THERMOMECHANICAL DESCRIPTION OF PSEUDOELASTICITY – THE THRESHOLD–TYPE DISSIPATIVE FORCE WITH DISCRETE MEMORY

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Introduction

Recently published experimental results [1-3] for pseudoelastic straining of CuZnAl monocrystals exhibit a very complicated history dependent behaviour inside the hysteresis loop. The thermodynamic theory of Müller [1-3] can describe only some details (for example the difference between stress values at which direct austenite (A) $\rightarrow$ martensite (M) and reverse $M \rightarrow A$ phase transitions (PT's) start) and a number of open problems exist [1-2], for example:
a) why PT's proceed at constant stress (ideal pseudoelasticity) rather than along the calculated equilibrium line AD (Fig.1, 2), although this line defines minima of the free energy ψ ?
b) What is the nature of metastability, i.e. why PT's do not occur inside the hysteresis loop ?
c) How to describe the whole $\sigma - \epsilon$ diagram at arbitrary strain history (Fig.2)?
In the paper using the concept of the threshold value of dissipative force k, which the thermodynamic stimulus of PT has to reach in order to proceed PT (Levitas [4,5]) two problems are solved:
a) all experimental details of the macroscopic material behaviour presented in [1-3] are described ;
b) a simple dependence of k on the volume fraction of M and PT's history is determined .
The possible generalizations of the simplest theory are considered (for example account for defects energy) which allow to describe additional features of non-ideal pseudoelastic behaviour. The necessity of the description of PT from the point of view of the choice of the stable post-bifurcation irreversible deformation process (rather than minima of ψ) is analyzed.

Experimental Results [1-3]

Experimental results for uniaxial strain controlled tension of CuZnAl single crystal may be rather

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adequately presented by ideal pseudoelastic behavior shown in Fig.1,2. The elastic properties of both phases are equal and direct and reverse PT's proceed at constant stress. Branch OA corresponds to the elastic behaviour of A, direct PT occurs along AB, on the line BC we have elastic deformation of M. At unloading, line CD corresponds to elastic behaviour of M, reverse PT occurs along DE and on the line EO we have elastic deformation of A. If unloading starts when direct PT is not finished, then we have on the line bd (point d lies on the diagonal AD) elastic behavior of $A+M$ mixture without PT and the curve de corresponds to $M \rightarrow A$ PT (Fig.1). If we interrupt the reverse PT at some point m (Fig.2), then along the line mn the elastic deformation of the $A+M$ mixture takes place, and along the line np $A \rightarrow M$ PT occurs. At a more complex deformation path $OEAbkdeaklBC$ (Fig.2) the lines bd and ea correspond to elastic behaviour of $A+M$ mixture without PT, on the lines de and al PT's $M \rightarrow A$ and $A \rightarrow M$, respectively, take place. Summarizing this results we can conclude that for arbitrary strain history:

1. PT's start always on the diagonal AD, direct PT starts at loading, reverse PT – at unloading and PT's proceed at constant stress.

2. Elastic behaviour without PT starts at unloading inside triangle ABD or loading inside triangle ADE. It takes place when the stress varies (may be cyclically) between the last of its value, when PT has proceeded, and the point on the diagonal AD.

