilon}^l + \boldsymbol{\varepsilon}^p) \cdot \mathbf{t} = 0.5\varepsilon_0 - \varepsilon^p = 0 \quad \text{and} \quad \varepsilon^p = 0.5\varepsilon_0. \quad (26)$$

Then from (25)

$$\begin{aligned} \frac{\gamma^p}{\varepsilon^p} &= \frac{2\gamma^p}{\varepsilon_0} = \frac{4\tau}{\sigma_n - \sigma_t} = \frac{4\tau}{\sqrt{\sigma_y^2 - 4\tau^2}} = 2 \frac{2\tau/\sigma_y}{\sqrt{1 - (2\tau/\sigma_y)^2}}, \\ \gamma^p &= \frac{\varepsilon_0 a}{\sqrt{1 - a^2}}, \quad a := \frac{2\tau}{\sigma_y}, \quad \tau = \frac{\sigma_y}{2} \frac{\gamma^p}{\sqrt{\varepsilon_0^2 + \gamma^{p2}}}, \quad \sqrt{\sigma_y^2 - 4\tau^2} = \frac{\sigma_y \varepsilon_0}{\sqrt{\varepsilon_0^2 + \gamma^{p2}}}. \end{aligned} \quad (27)$$

After substitution of (27) in (18) we obtain

$$\sigma_n^{1 \rightarrow 2} = \frac{\Delta\psi^\theta}{\varepsilon_0} + \frac{k_{1 \rightarrow 2}}{\varepsilon_0} + \frac{\sigma_{y2}}{2} \frac{\varepsilon_0}{\sqrt{\varepsilon_0^2 + \gamma^{p2}}} - \frac{\sigma_{y2}}{2} \frac{\gamma^l \gamma^p}{\varepsilon_0 \sqrt{\varepsilon_0^2 + \gamma^{p2}}}. \quad (28)$$

Equation (28) exhibits the experimentally observed (Bokarev *et al.*, 1986; Alexandrova *et al.*, 1987, 1988) decrease of PT pressure under the growing plastic shear; at $2\tau = \sigma_{y2}$, $\gamma^p \rightarrow \infty$ and the third term in (28) disappears.

If on the surface S the horizontal displacement u instead of τ is prescribed, then $\gamma^p = u/b - \gamma^l$, where b is the width of the transformed layer. The maximum value of $X - k$ at $k = \text{const.}$ and consequently the minimal value $\sigma_n^{1 \rightarrow 2}$ will be at $b \rightarrow 0$ and $\gamma^p \rightarrow \infty$, i.e. (according the postulate of realizability) PT starts in infinitesimally narrow layer (on the slip surface) which is in agreement with experiments (Bernshtein *et al.*, 1993).

Allowing for adiabatic heating leads to finite b and γ^p (Levitas, 1996d).

3.2. Evaluation of the dissipative threshold k

For the evaluation of the dissipative threshold k let us use the experimental evidence presented by Estrin (1993). The linear dependence between microhardness of materials and pressure hysteresis during the PT was obtained for a number of materials. The microhardness was measured after different types of plastic straining (hydroextrusion, PT) or at various temperatures. Pressure hysteresis was determined as the difference between points of the beginning of direct and reverse PT at compression in the cylinder-piston chamber [Fig. 2(a)]. The conclusion was drawn that due to linear dependence between the hysteresis and hardness (yield stress), hysteresis is completely caused by resistance to plastic deformation and at the zero yield limit the hysteresis would be absent. The additional dissipative threshold k is not considered by Estrin (1993). The above experiments allow us to relate k and yield stress.

The relation between the yield stress and the hardness $\sigma_y = 0.383 H_\mu$ follows from the solution of the axisymmetric problem of the indentation of rigid punch in a perfectly plastic half-space (Ishlinsky, 1944). This relation is in good agreement with experiments for perfectly plastic materials (Levitas, 1987, 1996b), for hardening materials $\sigma_y = (0.32 \div 0.37) H$ depending on the hardening modulus (Del, 1978).

