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Simulation of martensitic phase transition progress with continuous and discontinuous displacements at the interface [1]

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Abstract

The problem formulation for martensitic phase transition (PT) progress in elastoplastic materials at small strains, based on a recently proposed thermomechanical approach [V.I. Levitas, Mech. Res. Commun. 22 (1995) 87; V.I. Levitas, J. Phys. IV, Colloque C2, 5 (1995) 41.], is presented. Stress history dependence during the transformation process is a characteristic feature of the PT criterion. To define the PT progress a corresponding extremum principle for PT is used (without any kinetic equations). A relatively simple mechanical model for incoherence at interfaces is proposed. The problem of progress of PT in a cylindrical sample with a moving coherent and incoherent interface is analyzed by the finite element method (FEM) using a layer-by-layer progression technique. It is shown that the incoherent interface has low mobility or cannot move at all, which agrees with known experiments. Possible reasons of formation of discrete microstructure (discontinuously transformed subdomains) such as incoherence, perfect plasticity or plasticity with hardening are modeled and discussed. The elastic problem of progress of PT for the same cylindrical sample with coherent interface has also been solved using an element-by-element progression technique. It is shown that the shape variation of the transformed region during PT progress is insensitive to mesh refining. © 1997 Elsevier Science B.V.

Keywords: Phase transition; Elastoplastic material; Finite elements

1. Introduction

PT in elastoplastic materials are phenomena that are very widespread in nature, physical experiments and modern technologies. Practically all PTs with volumetric transformation strain exceeding 0.5% are accompanied by plastic strains, e.g. during heat treatment of steels. Thermomechanical treatment of materials involves consecutively or simultaneously occurring PT and plastic straining which results in the required microstructure and physical–mechanical properties. Strain-induced PT and transformation-induced plasticity (TRIP) are other important examples. Martensitic PT in elastoplastic materials is a complex thermomechanical process accompanied by the change of mechanical properties, transformation strain and a complicated distribution of local stresses and strains. The difficulties of a thermomechanical description of PT are related to the definition of the PT condition, the formulation of boundary value problems and their numerical solution.

We consider the instantaneous occurrence of PT in some volume based on thermodynamics, without introduction of volume fraction and prescribing the kinetic equations. There are only three known nu-

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[1] Dedicated to Professor Franz Ziegler on the occasion of his 60th birthday.

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merical approaches of such type of PT with coherent interface in elastoplastic materials. Ganghoffer et al. [1], Marketz and Fischer [2,3] and Marketz, Fischer and Tanaka [4] used FEM to compute PT progress in a grain (appearance of martensitic plates). Typical for these papers is that the PT conditions for elastoplastic materials are not related directly to the second law of thermodynamics and the dissipation due to the PT. The analysis of such approaches is given in Ref. [5]. In papers by Levitas [6,7] a thermomechanical description of PT in elastoplastic materials, based on the second law of thermodynamics, was proposed. Numerical realization of the approach for martensitic PT with fixed interface is presented in Refs. [5,8].

The aim of this paper is to show the possibility of modelling coherent and incoherent martensitic PT with moving interface for elastoplastic materials. Here we will not consider crystallographic peculiarities of PT, but we will deal with the more simple case of dilatational transformation strain only (shear components of transformation strain were taken into account at finite strains in Ref. [9]). The condition of nucleation (in contrast to known approaches) includes the history of local stress variation in the nucleus during the transformation process. Therefore, knowledge of stresses and strains before and after PT does not give sufficient information to calculate the PT condition. This fact causes additional difficulties for the numerical method.

Firstly the formulation of an elastoplastic problem with PT based on the recently proposed PT criterion and related maximum principle [6,7] is presented. Then we will consider the simplest model problem for coherent and incoherent PT in an elastic and elastoplastic cylindrical sample with moving interface between the new and old phase. It will be shown that incoherence at the interface and plasticity considerably change the PT process and can be possible reasons of formation of a discrete microstructure of the new phase. The interface motion is prescribed in advance by a number of intermediate interface positions during PT. The PT condition for such interface motion is defined and analyzed using the PT criterion and extremum principle, i.e., the inverse problem is solved. Then, another problem of determination of the coherent interface positions during the growth of new phase in cylindrical sample for elastic materials is considered. All the model problems under consideration are axisymmetric and restricted to small strains. To calculate PT condition for the above problems, elastoplastic contact problems are solved by FEM [10] to determine the variation of local stresses as function of growing transformation strain.

Note that some analytical solutions based on the above theory and interpretation of some experiments are presented in Ref. [11].

2. Problem formulation

Let us consider the problem formulation of martensitic PT in elastoplastic materials using the thermomechanical description of PT. The following assumptions are used: for new (nucleus) and old (matrix) phases the standard elastoplastic model with von Mises yield condition is assumed, elastic properties of both phases are the same [1–4] and the transformation strain is volumetric. PT is considered here as the thermomechanical process of growth of volumetric transformation strain from zero to a final value which is accompanied by change of thermal material properties. A set of equations includes the following relationships:

(1) Kinematic decomposition within geometrically linear theory:

$$\boldsymbol{\varepsilon} = 1/2(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathrm{T}}) = \boldsymbol{\varepsilon}^{\mathrm{e}} + \boldsymbol{\varepsilon}^{\mathrm{p}} + \boldsymbol{\varepsilon}^{\mathrm{t}}, \quad (1)$$

where $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}^{\mathrm{e}}$, $\boldsymbol{\varepsilon}^{\mathrm{p}}$ and $\boldsymbol{\varepsilon}^{\mathrm{t}}$ are the total, elastic, plastic and transformation strains, respectively and $\boldsymbol{u}$ is the displacement vector. For the case of pure dilatational transformation strain, $\boldsymbol{\varepsilon}^{\mathrm{t}} = \varepsilon_0^{\mathrm{t}}\mathbf{I}$, where $\mathbf{I}$ is a unit tensor, and $3\varepsilon_0^{\mathrm{t}}$ is the volumetric transformation strain.