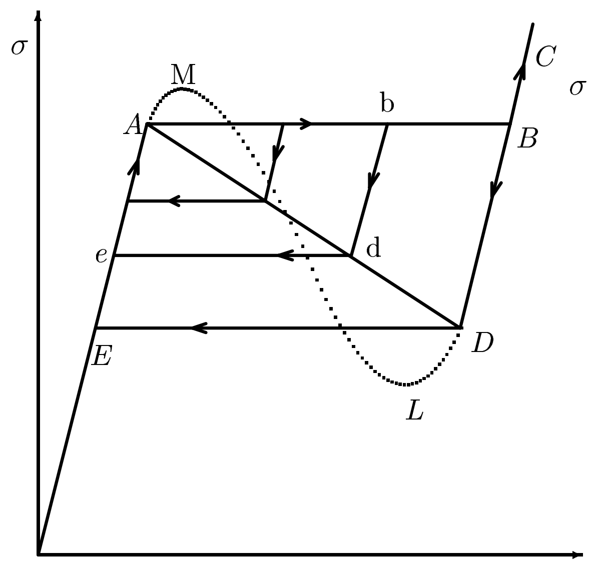

FIG.1

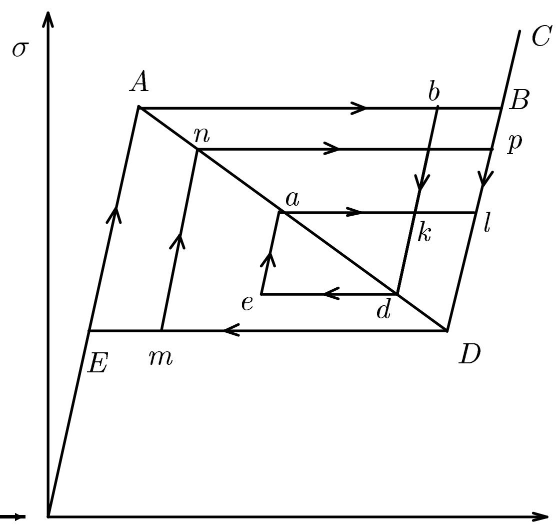

FIG.2

Thermomechanical Model

Let us develop the simple one-dimensional thermomechanical model for description of the above experiments. As in [1-3] we neglect thermal strains, the differences of Young moduli E of phases and the temperature dependence of E. For tensile stress σ assume $\sigma = \sigma_1 = \sigma_2$, for tensile strain

$\epsilon = c_1\epsilon_1 + c_2\epsilon_2$, where the subscripts 1 and 2 correspond to A and M, respectively, c_i is the volume fraction of i-th phase. For A $\epsilon_1 = \epsilon_1^e$, for M $\epsilon_2 = \epsilon_2^e + \eta$, for $A+M$ mixture adopt $\epsilon = \epsilon^e + \epsilon^f$, where the superscripts e and f denote the elastic and transformation strain, $\eta = \epsilon_2^f$. We have $\epsilon = c_1\epsilon_1 + c_2\epsilon_2 = (c_1\epsilon_1^e + c_2\epsilon_2^e) + c_2\eta = \epsilon^e + \epsilon^f$. Because $\sigma = \sigma_1 = \sigma_2 = 0$ results in $\epsilon^e = \epsilon_1^e = \epsilon_2^e = 0$, we get

$$\epsilon^f = c_2\eta \qquad \text{and} \qquad \epsilon^e = c_1\epsilon_1^e + c_2\epsilon_2^e \; . \tag{1}$$

For each phase assume the simplest expression for the free energy $\psi_i = \psi_{0i}(\theta) + 0.5E\epsilon_i^{e2}$, where $\psi_{0i}(\theta)$ is some function of the temperature θ. Assume that

$$\psi = c_1\psi_1 + c_2\psi_2 + \psi_r \; , \qquad \psi_r = 0.5Bc_1c_2 \; , \tag{2}$$

where ψ_r is the energy of internal stresses due to the presence of the transformation strain in M. For the three-dimensional case, at a uniform stress-strain state of each phase, the expression for ψ_r was obtained by Levitas [4,5]. For isotropic phases with equal elastic properties Eq.(2) for ψ_r follows with constant B, depending on the elastic moduli and proportional to η^2 [5]. In the papers [1-3] the same expression for ψ_r is adopted using other motivation and it is called the coherency energy. Let us transform the two first terms in Eq.(2): $c_1\psi_1 + c_2\psi_2 = c_1\psi_{01} + c_2\psi_{02} + 0.5E\left(c_1\epsilon_1^{e2} + c_2\epsilon_2^{e2}\right)$; $E\left(c_1\epsilon_1^{e2} + c_2\epsilon_2^{e2}\right) = c_1\epsilon_1^e E\epsilon_1^e + c_2\epsilon_2^e E\epsilon_2^e = \left(c_1\epsilon_1^e + c_2\epsilon_2^e\right)\sigma = \epsilon^e\sigma = E\epsilon^{e2}$ and, finally,

$$\psi = c_1\psi_{01} + c_2\psi_{02} + 0.5E\epsilon^{e2} + 0.5Bc_1c_2 \; . \tag{3}$$