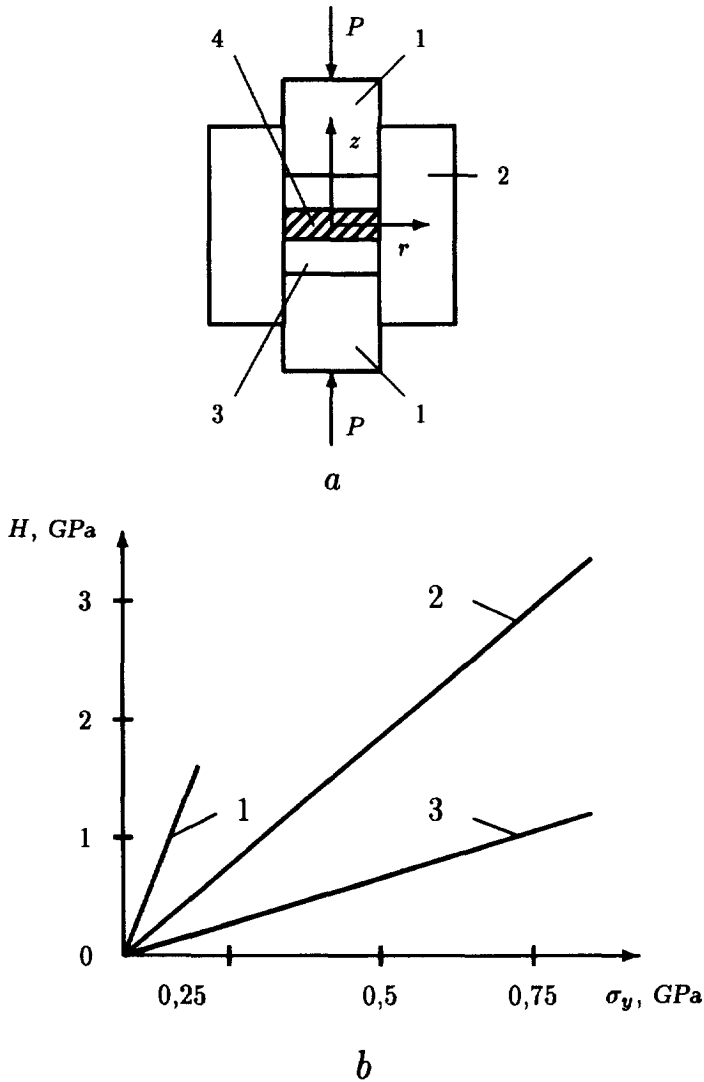


Fig. 2. (a) PT in the piston-cylinder chamber: 1, piston; 2, cylinder; 3, compressed material; 4, transformed region. (b) Relation between the pressure hysteresis and the yield stress for various materials (Estrin, 1993): 1, RbCl, KCl, KBr, KI; 2, CdS, CdSe; 3, Ce, InSb, Bi.

Using the coefficient 0.383 we present schematically experimental results by Estrin (1993) in the coordinates hysteresis H –yield stress σ_y [Fig. 2(b)].

For the interpretation of these results we assume that PT in the piston-cylinder chamber can be described by the axisymmetric problem of PT in a horizontal layer under prescribed pressure σ_n in a chamber [Fig. 2(a)], similar to that solved above for plane strain. Taking into account the complete plasticity condition $\sigma_r = \sigma_\theta$ (Hill, 1950) and yield condition $\sigma_n - \sigma_r = \sigma_y$ we obtain for hydrostatic pressure $\sigma_0 = (\sigma_n + 2\sigma_r)/3 = \sigma_n - 2/3\sigma_y$ (it is assumed for simplicity $\sigma_{y1} = \sigma_{y2}$). The nucleation criterion (11) gives

$$X = (\sigma_n - 2/3\sigma_y)\varepsilon_0 - \Delta\psi^\theta = k, \quad (29)$$

$$\sigma_n^{1 \rightarrow 2} = \frac{\Delta\psi^\theta}{\varepsilon_0} + \frac{k}{\varepsilon_0} + \frac{2}{3}\sigma_y, \quad \sigma_n^{2 \rightarrow 1} = \frac{\Delta\psi^\theta}{\varepsilon_0} - \frac{k}{\varepsilon_0} - \frac{2}{3}\sigma_y, \quad H = \frac{2k}{\varepsilon_0} + \frac{4}{3}\sigma_y. \quad (30)$$

Equation (30)₃ in comparison with Fig. 2(b) leads to the conclusion that

$$k = L\sigma_y\varepsilon_0 \quad \text{and} \quad H = \sigma_y(4/3 + 2L). \quad (31)$$

The value L is equal to 5.89 for materials of group 1 [Fig. 2(b)], 1.39 for materials of group 2 and 0.11 for materials of group 3. The coefficient L is a function of the volume fraction of a new phase. Note that the pressure dependence of yield stress should be taken into account.

It follows from the obtained results that plastic work can explain only 8% ($= \frac{4}{3}\sigma_y/H$), see (30)₃ of hysteresis for materials of group 1, 32% for materials of group 2 and 86% for materials of group 3; the remaining part in isothermal approximation is related to k . Consequently the dissipative threshold k is a very important parameter for the control of the PT condition and knowledge about its dependence on various parameters is very important. If we assume the validity of (31)₁ in the general case, then the dependence of k on temperature, plastic strain, plastic strain rate and history, volume fraction of martensite, grain size and so on are determined in terms of yield stress. It is known that the smaller the grain size or size of a single crystal, the worse the PT condition is, and in very small crystals temperature induced martensitic PT does not occur (Hornbogen, 1984). The usual explanation of these results is based on the decrease in the probability of stress concentrators, e.g. dislocations which improve the PT condition, with the reduction of grain size. We can give an additional reason based on the above equation. According to the Hall–Petch effect $\sigma_y = a + bd^{-0.5}$, where a and b are constants and d is some characteristic size (size of grain, subgrain, width of martensitic plate and so on) (Bernshtein *et al.*, 1993). Consequently, decrease in d results in increase in σ_y and especially k , which makes the PT condition worse.

3.3. Phase transition in a thin inclined layer

Let us consider an infinite rigid-plastic half-space with prescribed normal P and shear T stresses on the whole surface (Fig. 3). Assume that a coherent PT transforms the thin infinite layer $A'B'CD$ in $ABCD$, which is, in contrast to the previous problem, inclined at an angle α to surface S . Here we will define an “optimal” angle α and find a limitation related to fulfilment of the yield conditions outside the layer. In the local x – y coordinate system we assume $\mathbf{e}^i = (0.5\varepsilon_0\mathbf{i} + \gamma^i(\mathbf{tn})_s)\xi$. In this case, the PT criterion (11) results in

$$X = 0.5\varepsilon_0(\sigma_{xn} + \sigma_{xt}) + \tau_x\gamma^i - \Delta\psi^\theta = k(\alpha), \quad (32)$$

where function $k(\alpha)$ characterizes the anisotropy of a dissipative threshold; σ_{xn} , σ_{xt} and τ_x are the normal, tangential and shear stresses in the layer, and subscript α denotes that the stresses are defined in the local coordinate system x – y , inclined at an angle α .