(2) Hooke's law:

$$\boldsymbol{\sigma} = \mathbf{E}:\boldsymbol{\varepsilon}^{\mathrm{e}} = \lambda(\boldsymbol{\varepsilon}^{\mathrm{e}}:\mathbf{I})\mathbf{I} + 2\mu\boldsymbol{\varepsilon}^{\mathrm{e}}, \quad (2)$$

where $\boldsymbol{\sigma}$ is the stress tensor and λ and μ are the Lame coefficients.

(3) Von Mises yield condition:

$$f(\boldsymbol{\sigma}) = \sigma_i - \sigma_y(q) \le 0, \quad \dot{q} = (2/3\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}:\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}})^{1/2}, \quad (3)$$

where $\sigma_i = (3/2\boldsymbol{s}:\boldsymbol{s})^{1/2}$ is the equivalent stress, $\boldsymbol{s} =$

$\mathrm{dev}\,\boldsymbol{\sigma}$ is the stress deviator, q is the accumulated plastic strain and $\sigma_y(q)$ is the yield stress.

(4) The associated plastic flow rule:

$$\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \lambda \boldsymbol{s}, \quad \lambda \geq 0. \tag{4}$$

(5) Equilibrium equations for neglected body forces:

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = 0. \tag{5}$$

(6) PT criterion [6,7]:

$$\int_{V_n} X \,\mathrm{d}V_n := \int_0^{\boldsymbol{\varepsilon}_2^t} \int_{V_n} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}^t \,\mathrm{d}V_n - \int_{V_n} \Delta\psi^\theta \,\mathrm{d}V_n$$
$$= \int_{V_n} k \,\mathrm{d}V_n \;\Rightarrow\; \text{PT occurs}, \tag{6}$$

where X is the local dissipation increment in the course of PT due only to PT (excluding plastic and other types of dissipation), $\Delta\psi^\theta = \rho(\psi_2^\theta - \psi_1^\theta)$, ψ_2^θ and ψ_1^θ are the thermal parts of the specific Helmholtz free energy of new and old phases (function of temperature only), ρ is the mass density, V_n is the volume of nucleus, k is an experimentally determined threshold value of dissipation due to PT (which can depend on some parameters, for example θ, $\boldsymbol{\varepsilon}^{\mathrm{p}}$), $\boldsymbol{\varepsilon}_2^t$ is the transformation strain after PT. For the dilatational transformation strain, temperature and k, distributed homogeneously in the nucleus, Eq. (6) can be transformed into the following form:

$$\bar{X} := \int_0^{\varepsilon_{02}^t} 3\bar{\sigma}_0 \,\mathrm{d}\varepsilon_0^t - \Delta\psi^\theta = k \;\Rightarrow\; \text{PT occurs}, \tag{7}$$

$$\bar{\sigma}_0 = \frac{1}{V_n} \int_{V_n} \sigma_0 \,\mathrm{d}V_n, \tag{8}$$

where σ_0 and $\bar{\sigma}_0$ are the local pressure and pressure, averaged over the nucleus, $\bar{X}$ is the driving force of PT (averaged over the nucleus value of X). Eq. (7) is the final form of phase transformation criterion which is used in the present paper. The physical sense of the criterion in Eq. (6)) is the following: If PT and plastic flow in the given material point are thermodynamically independent, then at $X < 0$ the PT is impossible (contradicts to the second law of thermodynamics). At $X = 0$ the PT is possible, but it will be a PT without dissipation due to PT (dissipation due to plastic deformation is possible). Since usually rather large dissipation accompanies PT, we assume that the calculated increment of dissipation X, due to the PT, reaches the experimentally determined value k. This model is similar to the formulation of yield conditions, see Eq. (3).

(7) Extremum principle for PT: In the general case the position and volume V_n of new nucleus for each increment of the boundary conditions and temperature θ are unknown. To define them, we use the extremum principle

$$\bar{X}(V_n^*) - k < 0 = \bar{X}(V_n) - k, \tag{9}$$

which follows from the postulate of realizability [12], where V_n and V_n^* are the actual and physically possible volume of nucleus. The physical interpretation of the principle in Eq. (9) is as follows: when for some volume V_n the PT criterion in Eq. (7) is fulfilled for the first time, the PT occurs in this V_n. For all other V_n^* the inequality in Eq. (9) is valid, because in the opposite case the PT criterion in Eq. (7) will be met for this V_n^* earlier than for V_n. As only the work integral $\varphi := \int_0^{\varepsilon_{02}^t} 3\bar{\sigma}_0 \,\mathrm{d}\varepsilon_0^t$ depends on the volume V_n, then from the extremum principle in Eq. (9) it follows that

$$\varphi(V_n) \to \max. \tag{10}$$

(8) One of the mechanisms for getting a more favorable stress variation in the transforming particle is related to the possibility of displacement discontinuities across the interface. We show a simple way of admitting incoherence (sliding). Two types of the interfaces between new and old phases are considered: coherent (with continuous displacements across interface) and incoherent (with discontinuous tangential displacements across interface). We assume that PT and incoherence criteria are thermodynamically mutually independent and that these processes are coupled by the stress fields only. If, in the course of the growth of transformation strain and variation of material properties in nucleus, the incoherence criterion is satisfied, we admit sliding in this point until a value where the criterion is violated. After completing the PT we check using the PT criterion whether PT is thermodynamically admissible. Consequently, a growing transformation strain produces the stresses which are necessary for appearance of incoherence and the incoherence changes the stress variation in the transforming particle. For the simplest incoherence criterion we assume that, if shear stress at any interface point reaches some critical value, then slid-

ing occurs at this point. This condition for a two-dimensional problem in local coordinate system has the following form:

Sliding condition (incoherent interface) at the interface

$$|\boldsymbol{\tau}| < \tau_s \;\Rightarrow\; \dot{\boldsymbol{u}}^2 - \dot{\boldsymbol{u}}^1 = 0, \tag{11}$$

$$|\boldsymbol{\tau}| = \tau_s \;\Rightarrow\; \dot{u}_s^2 - \dot{u}_s^1 \neq 0,\; \dot{u}_n^2 = \dot{u}_n^1, \tag{12}$$

where $\boldsymbol{\tau}$ is the tangential stress at the interface, τ_s is the critical value of the shear stress, $\dot{u}_n$, $\dot{u}_s$ are the normal and tangential components of velocity at the interface. Indices 1 and 2 identify those belonging to the matrix and the nucleus.