For the rate of dissipation per unit volume D we obtain

$$D = \sigma\dot{\epsilon} - \dot{\psi} - s\dot{\theta} = \left(\sigma - \frac{\partial\psi}{\partial\epsilon^e}\right)\dot{\epsilon}^e + \sigma\dot{\epsilon}^f - \left(s + \frac{\partial\psi}{\partial\theta}\right)\dot{\theta} - \frac{\partial\psi}{\partial c}\dot{c} \geq 0 \; , \tag{4}$$

where $c = c_2 = 1 - c_1$, s is the entropy and $\Delta\psi_0 = \psi_{02} - \psi_{01}$. From Eq.(4) it follows

$$\sigma = \frac{\partial\psi}{\partial\epsilon^e} = E\epsilon^e \; ; \qquad s = -\frac{\partial\psi}{\partial\theta} = -c_1\frac{\partial\psi_{01}}{\partial\theta} - c_2\frac{\partial\psi_{02}}{\partial\theta} \; ; \tag{5}$$

$$D = X\dot{c} \geq 0 \; ; \qquad X = \sigma\eta - \Delta\psi_0 - 0.5B\left(1 - 2c\right) \; , \tag{6}$$

where X is a thermodynamic stimulus for PT (dissipative force conjugated with $\dot{c}$). From the conventional condition of phase equilibrium $X = 0$ we receive

$$\sigma = \sigma_e\left(c\right) := \left(\Delta\psi_0 + 0.5B\left(1 - 2c\right)\right)\eta^{-1} \; . \tag{7}$$

Substituting $c = \epsilon^f\eta^{-1} = \left(\epsilon - \epsilon^e\right)\eta^{-1} = \left(\epsilon - \sigma E^{-1}\right)\eta^{-1}$ into Eq.(7), we obtain

$$\sigma = \frac{E}{E\eta - B}\left(\left(\Delta\psi_0 + 0.5B\right)\eta - B\epsilon\right) \; . \tag{8}$$

Eq.(8) coincides with the corresponding expression in Müller's theory [1-3] and describes the diagonal AD (Fig.1,2). It is evident, that due to the negative slope of this diagram the phase equilibrium is unstable at fixed σ and θ and there is no hysteresis. The same conclusions were made by Levitas [4,5] after consideration of a three-dimensional model. This was the reason to introduce the concept of the threshold value of dissipative force, which the thermodynamic stimulus X has to reach in order to proceed the PT. Thus, it is assumed that

$$\text{at} \quad \dot{c} > 0 \qquad X = k_{1\to 2}\,(c, ...) > 0\;; \tag{9}$$

$$\text{at} \quad \dot{c} < 0 \qquad X = k_{2\to 1}\,(c, ...) < 0\;; \tag{10}$$

$$\text{at} \quad \dot{c} = 0 \qquad k_{2\to 1}\,(c, ...) \leq X \leq k_{1\to 2}\,(c, ...)\;; \tag{11}$$

where $k_{1\to 2}$ and $k_{2\to 1}$ are the threshold value of X at $A \to M$ and $M \to A$ PT, correspondently, dots denote unspecified parameters. Note, that the cases $X > k_{1\to 2}$ and $X < k_{2\to 1}$ are impossible by definition. The analogy with the threshold value of external force, applied to the body lying on a rough surface and equal to the maximum static friction force is evident. There is also the similar analogy to the threshold value of stress, equal to the yield limit in an elastoplastic material. Using this concept and Eqs. (9)-(11) we can solve two problems, mentioned in Introduction.
Assume $k_{1\to 2} = k_{2\to 1} = k$ and

$$k = B(c - c_0)\;, \tag{12}$$

where c_0 is the volume fraction of M at the beginning of the last type of PT ($A \to M$ or $M \to A$), i.e. at the last intersection with the diagonal AD. For example in Fig.2 the first PT starts at a point A (before A we assume $c_0 = 0$) in which $c = 0$ and for whole following deformation above the line AD (path $AbBC$ or Abk) we have $c_0 = 0$. For a path $Abde$ at the point d PT $M \to A$ starts and for the following deformation dea $c_0 = c_d$, where c_d is the c in a point d. After point a (path $aklBC$ or $aklD$) we obtain $c_0 = c_a$. Thus, by definition when the $\sigma - \epsilon$ diagram intersects the diagonal $X = 0$ and $\dot{\epsilon}$ does not change sign, c_0 has a jump till the current value of c and at the beginning of each type of PT we have $c = c_0$ and $k = 0$. Combining Eqs. (9)-(11) and (12) we have

$$\text{at} \quad \dot{c} > 0 \quad \text{or} \quad \dot{c} < 0 \qquad X = B(c - c_0)\;; \tag{13}$$

$$\text{at} \quad \dot{c} = 0 \qquad (\text{ after } \quad \dot{c} > 0\,) \qquad 0 < X < B(c - c_0)\;; \tag{14}$$

$$\text{at} \quad \dot{c} = 0 \qquad (\text{ after } \quad \dot{c} < 0\,) \qquad B(c - c_0) < X < 0\;. \tag{15}$$