Let a slip line in the layer be inclined at an angle β with respect to the surface S

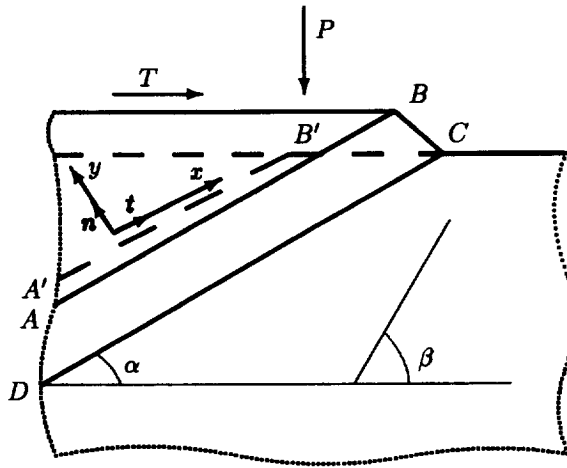


Fig. 3. Coherent PT layer in thin layer ABCD.

(Fig. 3). By definition, for a slip line the condition $\tau_\beta = 0.5 \sigma_y$ is valid. We will use known relations based on Mohr's circle (Hill, 1950).

$$\sigma_{\alpha n} = \sigma \pm 0.5 \sigma_y \sin 2(\beta - \alpha), \quad \sigma_{\alpha t} = \sigma \mp 0.5 \sigma_y \sin 2(\beta - \alpha), \quad (33)$$

$$\tau_x = 0.5 \sigma_y \cos 2(\beta - \alpha) \quad \text{and} \quad \sigma := 0.5(\sigma_{\alpha n} + \sigma_{\alpha t}) = 0.5(\sigma_1 + \sigma_2), \quad (34)$$

where σ_1 and σ_2 are the main stresses. The sign + or - in (33) should be chosen, reasoning from the knowledge, which of the two inequalities ($\sigma_{\alpha n} > \sigma_{\alpha t}$ or $\sigma_{\alpha n} < \sigma_{\alpha t}$) is valid for the problem under consideration. The stresses (33), (34) meet automatically the Tresca yield condition

$$(\sigma_{\alpha n} - \sigma_{\alpha t})^2 + 4\tau_x^2 = \sigma_y^2, \quad (35)$$

as well as the condition $\tau_\alpha = 0.5 \sigma_y$, when $\alpha = \beta$. The line BC remains horizontal for a small displacement approximation. According to the boundary conditions in the line BC,

$$\text{for } \alpha = 0 \quad \sigma_{\alpha n} = P > \sigma_{\alpha t} \quad \text{and} \quad \tau_x = T \text{ are valid.} \quad (36)$$

Consequently, $0.5 \sigma_y \cos 2\beta = T$; $\sigma + 0.5 \sigma_y \sin 2\beta = P$, whence it follows that

$$\cos 2\beta = 2T/\sigma_y \quad \text{and} \quad \sigma = P - 0.5 \sigma_y \sqrt{1 - 4T^2/\sigma_y^2}. \quad (37)$$

Equation (37)₁ determines an orientation of two orthogonal slip lines. Substitution of (34)₂ into (32) gives

$$X = \sigma \varepsilon_0 + \tau_x \gamma^t - \Delta \psi^0 = k(\alpha). \quad (38)$$

From the postulate of realizability it follows that

$$X(\alpha) - k(\alpha) \rightarrow \max, \quad \text{whence} \quad \sin 2(\beta - \alpha) = \frac{k'}{\sigma_y \gamma^t} \quad (39)$$

is valid with $k' := \partial k / \partial \alpha$. Equation (39) allows us to define the function $\alpha = q(\beta)$. Substitution of σ from (37)₂ and $\alpha = q(\beta)$ into (38) yields the PT criterion

$$X = P\varepsilon_0 - 0.5\varepsilon_0\sqrt{\sigma_{y2}^2 - 4T^2} + 0.5\sigma_{y2}\gamma^l \cos 2(\beta - q(\beta)) - \Delta\psi^\theta = k(q(\beta)), \quad (40)$$

or

$$(P - A)^2 + T^2 = 0.25\sigma_{y2}^2, \quad P \geq A,$$

where

$$A := [\Delta\psi^\theta + k(q(\beta)) - 0.5\sigma_{y2}\gamma^l \cos 2(\beta - q(\beta))]/\varepsilon_0, \quad (41)$$

which represents in the P - T plane of a semicircle of $0.5 \sigma_{y2}$ radius, shifted to the vector A along the axis P (Fig. 4). When $k' \equiv 0$, $\alpha = \beta$ (the layer coincides with a slip line) and

$$A = \Delta\psi^\theta + k - 0.5\sigma_{y2}\gamma^l/\varepsilon_0. \quad (42)$$

We should also take into account the inequality

$$P^2 + 4T^2 \leq \sigma_{y1}^2, \quad (43)$$

which denotes that the applied stresses cannot violate the yield condition for the first phase, and material outside the layer is rigid. In the P - T plane (43) represents an ellipse with semiaxis σ_{y1} and $0.5 \sigma_{y1}$. Consequently, the PT criterion represents in the P - T plane the part of a semicircle (41) lying inside the ellipse (43) (Fig. 4).