It is necessary to note that the PT condition in Eq. (7) has formally the same form for elastic and elastoplastic materials with coherent and incoherent interfaces; plasticity and incoherence effect on a variation of stresses in the course of PT and, hence, on the value of the work integral φ [6,7]. To calculate the variation of local stress distributions as function of the growing transformation strain we solve numerically by FEM the standard elastoplastic contact problem with given volumetric transformation strain and contact condition at the interface [10]. Quadratic triangular finite displacement elements are used.

3. Progress of PT (layer by layer) in a cylindrical sample (moving coherent and incoherent interfaces)

In the case where k is a function of temperature only, at given temperature the values of k and $\Delta\psi^\theta$ are known and, hence, the value of the work integral φ (due to the PT condition in Eq. (7) and the extremum principle in Eq. (10)) gives full information to evaluate the possibility of PT. We will also analyze the more complicated case of when k is a function of yield stress [11], averaged over the transforming volume and temperature.

Let us consider the problem of PT progress through a cylindrical sample with a moving straight interface. Fig. 1 shows the cross section of a cylindrical sample divided into layers. The following boundary conditions are applied:

- Along CD and DE boundaries $u_n = 0$, $\tau_n = 0$.
- Along EF boundary $\sigma_n = \tau_n = 0$ (free surface).
- Along CF boundary $\sigma_n = P = 100$ MPa, $\tau_n = 0$ (prescribed compressive stress P).

The elastic properties are: Young's modulus $E = 2 \cdot 10^5$ MPa and Poisson ratio $\mu = 0.3$. The moving interface is modeled by a number of intermediate predefined interface positions. For this example we

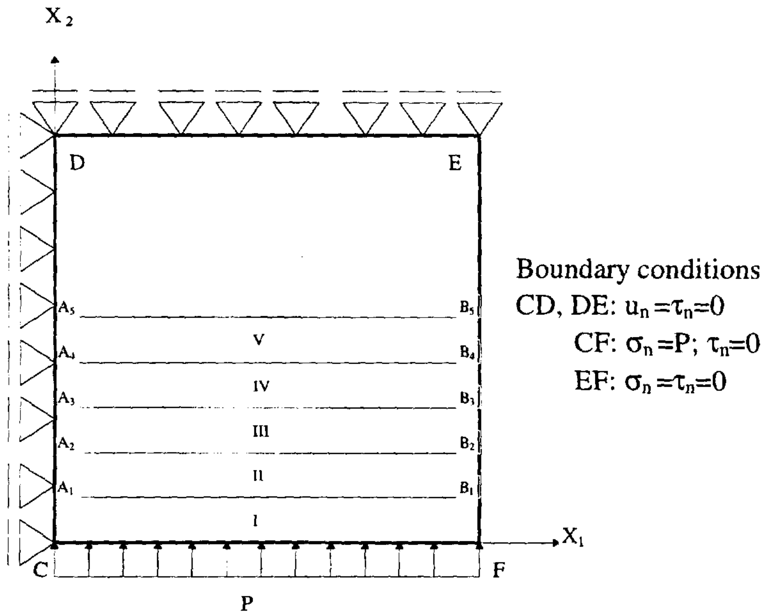
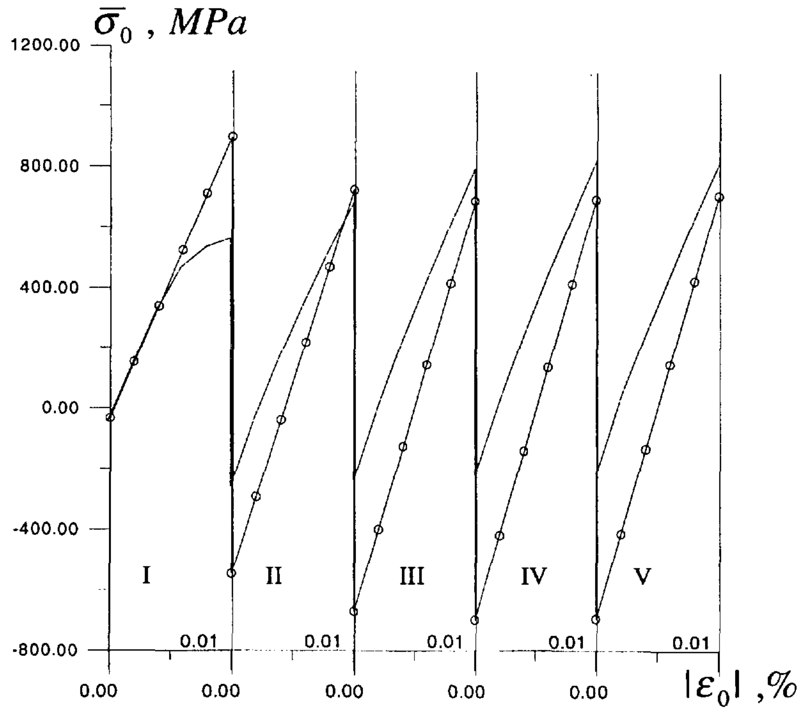
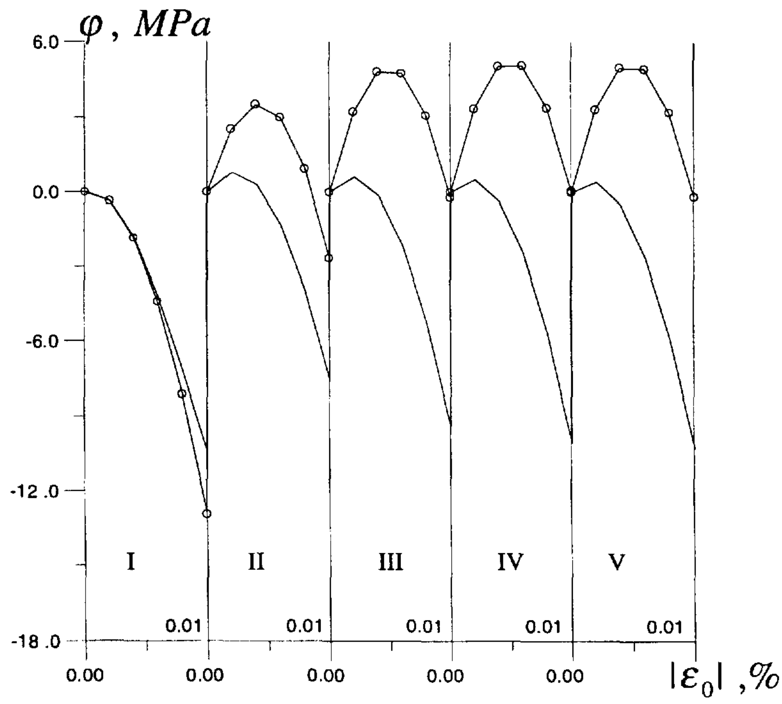