In Eq.(14) we take into account that at $\dot{c} > 0$ we have $X > 0$ and $\dot{c} = 0$ is possible at $X < B(c - c_0)$, but $X > 0$, because at $X = 0$ the stress-strain path intersects the diagonal AD, $c_0 = c$, $k = 0$ and $M \to A$ PT could start (similarly, in Eq.(15)). Using Eq.(7) we obtain:

$$\text{at} \quad \dot{c} \neq 0 \qquad \sigma = \sigma_0(c_0) := \eta^{-1}\left(\Delta\psi_0 + 0.5B(1 - 2c_0)\right)\;; \tag{16}$$

$$\text{at} \quad \dot{c} = 0 \qquad (\text{ after } \quad \dot{c} > 0\,) \qquad \sigma_e(c) < \sigma < \sigma_0(c_0)\;; \tag{17}$$

$$\text{at} \quad \dot{c} = 0 \qquad (\text{ after } \quad \dot{c} < 0\,) \qquad \sigma_0(c_0) < \sigma < \sigma_e(c)\;. \tag{18}$$

Eqs.(16)-(18) describe all the above details of the materials behaviour . Thus, when PT's start $c_0 = c$ and Eq.(16) describes the diagonal (7), i.e. PT's start on the diagonal AD. Then the PT's proceed at the same constant stress σ_0 (Eq.(16)). If σ become less than σ_0 (after $\dot{c} > 0$) or grater than σ_0 (after $\dot{c} < 0$) or varies between σ_0 and σ_e, then $\dot{c} = 0$ (Eqs.(17)-(18)) and we have elastic behaviour without PT.
To evaluate the value B note that $B = 2A\rho$, where A is the coherency coefficient in [3], ρ is a mass density. As $A = 82\ J/kg$, $\rho = 7745\ kg/m^3$ [3], then $B = 635090\ J/m^3$. This value does not depend on θ [2,3].

Consistency Condition and PT Criteria

Conditions (9)-(11) and (13)-(18) are not precise PT criteria, because they show which diagram has material at $\dot{c}$ grater, less or equal to zero, but not at which ϵ and $\dot{\epsilon}$ value $\dot{c}$ is grater, less or equal to zero. In plasticity theory it is necessary to consider additionally the consistency condition, the loading criterion and the plastic flow rule [6]. Let us find their counterparts for PT's theory. Due to the fact that at PT $\dot{\sigma} = 0$ and PT criteria may be formulated in term of $\dot{\epsilon}$, let us express X in terms of ϵ and c: $X = E(\epsilon - c\eta)\eta - \Delta\psi_0 - 0.5B(1-2c)$. If at some c condition (9) is met, than for $\dot{c} > 0$ it is necessary that at time $t + \Delta t$ this condition is met at $c + \Delta c$, i.e. $X(t + \Delta t) = k_{1\rightarrow 2}(c + \Delta c, ...)$. For infinitesimal Δt combining this equation with Eq.(9) we obtain $\dot{X} = \dot{k}_{1\rightarrow 2}$ or

$$\frac{\partial X}{\partial \epsilon}\dot{\epsilon} = \left(\frac{\partial k_{1\rightarrow 2}}{\partial c} - \frac{\partial X}{\partial c}\right)\dot{c}, \qquad \text{or} \qquad E\eta\dot{\epsilon} = \left(E\eta^2 - B + \frac{\partial k_{1\rightarrow 2}}{\partial c}\right)\dot{c}\ . \tag{19}$$