Let us analyze the results obtained. When the restriction (43) is not taken into account, the increase of T decreases the PT pressure, and maximal decrease is equal to $0.5 \sigma_{y2}$ at $T = 0.5 \sigma_{y2}$. Inequality (43) results in several important limitations (see Fig. 4).

- (1) The PT is possible when $-\sigma_{y1} \leq A + 0.5 \sigma_{y2} \leq \sigma_{y1}$.
- (2) The increase of T decreases the PT pressure when the circle (41) lies inside the ellipse (43). An additional increase of T makes the PT impossible. In particular when $\sigma_{y2} \geq \sigma_{y1}$ and $A = \sigma_{y1} - 0.5 \sigma_{y2}$ or $A = -\sigma_{y1} - 0.5 \sigma_{y2}$ the PT is possible at $T \equiv 0$ only (points $P = \pm \sigma_{y1}$).
- (3) The higher $(\sigma_{y1})/(\sigma_{y2})$, the more significant is the contribution of T . For $\sigma_{y1} \leq 0.5 \sigma_{y2}$, T has little or no effect on the P .

A comparison between equations for the "optimal" angle α and the results obtained for $\alpha = 0$ shows that

- (1) The term $\sqrt{\sigma_y^2 - 4T^2}$ in (40) is independent of α ;
- (2) The term $(\tau\gamma^l)/(\varepsilon_0)$ (for $\alpha = 0$) reaches its maximal value $(0.5 \sigma_y\gamma^l)/(\varepsilon_0)$ (42) for the "optimal" angle α .

The term $0.5 \sigma_y\gamma^l$ is a rather large positive contribution to the driving force of PT. At $\gamma^l = 0.2$ and $\varepsilon_0 = 0.01 \div 0.04$ (typical value for steels), the coefficient $(0.5 \gamma^l)/(\varepsilon_0) = 2.5 \div 10$ is of the same order as, or significantly exceeds the coefficient L in (31)₁, and parameter A in (42) can be less than $(\Delta\psi^\theta)/(\varepsilon_0)$. This contribution is independent of T and it is impossible to control it (in contrast with the case of a

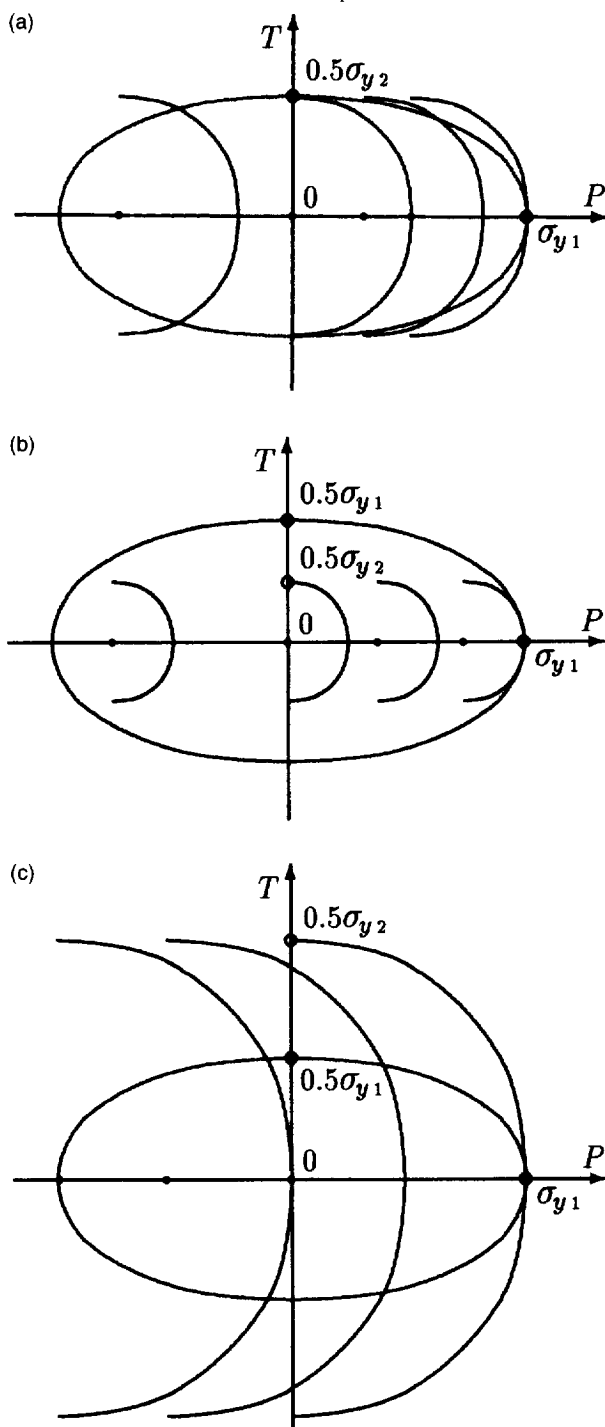


Fig. 4. PT criterion (semicircle of $0.5 \sigma_{y2}$ radius and a center at point A) and yield condition (an ellipse):
 (a) $\sigma_{y1} = \sigma_{y2}$; (b) $\sigma_{y1} = 2\sigma_{y2}$; (c) $\sigma_{y1} = 0.5 \sigma_{y2}$.

horizontal layer). Consequently, applied shear stresses T contributes to the yield condition and PT criterion (41) in a way equivalent to the decrease of the yield limit and this is the main mechanism of an increase in the driving force of PT.