Fig. 1. Half of the cross section of a cylindrical sample. A_1B_1, $A_2\ B_2$, A_3B_3, A_4B_4, A_5B_5 are the positions of the interface at different time instants (I, II, III, IV, V are the regions where PT occurs after corresponding displacement of the interface). X_2 is the rotation axis.


$\overline{\sigma}_0$, MPa
1200.00
800.00
400.00
0.00
-400.00
-800.00
I
II
III
IV
V
0.01
0.01
0.01
0.01
0.01
0.00
0.00
0.00
0.00
0.00
$|\varepsilon_0|$,%

a


φ , MPa
6.0
0.0
-6.0
-12 .0
-18 .0
I
II
III
IV
V
0.01
0.01
0.01
0.01
0.01
0.00
0.00
0.00
0.00
0.00
$|\varepsilon_0|$,%

b

consider the inverse problem, i.e. we specify a priori the sequence of the interface positions during PT progress. For every interface position the PT condition is calculated as nucleation condition Eq. (6) or Eq. (7) for the corresponding layer (where PT occurs for one interface displacement). We specify 5 different sequential positions of the interface. At the beginning PT occurs in the 1st layer with interface A_1B_1, then in the 2nd layer with interface A_2B_2 and so on (Fig. 1). We assume that sliding can occur at the current interface position between a transforming layer and the matrix only (critical value of shear stress at the interface $\tau_s = 200$ MPa is accepted). The interface between a transforming layer and the layers of a new phase is coherent.

The PT in a layer is simulated by the growth of compressive transformation strain ε_0 from 0 to -0.01. To obtain the value of work integral φ the elastoplastic contact problems are solved incrementally with a transformation strain increment $|\varepsilon_0| = 0.002$ under fixed P. In the finite element code the transformation strain can be taken into account as a fictitious thermal strain. After determination of the PT condition for one layer calculations continue for the next layer with new position of the interface. The local stresses in whole volume due to the PT in the transformed layers are used as initial data for the calculation of the PT condition of the subsequent layer.

3.1. Coherent interface (elastic and elastoplastic material)

Let us consider at first the case of elastic material. Fig. 2 shows the variation of hydrostatic pressure (a), averaged over the layer and the variation of the work integral φ (b) in the course of PT (as a function of growing transformation strain) for different layers. We obtained linear variation of $\bar{\sigma}_0$ with the growth of the transformation strain for every layer (due to linear elasticity). Therefore, variation of $\bar{\sigma}_0$ and φ for every layer i can be presented as

$$\bar{\sigma}_0^i = a_i + b_i\varepsilon_0, \quad \varphi_i = 3a_i\varepsilon_0 + 1.5b_i(\varepsilon_0)^2, \qquad (13)$$

where a_i, b_i can be calculated using, for example, values of $\bar{\sigma}_0$ at $\varepsilon_0 = 0$ and $\varepsilon_0 = \varepsilon_{02}$ (ε_{02} is the transformation strain after PT). PT for a coherent interface at $k =$ constant is unstable (according to the maximum principle, Eq. (10)), i.e. if PT occurs in the 1st layer, then at the same temperature and external stresses, PT should occur in all the remaining layers, because the value of work integral φ (and, hence, driving forces $\bar{X}$) at transformation strain $|\varepsilon_0| = 0.01$ is larger for the remaining layers than for the 1st one. Consequently, to describe the stable phase equilibrium we should assume heterogeneous k distribution, or assume that k grows with increasing total volume fraction c of new phase in a specimen. As the final value of φ is almost constant from the third layer, the interface can be arrested in position A_3B_3 or A_4B_4.