This is the consistency condition. As $E\eta^2 \gg B$ (it is easy to prove geometrically) then the term in the bracket in Eq.(19) is positive. Then for $\dot{c} > 0$ it is necessary that $\dot{\epsilon} > 0$ and at $\dot{\epsilon} < 0$ the consistency condition will be violated and $\dot{c} = 0$. Eq.(19) allows also to determine $\dot{c}$ at prescribed $\dot{\epsilon} \geq 0$, i.e. it serves as a counterpart of the flow rule as well. When Eq.(12) is valid, than Eq.(19) results in $\dot{\epsilon} = \eta\dot{c}$. Generalizing the above results we can formulate the following PT criteria:

$$X = B(c - c_0) \geq 0 \qquad \text{and} \qquad \dot{\epsilon} > 0 \longrightarrow \dot{c} > 0\ ; \tag{20}$$

$$X = B(c - c_0) \leq 0 \qquad \text{and} \qquad \dot{\epsilon} < 0 \longrightarrow \dot{c} < 0\ . \tag{21}$$

$$\dot{c} = 0 \qquad \text{when :}$$

$$1.\ \underline{\text{After}\quad \dot{c} > 0\ :} \qquad 0 < X < B(c - c_0) \qquad \text{or} \tag{22}$$

$$X = B(c - c_0) > 0 \quad \text{and} \quad \dot{\epsilon} < 0 \qquad \text{or} \qquad X = 0 \quad \text{and} \quad \dot{\epsilon} > 0\ .$$

$$2.\ \underline{\text{After}\quad \dot{c} < 0\ :} \qquad B(c - c_0) < X < 0 \qquad \text{or} \tag{23}$$

$$X = B(c - c_0) < 0 \quad \text{and} \quad \dot{\epsilon} > 0 \qquad \text{or} \qquad X = 0 \quad \text{and} \quad \dot{\epsilon} < 0\ .$$

$$3.\ \underline{\text{At}\quad c = 0 \quad (\text{ before any PT })\ :} \quad X < 0 \quad \text{or} \quad X = 0 \quad \text{and} \quad \dot{\epsilon} < 0\ . \tag{24}$$

Using Eq.(6) for X we obtain the following form of Eqs. (20)-(24)

$$\sigma = \sigma_0(c_0)\ , \qquad X \geq 0 \qquad \text{and} \qquad \dot{\epsilon} > 0 \longrightarrow \dot{c} > 0\ ; \tag{25}$$

$$\sigma = \sigma_0(c_0)\ , \qquad X \leq 0 \qquad \text{and} \qquad \dot{\epsilon} < 0 \longrightarrow \dot{c} < 0\ . \tag{26}$$

$$\dot{c} = 0 \qquad \text{when :}$$

$$1.\ \underline{\text{After}\quad \dot{c} > 0\ :} \qquad \sigma_e(c) < \sigma < \sigma_0(c_0) \qquad \text{or} \tag{27}$$

$$\sigma = \sigma_0(c_0)\ , \quad X > 0 \quad \text{and} \quad \dot{\epsilon} < 0 \qquad \text{or} \qquad \sigma = \sigma_e(c) \quad \text{and} \quad \dot{\epsilon} > 0\ .$$

$$\text{2. } \underline{\text{After} \quad \dot{c} < 0\ :} \qquad \sigma_0(c_0) < \sigma < \sigma_e(c) \qquad \text{or} \tag{28}$$

$$\sigma = \sigma_0(c_0)\ , \quad X < 0 \quad \text{and} \quad \dot{\epsilon} > 0 \qquad \text{or} \qquad \sigma = \sigma_e(c) \quad \text{and} \quad \dot{\epsilon} < 0\ .$$

$$\text{3. } \underline{\text{At} \quad c = 0\ :} \qquad \sigma < \sigma_e(0) \quad \text{or} \quad \sigma = \sigma_e(0) \quad \text{and} \quad \dot{\epsilon} < 0\ . \tag{29}$$

It is now easy to describe the whole complicated behaviour, as for example shown in Fig.2. On the line OA $c_0 = 0$ and according to Eq.(29) $\dot{c} = 0$. At point A at $\dot{\epsilon} > 0$ we have $\dot{c} > 0$ (Eq.(25)). At increasing ϵ we obtain $\sigma = \sigma_0$ (otherwise, $X > k$, which is impossible) and in all points of the line Ab Eq.(25) is met, $c_0 = 0$ and $\dot{c} = \dot{\epsilon}\eta^{-1}$. At point b we have $\dot{\epsilon} < 0$ and $\dot{c} = 0$, as well as on the line bd (Eq.(27)). At point d according to Eq.(26) $\dot{c} < 0$ and $c_0 = c_d$. On the line de we obtain $\sigma = \sigma_0(c)$ (otherwise $X < k < 0$) and $\dot{c} < 0$ (Eq.(26)). At point e we have $\dot{\epsilon} > 0$ and $\dot{c} = 0$, as well as on the line ea (Eq.(28)). At point a condition (25) gives $\dot{c} > 0$, as well as on the whole line akl.