At $T = 0$ (41) and (42) result in

$$P = \frac{\Delta\psi^\theta + k}{\varepsilon_0} + \frac{1}{2}\sigma_{y2}\left(1 - \frac{\gamma^l}{\varepsilon_0}\right). \quad (44)$$

when $\gamma^l > \varepsilon_0$ mechanical work reduces the PT pressure.

Evidently, if we allow the rotation of the transformation strain tensor independent of the rotation of the layer, it is always possible at $\gamma^l > 0.5|\varepsilon_0|$ to find the orientation, when a normal component of transformation strain along the lines AB and CD is zero (AB and CD are the invariant lines) and plastic strain at $\sigma_{y2} \geq \sigma_{y1}$ will not occur. Usually the transformation strain tensor is not plane and in this case it is impossible to find invariant lines and planes and plastic flow will occur in the layer obligatorily. To avoid the complicated analysis of three-dimensional problems and to find the main features of PT under complex loading we have considered a simplified two-dimensional problem with obligatory plastic flow in the transforming layer. The three-dimensional problem will be considered elsewhere.

4. PHASE TRANSITIONS UNDER COMPRESSION AND SHEAR OF MATERIALS IN BRIDGMAN ANVILS

4.1. Phenomenon

After compression of materials in Bridgman anvils (Fig. 5), especially in diamond anvils, a very high pressure in the center can be reached. A number of PT can occur under such conditions. It is known that:

- (1) additional rotation of an anvil and consequently plastic strain lead to significant reduction of PT pressure and to fundamentally new materials, which cannot be produced without additional plastic strains (Bokarev *et al.*, 1986; Alex-

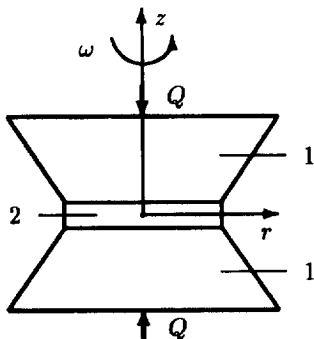


Fig. 5. Compression and shear of materials in Bridgman anvils: 1, anvils; 2, compressed material.

androva *et al.*, 1987, 1988; Blank *et al.*, 1994; Serebryanaya *et al.*, 1995; Batsanov *et al.*, 1995).

- (2) volume fraction of the new phase is an increasing function of the rotation angle and consequently plastic shear strain (Bokarev *et al.*, 1986; Aleksandrova *et al.*, 1987).

That is why plastic strain is considered as a factor, producing new physical mechanisms of PT. There is, for example, a quantum mechanical theory based on the assumption that large plastic shears produce a so-called atom-ion state, which allows qualitative interpretation of material behaviour under such conditions (Panin *et al.*, 1985).

It seems to us a little bit unrealistic. During the compression of materials in Bridgman nonrotating anvils, the mean value of plastic strain reaches 1000%, additional plastic shear strains near surfaces of anvils due to a contact friction exceed several thousand percent and have completely the same character, as a shear strain in rotating Bridgman anvils. Why is it that no one of the physical mechanisms of effect of plastic strains on PT manifests itself at such large plastic shear strain, but appears at rotation of an anvil, giving additional 10–100% plastic strain only?

In the paper, a simple theory is developed, which gives a new look on the above phenomena. We will use the PT criterion (11) for the case of equal elastic properties of phases. Let

$$\boldsymbol{\varepsilon}^t = (1/3\varepsilon_0 \mathbf{I} + \gamma^t (\mathbf{t}\mathbf{n})_s) \xi \quad \text{and} \quad \boldsymbol{\sigma} = p\mathbf{I} + 2\tau (\mathbf{t}\mathbf{n})_s, \quad (45)$$

where \mathbf{I} is the unit tensor, \mathbf{n} and $\mathbf{t} = \boldsymbol{\tau}/\tau$ are the unit vectors in the directions z and shear stress $\boldsymbol{\tau}$, $\tau = |\boldsymbol{\tau}|$, and p is the hydrostatic pressure. In this case

$$\boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^t = (p\varepsilon_0 + \tau\gamma^t) d\xi, \quad \tau\gamma^t > 0. \quad (46)$$

Assuming that transformation strain and k are homogeneous in the nucleus, (11) can be transformed into the form

$$\varepsilon_0 \int_0^1 \bar{p} d\xi + \gamma^t \int_0^1 \bar{\tau} d\xi - \Delta\psi^0 = k, \quad \bar{p} = \frac{1}{V} \int_V p dV, \quad \bar{\tau} = \frac{1}{V} \int_V \tau dV, \quad (47)$$

where \bar{p} and $\bar{\tau}$ are averaged over the nucleus pressure and modulus of shear stresses.