Now consider the case of elastoplastic material with yield stresses for matrix $\sigma_y^m = 2.5 \cdot 10^2$ MPa and for nucleus $\sigma_y^n = 1 \cdot 10^3$ MPa (for simplicity we assume that the yield stress for the nucleus changes instantaneously to the value of phase 2 after the beginning of PT). As we can see from Fig. 2a almost linear variation of the averaged hydrostatic pressure $\bar{\sigma}_0$ with the growth of PT strain takes place for 2–5 layers. For these layers we can also use the analytical relation Eq. (13). But plasticity increases considerably the values of averaged hydrostatic pressure $\bar{\sigma}_0$ at the beginning of PT. It causes an essential decrease in the value of the work integral φ (and, hence, driving force $\bar{X}$) for 2–5 layers with respect to the case of elastic material. Therefore, at $k =$ constant according to the maximum principle (Eq. (10)), the PT in the second layer will occur immediately after the PT in the first layer at the same external condition (temperature and loading), be-

Fig. 2. Variation of hydrostatic pressure $\bar{\sigma}_0$ (a), averaged over the layer and variation of the work integral φ (b) for ith layer in the course of PT in ith layer for moving coherent interface, i = I, II, III, IV, V ((○) elastic matrix; (———) elastoplastic matrix).

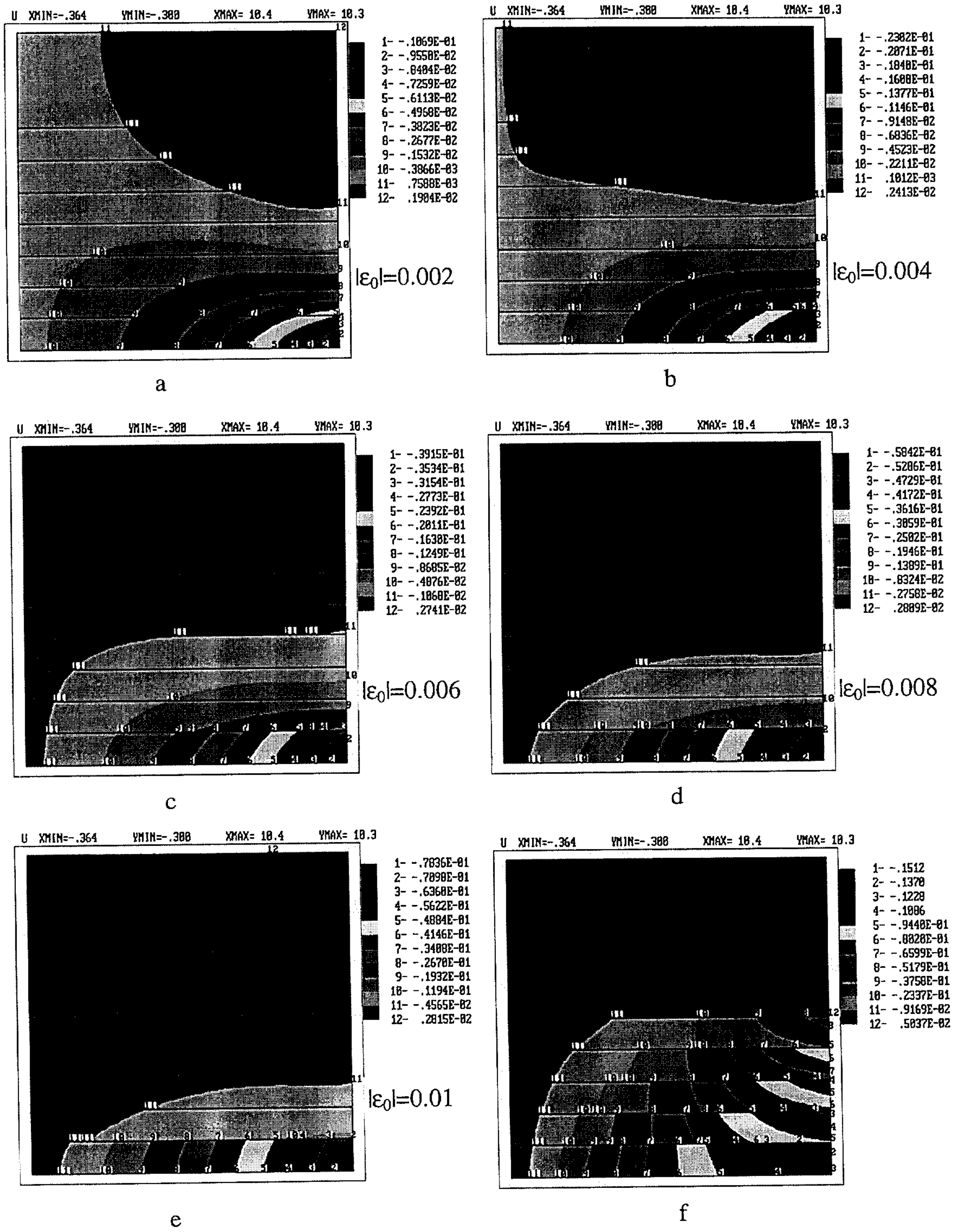


Fig. 3. Isobands of radial displacement distribution for incoherent interface at different values of transformation strain in course of PT within the first layer (a–e) and at the interface motion until the middle of a sample (f).

cause the value of work integral φ for the second layer is higher than the value of φ for the first one. But for the PT in 3–5 layers it is necessary to change the external condition to enforce PT (the values of work integral φ for the 3–5 layers are less than for the first one), i.e. due to plasticity it is possible to get stable interface motion.