Some Generalizations and Interpretations

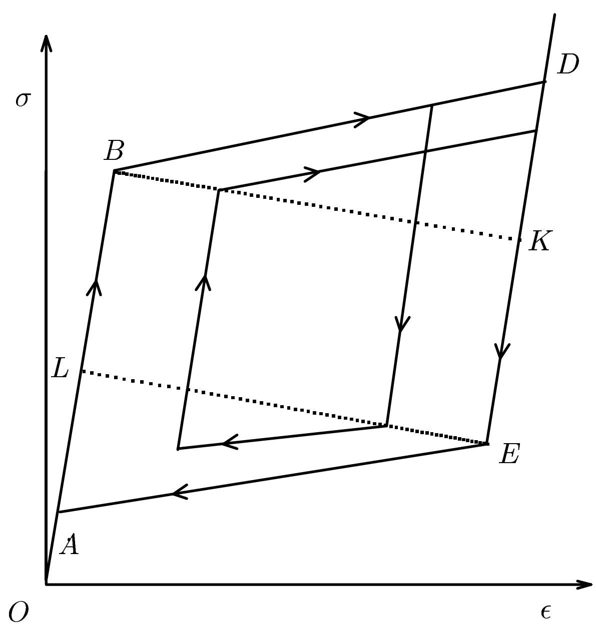

FIG.3

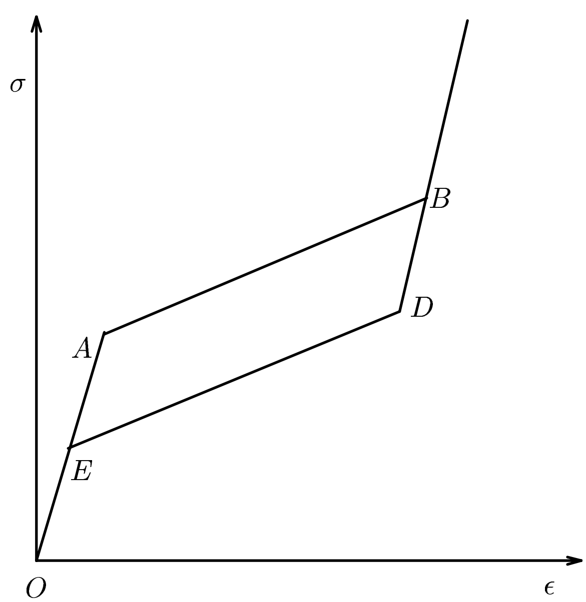

FIG.4

A more complicated behaviour than ideal pseudoelastic is possible even for the same alloy [2] and it is interesting to examine, which type of the diagram corresponds to more complex dependence $k(c, c_0)$, than in Eq.(12). Assume

$$k = P + L(c - c_0) \quad \text{at} \quad \dot{c} > 0 \quad \text{and} \quad k = -P + L(c - c_0) \quad \text{at} \quad \dot{c} < 0\ . \tag{30}$$

Corresponding to this case the behaviour is shown in Fig.3. At $L > B$ we have hardening, and at $L < B$ softening at $A \rightarrow M$ PT. Hardening behaviour is known in the literature, for example