4.2. Stress state of a thin cylindrical disk under compression and shear in anvils at $\gamma^t = 0$

The solution of this problem without PT is known (Ogibalov and Kiyko, 1962); we will generalize it to the case of PT. We will neglect the elastic deformations of anvils and deformed disk, pressure nonhomogeneity in the z -direction and use the simplified equilibrium equation well-known in the metal forming theory (Ogibalov and Kiyko, 1962; Levitas, 1987, 1996b)

$$\frac{\partial p}{\partial r} = -\frac{2\tau_{fr}}{h}, \quad (48)$$

where r is the radial coordinate, h is the current thickness of the disk, τ_{fr} is the radial component of the shear frictional stress $\boldsymbol{\tau}_f$ on the boundary S between anvils and a

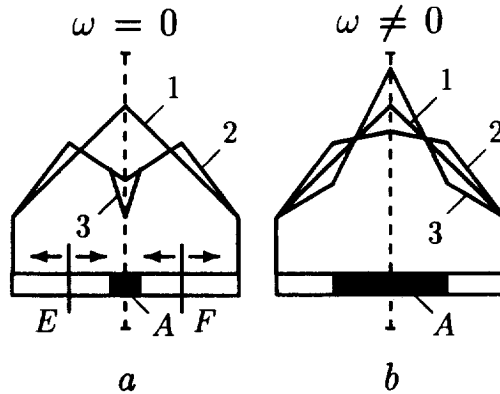


Fig. 6. Pressure distribution: (a) 1, before PT, 2, after PT at $\sigma_{y1} = \sigma_{y2}$, 3, after PT at $\sigma_{y1} < \sigma_{y2}$; (b) 1, $\sigma_{y1} = \sigma_{y2}$, 2, $\sigma_{y1} > \sigma_{y2}$, 3, $\sigma_{y1} < \sigma_{y2}$.

disk. Shear frictional stresses τ_r are directed opposite to the velocity \mathbf{v} of relative sliding of a compressed material on the boundary S . For a thin disk, the modulus τ_r usually reaches its possible maximum value equal to half of yield limit σ_y , i.e. $\tau_r = (\mathbf{v})/|\mathbf{v}|(\sigma_y)/2$. In the case without rotation of the anvil, $\tau_{fr} = 0.5 \sigma_y$ and (48) yields [Fig. 6(a)]

$$\frac{\partial p}{\partial r} = -\frac{\sigma_y}{h}, \quad p = \sigma_o + \sigma_y \left(1 + \frac{R-r}{h}\right), \quad (49)$$

where the boundary condition $p = \sigma_o + \sigma_y$ at the external radius of anvil $r = R$ is taken into account, σ_o being the pressure at $r = R$ due to the external support of material outside the working region of anvils $r > R$. The applied load is determined by integration of $p(r)$ over S

$$Q = \pi R^2 \left(\sigma_o + \sigma_y \left(1 + \frac{R}{3h}\right) \right). \quad (50)$$

Radial velocity v_r is defined from the incompressibility condition and condition $v_r = 0$ at $r = 0$ by the equation $v_r = -\dot{h}r/h$. During rotation of an anvil with an angular velocity ω , this expression for v_r is still valid, but the circumferential velocity $v_\theta = \omega r$ appears. Then, velocity vector \mathbf{v} and shear stress $\tau_r = 0.5 \sigma_y \mathbf{v}/|\mathbf{v}|$ are inclined at an angle α to the radius with

$$\cos \alpha = \frac{v_r}{\sqrt{v_r^2 + v_\theta^2}} = \frac{1}{\sqrt{1 + (\omega h/\dot{h})^2}} \quad (51)$$

and consequently

$$\tau_{fr} = 0.5 \sigma_y \cos \alpha. \quad (52)$$

Application of (48), taking into account (52), leads to

$$p = \sigma_o + \sigma_y(1 + (R-r)/H), \quad Q = \pi R^2(\sigma_o + \sigma_y(1 + R/(3H))), \quad (53)$$

$$H = \frac{h}{\cos \alpha} = h \sqrt{1 + (\omega h / \dot{h})^2}, \quad (54)$$

i.e. it is equivalent to the substitution of H for h . Let rotation occur at the fixed axial load Q . Then condition $Q = \text{const.}$ at $\sigma_o = \text{const.}$ results in $H = \text{const.} = h_o$, where h_o is the thickness of the disk at the beginning of rotation, and [together with (54)] in differential equation of reduction of thickness

$$d\varphi := \omega dt = -\frac{dh}{h} \sqrt{\left(\frac{h_o}{h}\right)^2 - 1}. \quad (55)$$

Equation (54) shows that at $Q = \text{const.}$ due to $H = \text{const.}$, pressure distribution is independent of rotation, which corresponds to experiments by Blank *et al.* (1984).

Consequently, rotation is equivalent to *reduction of friction* in the radial direction and results in a *decrease* of the *disk thickness* and this decrease is uniquely related to the rotation angle φ .

Let us consider PT in the central part of the disk (Fig. 6). We let c be the volume fraction of a new phase in the transforming region A . In the case without rotation of the anvil one part of the disk material moves to the center of the anvil. A neutral circle EF with zero velocity of relative sliding can be easily found using a volume balance. Equation (48) is valid, but shear stress in the region EF changes sign and in the region A the yield stress σ_{y2} of a new material, which depends on c , should be used. We assume that the pressure is continuous across the interface.

A complete analytical solution looks rather complicated, but its properties can be easily analyzed without explicit formulas. This is sufficient for the explanation of the above experiments.