3.2. Incoherent interface (elastic and elastoplastic material)

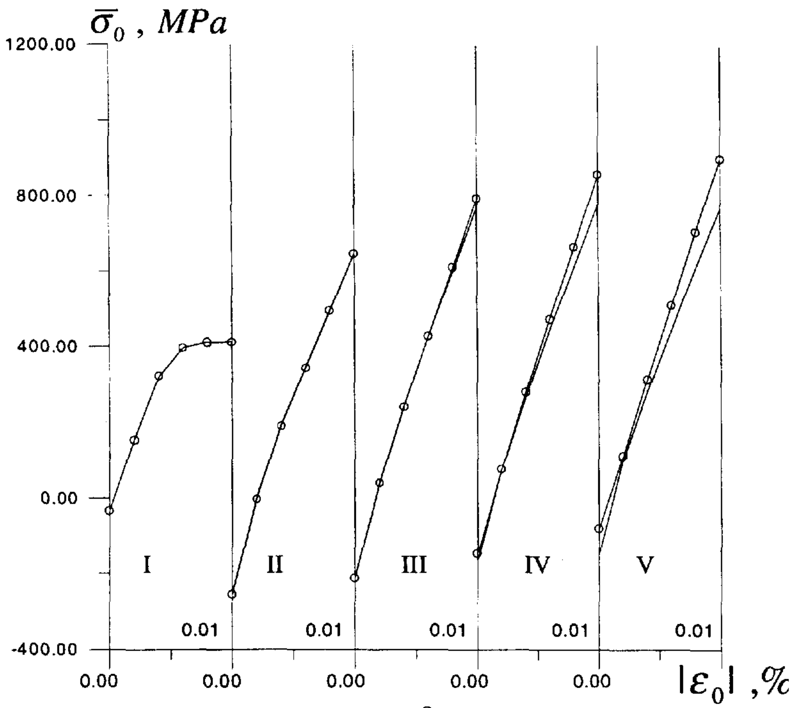
Let us consider an incoherent interface. Fig. 3 (elastic material) shows isobands of radial (along X_1 axes) displacement distributions at different values of transformation strain in the course of PT of the layer *I* (Fig. 3a–e) and at the motion of the interface until the middle of a sample (Fig. 3f). With the increase of the transformation strain the growth of the sliding zone takes place (different shades across interface correspond to the jump of displacements). The greatest amount of sliding at the interface takes place for PT in the 1st layer. For subsequent positions of interface the sliding zone size decreases. Fig. 4 shows the variation of hydrostatic pressure (Fig. 4a), averaged over the layer and the variation of the work integral φ (Fig. 4b) in the course of PT for every transforming layer (moving incoherent interface). For elastic materials nonlinear change of $\bar{\sigma}_0$ with the growth of the transformation strain within the layer (due to variation of sliding zone) takes place (curve for layer I, Fig. 4a). The more linear character of the curves for layers II–V in Fig. 4a is connected with the influence of the region where PT has already occurred (because at the interface between the layer of new phase and the layer where PT is still occurring, there are no additional displacement discontinuities). Comparison of Figs. 2 and 4 shows that the incoherence significantly stimulates the PT condition in the first layer (φ increases). The PT condition in the second layer for incoherent interface is worse than for the coherent interface, but a little bit better than for the first layer of incoherent interface. That is why at $k=$ constant or slightly growing k (c) the incoherent PT in the second layer can occur immediately after the PT in the first layer at the same external condition (temperature or loading). The value φ for incoherent PT in the third layer is smaller than for the first and the second layers and much smaller than for the third layer for coherent PT. If the value k (c) is large enough to stop coherent interface motion at fixed external parameters in positions A_2B_2, A_3B_3 or A_4B_4 ($\varphi = 0$ MPa), then it is necessary to very significantly change the external parameters to shift the incoherent interface ($\varphi \simeq -12$ MPa). But at such a change of external parameters the PT can occur in other places of a sample.

The reason for the decreasing value φ for a moving incoherent interface is the change of internal stresses. So the initial negative internal stresses in the transforming layer (due to transformation strain in the previous layer), which promote the PT, decrease (in absolute value) considerably due to stress relaxation during the sliding at the interface (compare initial values $\bar{\sigma}_0$ for layers in Fig. 2a and Fig. 4a). The effect of the incoherent interface is similar to the effect of plastic deformation during PT presented above. The slight difference of results for elastic and elastoplastic materials (difference only seen for PT in layers 3–5, Fig. 4) is explained by the fact that with the chosen mechanical properties sliding at the interface is more important than plastic deformation. Thus, incoherence changes PT conditions considerably.

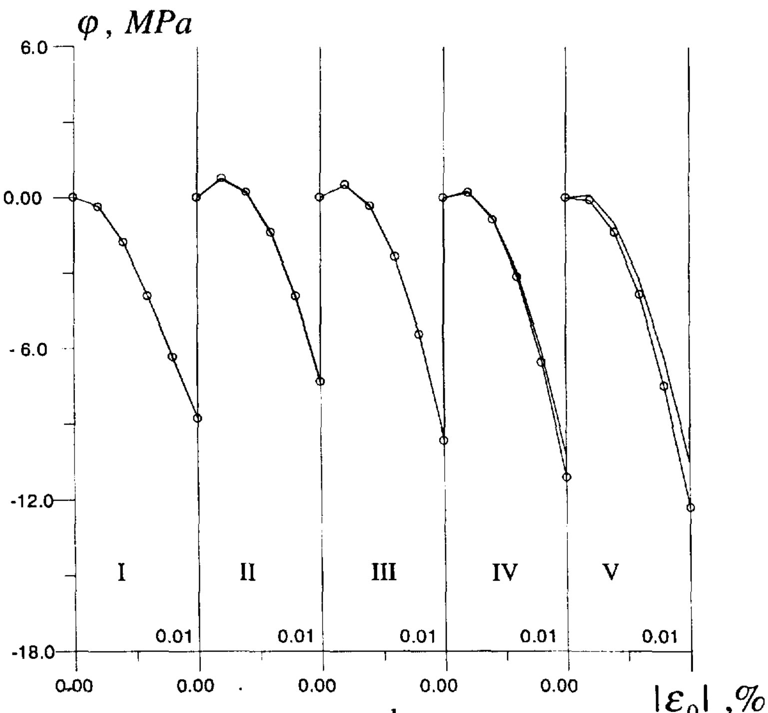
3.3. Possible reasons of formation of discrete microstructure

For an elastic material with a coherent interface field, the initial pressure promoting PT is larger for the layer adjoining the interface than for a layer remote from the interface. Therefore, in this case PT occurs sequentially layer by layer (a single connected region of new phase is formed). But incoherence and plasticity considerably change the distribution of the stress–strain state during PT.