[7]. At $P \neq 0$ $A \rightarrow M$ and $M \rightarrow A$ PT's start on the different lines, BK and LE respectively, which also takes place in reality [8]. Consequently, the simplest generalization of Eq.(12) can be useful, and more general dependence $k(c, c_0)$ (for example different for $A \rightarrow M$ and $M \rightarrow A$ PT, nonlinear) can be used to describe more complicated behaviour. Parameter c_0 characterizes the history dependence of the PT. Material memory has discrete character and after intersecting of line AD in Fig.1,2 or lines BK (at $\dot{\epsilon} > 0$) or EL (at $\dot{\epsilon} < 0$) in Fig.3 the material does not remember the previous straining. This behaviour is possible only in the absence of any irreversible changes (for example plastic deformation) in the material. As shown in [4,5], k is equal to the resistance force to the interface motion $\tilde{k}$, which is averaged over the volume , in which during the time increment Δt the PT occurs. The resistance force $\tilde{k}$ in the general case can be caused by the intersection of the interface with boundary of grains and subgrains, with dislocations and point defects, by accommodation plastic strain and lattice friction, emission of acoustic waves and so on. For the coherent interface $\tilde{k}$ is much smaller than for a noncoherent one. Consequently, the origin of the hysteresis and dissipation is related with the resistance to the interface motion, but not with the coherency energy as mentioned in [1,2]. Hysteresis will takes place at $B = 0$, but $k \neq 0$ (for k Eq.(30) can be used), but at $k = 0$ and $B \neq 0$ not.
The above model considers hardening behaviour only due to a dissipation mechanism, because at $k = 0$ the $\sigma - \epsilon$ diagram exhibits softening (line AD). But it is also necessary to assume the possibility of the reversible mechanism of hardening. During direct PT the defects of A are kept in M, as well as the new ones (for example accommodation twins) appear and the internal energy varies. At reverse $M \rightarrow A$ PT the new defects disappear and the kept defects, mentioned above, are returned in a initial condition and the whole accumulated energy is recovered. This type of energy was considered, for example in [9] as responsible one for the realization of reverse PT "exactly back". If we assume the simplest expression for energy of defects $\psi_d = -0.5Mc(1-c)$, $M > 0$, similar to the energy of internal stresses, but with opposite sign, then in all the above equations B has to be replaced with $(B - M)$. At $B < M$ direct PT starts at σ, which is less than its value for $B = M = 0$, but the material exhibits hardening (even at $k = 0$).Only when we include in our consideration the reversible hardening mechanism, it is possible to describe the situation, when reverse PT starts at stress higher than σ at the beginning of the direct PT (Fig.4), $\sigma_D > \sigma_A$. This phenomenon is observed in some experiments [7].

Concluding Remarks

Usually as initial information about the behaviour of the material with PT's the nonmonotone diagram of uniform straining is presented (line $OAMLDC$ in Fig.1). Point A is the bifurcation point after which two continuations are possible– with uniform strain (along $AMLDB$) or with nonuniform one (along AB) , if two-phase mixture appears with the different strains in each phase. For the reversible processes there is the principle of minima of ψ, using which we can find more stable solution. If we introduce the dissipative force k, than the irreversible process occurs and this principle is not applicable. The extremum principle for choosing the stable post-bifurcation process for irreversible elastoplastic system was substantiated in [10] and applied for a direct PT process

at simple shearing. It is easy to show, that the similar conclusions are valid in the given case. Thus if the stress on the line AB is less then σ_M in a point M, then the deformation process AB with varying c (moving interfaces) is more stable. If the stress at the part of the line AB exceeds σ_M , then at $\sigma = \sigma_M$ the straining at $\dot{c} = 0$ is more stable, A is deformed in accordance with the branch ML, M – in accordance with the line BL, stress decrease up to value σ_L. Then material becomes uniform and the following loading occurs along the line $LDBC$. Note, that it is necessary the choice of the more stable deformation process to make at the every point of the post-bifurcation processes AB. At the more detailed micromechanical approach the above extremum principle allows us to choose at every ϵ and $\Delta\epsilon$ which process is more stable: with appearance of the new martensitic plate (in which place and how orientated) or interface motion.
The results obtained could be generalized for the three-dimensional case, using the developed in [4,5] approach. To determine the transformation strain tensor the same extremum principle, as for choosing the more stable post-bifurcation process [10], could be applied. It is unclear, why cyclic deformation reduces dissipation. According to the model, it is possible to transform the whole A into M and back with a infinitesimal dissipation and hysteresis, organizing a infinite number of corresponding infinitesimal cycles around the diagonal AD. The key open problem is the micromechanical basis of the dependence $k(c, c_0)$, i.e. the dependence $\tilde{k}$ on the interface displacement and its history for mono- and polycrystalline materials with various types of defects and microheterogeneties.

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