Results of an analytical solution are shown schematically in Fig. 6. It is important that under a fixed axial force Q , pressure in the transforming region and the work integral in (47) decrease significantly, which makes PT condition worse. The higher σ_{y2} , the larger pressure the reduction in the transforming region.

Rotation decreasing the *thickness* reduces the negative pressure variation in the transforming particle, *increases* the work integral and the driving force for PT. This explains why the *rotation* (and not plastic strain) improves the PT condition.

We will show that the actual pressure variation which satisfies the postulate of realizability will be when infinitesimal radial flow from the disk center occurs. In this case, shear stress does not change sign, pressure grows monotonically with decreasing radius and volume decrease due to PT is completely compensated by the thickness reduction. The last condition results in the equation

$$dc\varepsilon_o = -\frac{dh}{h}, \quad (56)$$

and taking into account (55) at $\sigma_{y1} = \sigma_{y2}$ in the differential equation

$$dc\varepsilon_o = -\frac{dh}{h} = d\varphi \left(\left(\frac{h_o}{h} \right)^2 - 1 \right)^{-0.5}, \quad (57)$$

which relates uniquely the variation of the volume fraction of a new phase in the transformed region and the rotation angle, as is observed in experiments by Alexandrova *et al.* (1987) and Bokarev *et al.* (1986).

Equation (56) is valid only when PT criterion (47) is fulfilled. For $\sigma_{y1} \neq \sigma_{y2}$ the equation similar to (57) looks more complicated, but it also relates uniquely the variation of the volume fraction of a new phase in the transformed region and the rotation angle.

According to (48) if both phases have the same yield limit, the pressure distribution after PT is the same as before PT [Fig. 6(b)]. If the new phase is weaker, pressure decreases in the center; if the new phase is harder, pressure increases in the center. Consequently, despite the volume decrease due to PT, pressure increases due to appearance of the harder phase and additional plastic flow, which agrees with experiments [effects of pressure self-multiplication (Blank *et al.*, 1984)].

The above solution allows us easily to explain why rotation of an anvil gives us a way to obtain fundamentally new materials which cannot be produced under compression without rotation. If two materials can appear as a result of PT which differ by the yield stress only, then the material with the smaller yield strength appears under compression without rotation [as pressure is higher at $\sigma_{y1} > \sigma_{y2}$, see Fig. 6(a)], and the stronger phase will be obtained under compression with rotation [as pressure is higher at $\sigma_{y2} > \sigma_{y1}$, see Fig. 6(b)]. Consequently, the method based on the compression of materials with rotation of an anvil is especially important for the production of high strength materials.

Let us prove that (56) follows from the postulate of realizability, i.e. maximizes the driving force for PT in criterion (47). When $d\epsilon_0 > -(dh)/h$, i.e. the volume decrease due to PT is not completely compensated by the thickness reduction, part of the disk material moves to the center of the anvil, pressure in the transforming particle [Fig. 6(a)] and the driving force for PT in criterion (47) decreases in comparison with the case shown in Fig. 6(b), which contradicts the postulate of realizability.

In the case $d\epsilon_0 < -(dh)/h$, material moves from the disk center and the pressure distribution is shown in Fig. 6(b). For $\sigma_{y1} \leq \sigma_{y2}$, additional growth of c increases or does not change the pressure in the transforming particle after PT and consequently the driving force for PT. According to the postulate of realizability, as only PT can occur it will occur, i.e. the volume fraction increment dc should be increased. This increase is possible up to the value $d\epsilon_0 = -(dh)/h$, because then we come to the previous case and the decrease in the driving force. In the case $\sigma_{y1} > \sigma_{y2}$, additional growth of c decreases σ_{y2} , the pressure in the transforming particle and the driving force. If, for dc determined from the (56), the PT criterion is fulfilled, then this increment dc will occur (according to the postulate of realizability). When the PT criterion is violated and PT does not occur, the pressure distribution is independent of additional anvil rotation and thickening of the disk. Consequently the last infinitesimal increment dc proceeds at constant (independent of ϵ_0) averaged pressure \bar{p}^* , which is determined by (47)

$$\bar{p}^* \epsilon_0^t - \Delta \psi^\theta = k. \quad (58)$$

Knowledge of \bar{p}^* , σ_{y1} , $\sigma_{y2}(c)$, Q and the radius of the transforming region A determines

the unique stress distribution and the maximum volume fraction of a new phase c^* , which is independent of the kinetic equation for c and in particular valid for (56). Consequently at $c \leq c^*$ the value dc determined from (56) will not violate the PT criterion and this increment dc (according to the postulate of realizability) will occur. At $c > c^*$, $dc = 0$.

We have proved that (56) follows from the postulate of realizability. It follows from the above results that experimentally observed relations between the volume fraction of the new phase and rotation angle (but not plastic strain) do not represent a new physical law, but the consequence of the *volume balance* equation (56) (which follows from the postulate of realizability) and (55), which relates thickness of disk and rotation angle.

Note that the explanation of the pressure self-multiplication effect based on increasing of elastic moduli after PT (Blank *et al.*, 1984) is not correct, because it does not take into account the plasticity. Even at infinite moduli (as in our model), the pressure is limited by solution of the problem of plastic equilibrium, as presented here. If $\sigma_{y1} > \sigma_{y2}$ or material flows to the center of the disk, the pressure in the new phase cannot be increased irrespective of the increase in elastic moduli.