Let us consider the influence of incoherence for an elastic material. We have investigated the problem for the following sequence of PT in layers for coherent and incoherent interfaces: (a) after PT in the first layer, PT occurs in the second layer; (b) after PT in the first layer, PT occurs in the third layer. For the coherent interface the work integral φ in the transforming layer is bigger for case (a) than for case (b). For the incoherent interface at some small value of critical shear stress τ_s, the value of


$\bar{\sigma}_0$, MPa
1200.00
800.00
400.00
0.00
-400.00
I
II
III
IV
V
0.01
0.01
0.01
0.01
0.01
0.00
0.00
0.00
0.00
0.00
$|\varepsilon_0|$,%

a


φ, MPa
6.0
0.00
- 6.0
-12.0
-18.0
I
II
III
IV
V
0.01
0.01
0.01
0.01
0.01
0.00
0.00
0.00
0.00
0.00
$|\varepsilon_0|$,%

b

work integral φ for the transforming layer was bigger for case (b) than for case (a), i.e. PT can be more favorable in the layer which is not in contact with a transformed one.

Now we consider this problem with $P=0$ and $\tau_s=0$ (limit case). Then for any layer, if it is not in contact with a transformed layer (the interface between matrix and transforming layer is incoherent), the work integral φ is zero (because stresses are zero due to $\tau_s=0$). But if the transforming layer is in contact with a transformed one (interface between these layers is coherent according to the problem formulation), the work integral φ is negative (because of the jump of the negative transformation strain across the interface we have a positive average pressure in the transforming layer). Thus, incoherence relaxes the stresses and can enforce the complicated kinetics of a new phase, i.e. variation of the critical shear stress τ_s can change the kinetics of PT.

These results explain the known experimental observation that incoherent interfaces have low mobility or cannot move at all [13].

Another possible reason for formation of discrete microstructure for a plastically hardening material is related to the linear dependence of k on yield stress $\bar{\sigma}_y$, averaged over the transforming layer at the beginning of PT [11]:

$$k=3L\bar{\sigma}_y\varepsilon_0, \tag{14}$$

where the value L is equal to 7.48 for steel [11]. For linear hardening materials it is equivalent to the dependence $k(\bar{q})$ on accumulated plastic strain $\bar{q}$, averaged over the transforming layer at the beginning of PT. For example, we have solved the problem for hardening elastoplastic matrix with $\sigma_y(q)=250+2000q$ and elastic nucleus with a coherent interface. The results are such that after PT in the first layer the value of $\bar{q}$ for the second layer is $\bar{q}=0.17\cdot10^{-1}$, for the third layer $\bar{q}=0.1\cdot10^{-2}$, for the fourth layer $\bar{q}=0.48\cdot10^{-4}$ and for the fifth layer $\bar{q}=0.55\cdot10^{-6}$. Hence according to Eq. (14) for the second layer the value $k(\bar{q})$ is 7.18 MPa larger than for the third one and 7.63 MPa larger than for the fourth one. It can cause the PT in the third layer after PT in the first one, i.e. we can obtain a multiple connected region of the new phase.

4. Progress of PT (element by element) in a cylindrical sample (coherent interface)

Let us consider the same sample as in the previous problem for elastic material and coherent interface after PT in the first two layers (interface has position A_2B_2, Fig. 1). The boundary conditions are also the same. Now we will not prescribe the next interface position, but investigate further PT progress (finite element by finite element) in the remaining region of the matrix. The internal stresses in the sample (due to PT in the first two layers) are used as initial conditions. For example, the axial stress and the pressure are shown in Fig. 5; axial stress (Fig. 5a) is continuous with large regions of positive and negative values; hydrostatic pressure (Fig. 5b) is discontinuous across the interface with positive values in almost all of the new phase (layers I and II) and negative values in almost all of the matrix and has maximum positive value at the right side of the interface and a maximum negative value at the center of the interface.

The following assumption is used for calculation of PT progress: PT occurs at any time instant in one finite element (FE) only. For this state, the variation of stress–strain state due to PT in the FE has to be computed. Every FE in the remaining region of matrix is considered as a possible new nucleus. To choose the FE where PT can occur, we should find the FE for which the functional φ has maximum value (see Eq. (10)). Only after finishing PT in one element can the PT start in another one. The solution algorithm for this problem is described briefly in Ref. [5]. In contrast to the paper by Marketz and Fischer [3] where the place of subsequent transforming region is determined using initial stress–strain state before PT (without solving boundary value problem) we should solve boundary value problems for all admissible positions of subsequent transform-

Fig. 4. Variation of hydrostatic pressure $\bar{\sigma}_0$ (a), averaged over the layer, variation and of the work integral φ (b) in the course of PT in different layers for moving incoherent interface ((○) for elastic matrix; (————) elastoplastic matrix).

ing region (finite elements in our case) because of the stress history dependent value of work integral φ. Then we choose the actual position of the subsequent transforming region according to the extremum principle, Eq. (9) or Eq. (10).

To investigate the dependence of the solution on the FE mesh we use two meshes: the first one is shown in Fig. 6e and includes 673 finite elements and 1408 nodes, the second mesh (Fig. 6a) has 284 finite elements and 599 nodes. Fig. 6 shows the PT progress in the matrix. The first nucleus appears in the matrix near the middle of the interface where the negative value of initial pressure reaches a maximum. Then the PT region extends to the axes of