4.3. Estimation of the effect of $\gamma^l \neq 0$

As the solution to the problem in this case is unknown, we will make the simplest estimations. Assume that $\gamma^l = \text{const}$ in the transforming region and the stress state is independent of γ^l . Let the shear stress be independent of r . In the case without rotation of the anvil it is usually accepted that

$$\tau = \sigma_{y2} z/h \quad \text{and consequently} \quad \bar{\tau} = 0.25\sigma_{y2}. \quad (59)$$

During rotation of the anvil only the radial component of shear stress varies linearly, $\tau_r = \sigma_{y2} \cos \alpha z/h$, a circumferential shear stress $\tau_{z\theta} = 0.5 \sigma_{y2} \sin \alpha$ is constant (similar to the case of plastic torsion of a rod) and $\tau = \sqrt{\tau_r^2 + \tau_{z\theta}^2}$. That is why the value

$$\begin{aligned} \bar{\tau} &= \frac{2}{h} \int_0^{0.5h} \tau dz = \frac{2}{h} \sigma_{y2} \int_0^{0.5h} \sqrt{0.25 \sin^2 \alpha + \cos^2 \alpha \frac{z^2}{h^2}} dz \\ &= 0.25\sigma_{y2} \left(1 + \cos \alpha \tan^2 \alpha \ln \left| \frac{1 + \cos \alpha}{\sin \alpha} \right| \right) \end{aligned} \quad (60)$$

during rotation exceeds the corresponding value without rotation and the driving force for the PT in (47) increases. For large enough γ^l PT can proceed under pressure which is less than thermodynamic equilibrium pressure (as in the problem of PT in the layer), which corresponds to the results obtained in some experiments (Alexandrova *et al.*, 1988). In the case $\sigma_{y1} < \sigma_{y2}$ this situation can be achieved more easily due to the growth of \bar{p} .

Let us summarize the results. Improvement of the PT conditions due to rotation of the anvil is related to the possibility of additional displacement, compensating a volume decrease. It is connected with a decrease of friction stress in a radial direction. But when we understand that the reason lies in additional displacement (and not in a

plastic straining), it is possible to find other ways to obtain additional displacement without rotation.

One possibility is to decrease the yield stress at constant external force, e.g. due to heating of the external part of the disk or of the whole disk. Equation (50) determines the variation of disk thickness (56) defines the volume fraction of a new phase. As in the case with the rotating anvil, if a new phase is harder, pressure increases in the center of the disk. Such a situation is observed in experiments by Blank *et al.* (1989): the increase in pressure caused by PT $B1 \rightarrow B2$ in KCl during heating from 300 up to 600 K and initial pressure 6 GPa at the center was 30%.

Another possibility may be based on the use of transformation induced plasticity (TRIP) (Mitter, 1987; Padmanabhan and Dabies, 1980). Let us consider a two-phase material consisting of inclusions in a plastic matrix. If, under cyclic temperature variation, inclusions undergo the cyclic direct—reverse PT with large enough volumetric transformation strain, then the matrix will be deformed plastically even without external stresses. External stress produces plastic strain in the direction of its action, which is proportional to the value of applied stress and number of thermal cycles, i.e. is practically unlimited. If we introduce the transforming particles into the disk compressed in anvils, then it is possible to use the thermal cycles instead of rotation of the anvil to get additional displacement and to improve the PT condition in the center of the disk.

It is necessary to note that the above problem shows a good example of stress (pressure) concentration due to external friction during plastic loading. At large R/h (in experiments $R/h = 10 \div 100$) pressure in the disk center exceeds the yield stress by a factor of $10 \div 100$ and the specific applied force $Q/(\pi R^2)$ by a factor of 3. For materials with pressure dependent yield stress these values can be several times higher (Levitas, 1987, 1996b).

The pressure dependence of the yield stress and elastic strain will be taken into account elsewhere. The problem of compression of a rigid-plastic disk for pressure-sensitive materials is solved numerically by Levitas (1987, 1996b).

5. CONCLUDING REMARKS

It follows from the solution of the above problems that the generally accepted statement concerning the improvement of the PT condition by large plastic shear is not always correct. Under homogeneously distributed pressure and shear stress this is indeed the case. According to the plastic flow rule, shear stresses and shear plastic strain (or plastic strain increment) are related uniquely and are in monotone relation with each other (27)₁, i.e. they produce equivalent contribution to the driving force of PT. In the problem of the compression of materials in Bridgman anvils, all impressive experimental results are described (at least qualitatively) without the appearance of plastic strain in any equation. Consequently each experimental situation should be simulated carefully before any conclusion is made.

The phenomena enumerated in Section 4.1 take place not only for martensitic PT, but for various chemical reactions in polymers (Zharov, 1984, 1989) and for oxide decomposition (Vereschagin *et al.*, 1971). In these cases plastic shear accelerates the

kinetics of reactions by several orders, making it practically “instantaneous” (like for martensitic PT), because the volume fraction of product depends not on the time, but on the value of shear. This means of course the appearance of new physical (or chemical) mechanisms. For martensitic PT this is not the case, because the “instantaneous” time-independent kinetics is typical for them without plastic strain as well. The existence of a physical effect of plastic shear on martensitic PT can be proved only in the case of disagreement of experiment with the solution to the same problem, when all the material parameters and boundary conditions are determined independently.

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