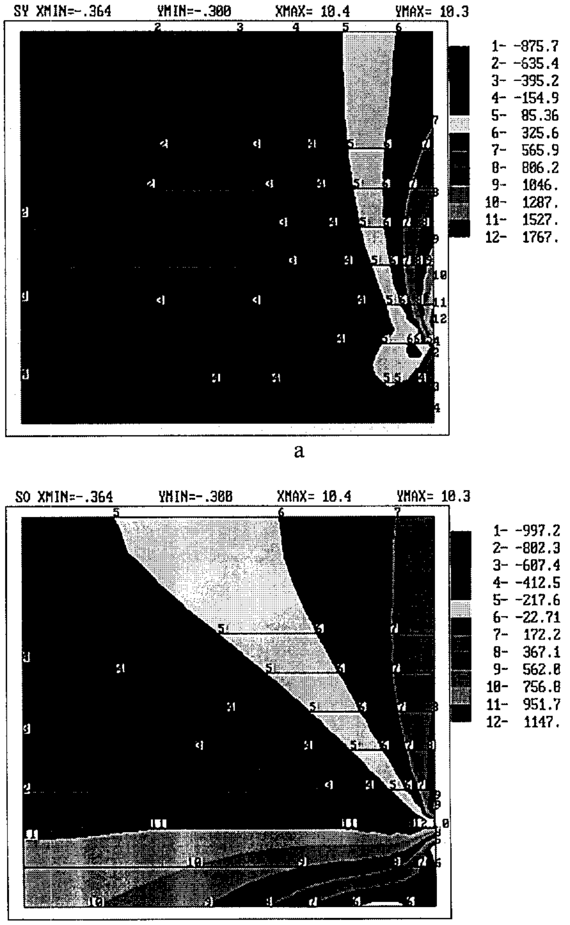


Fig. 5. Isobands of axial stress σ_2 (a) and hydrostatic pressure σ_0 (b) distribution in a sample after PT in layers I and II.

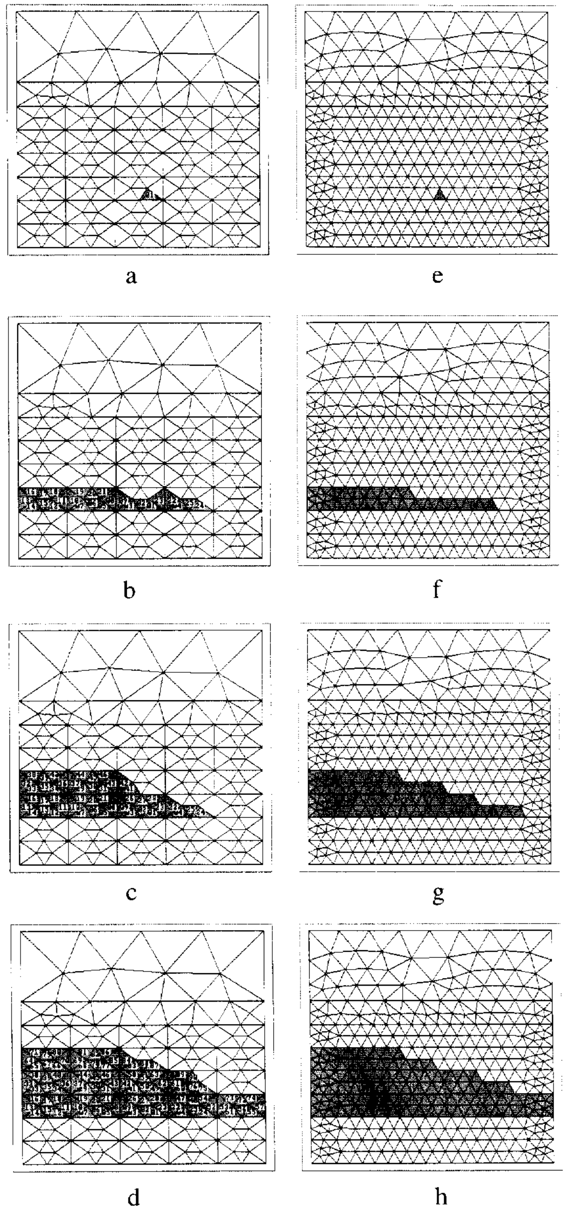


Fig. 6. Progress of PT (element by element) in an elastic sample for two different finite element (FE) meshes. Transformed FEs are shaded. The numbers in the left figures indicate the sequence of FEs where PT occurs.

rotation. Further PT progress proceeds in a such way that the thickness of the transformed region increases to the center of the sample (to the axes of rotation). During PT progress the interface has a complicated shape. We can consider the assumption that the interface is a straight line (which is used for problem solution in Section 3 as the first approximation or an additional constraint). Analysis of the driving forces of PT has shown that the value of work integral is minimal for the first transformed finite element. This means that at $k=\text{constant}$ after PT in the first element, PT should occur in the other elements, i.e. phase equilibrium is unstable. Consequently, to describe the stable phase equilibrium we should assume that k grows with an increasing total volume fraction c of the new phase in a specimen.

Comparison of the transformed region during PT progress for two different meshes (Fig. 6) shows that for the problem under consideration the variation of interface shape is practically insensitive to mesh refining.

5. Conclusions

(1) A numerical study of martensitic PT progress in elastic and elastoplastic materials, based on a recently proposed thermomechanical approach [6,7] is presented, using the finite element method. PT condition based on the second law of thermodynamics and the related maximum principle are used. Stress history dependence during the transformation process is a characteristic feature of new PT criterion. A simple way for incorporating incoherence at the interface is proposed.

(2) The problem of progress of the PT with a layer-by-layer technique in a cylindrical sample with moving both coherent and incoherent interfaces is simulated. The driving force for PT in elastic materials grows during the coherent interface propagation and, consequently, at $k=\text{constant}$ PT should occur in the whole sample for fixed external parameters. It is shown that an incoherent interface has low mobility or cannot move at all, which agrees with known experiments. In the problem under consideration, plastic deformation produces a similar effect as incoherence. Possible reasons of formation of discrete microstructure (due to plasticity, incoherence and dependence of threshold value k on yield stress) are discussed.

(3) The elastic problem of PT progress with an element-by-element technique in a cylindrical sample with a coherent interface is computed, as well as the shape variation of the transformed region during PT. It is shown that the solution obtained is practically insensitive to mesh refining.

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