



## SIMPLE MICROMECHANICAL MODEL OF THERMOELASTIC MARTENSITIC TRANSFORMATIONS

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### 1. Introduction

A number of descriptions of phase transitions (PT) in elastic materials under three-dimensional loading are known. In [1, 2] some general relations are obtained for anisotropic materials, but results were not applied for the description of experiments. Thermodynamical theory [3] can rather adequately describe one-dimensional experiments. It seems to be a little oversimplified for the description of PT under three-dimensional loading (see Section 7).

Closed to the present paper are the results obtained in [4]; detailed comparison will be made in Section 7. The important features of our consideration are the following:

- a new PT criterion derived in [5, 6] is applied;
- new extremum thermomechanical principles and explicit formulas for jump of transformation strain in transforming particles and macroscopic transformation strain are derived based on a postulate of realizability [5] – [7];
- five real micromechanical mechanisms of PT (nucleation at direct austenite ( $A$ )  $\rightarrow$  martensite ( $M$ ) and reverse  $M \rightarrow A$  PT, interface motion at direct and reverse PT and reorientation of martensitic variants) are taken into account;
- the constant in obtained expressions for stresses in  $A$ ,  $M$  and transforming particle (characterizing a level of internal stresses) is calibrated from experiments; known theoretical formulas for this constant [2, 4] overestimate it in one to two orders.

Based on the above features, the thermodynamical criteria of occurrence of all five enumerated micromechanical processes are derived. These criteria describe the evolution of five PT surfaces in the macroscopic stress space. Comparisons of the theory with some known experimental results show qualitative and quantitative agreement. The similarity between PT theory (for the direct PT due to nucleation) and plasticity theory, established in Section 6, allows the application of numerical algorithms – which were developed for the solution of elastoplastic boundary-value problems – for the solution of boundary-value problems for materials with PT.

Note that some preliminary results were published in [8]–[10].

## 2. Phase transitions criterion and extremum principle

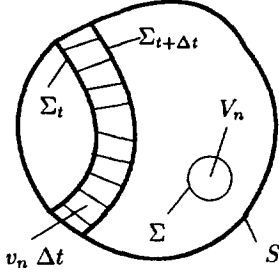


FIG. 1. Volume with PT

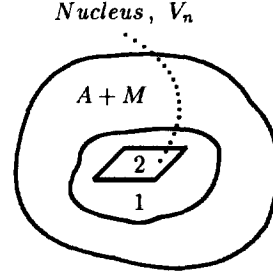


FIG. 2. Scheme of averaging over volume with PT

Consider the volume  $V$  of  $A + M$  mixture. During the time  $\Delta t$  some PT occurs in a volume  $V_n \in V$ ,  $V_n \ll V$  with a boundary  $\Sigma$  (Fig.1) ( $A \rightarrow M$  and  $M \rightarrow A$  due to nucleation or interface motion or reorientation of  $M$  particles). The following conditions for the driving force  $X_n$

$$X_n := \frac{1}{V_n} \int_{V_n} \int_{\tilde{\epsilon}_1}^{\tilde{\epsilon}_2} \tilde{\sigma} : d\tilde{\epsilon} dV_n - (\psi_2 - \psi_1) = k_n; \quad \dot{X}_n = \dot{k}_n \quad (1)$$

are substantiated in [5, 6] as PT criteria. Here  $\tilde{\sigma}$  and  $\tilde{\epsilon}$  are the local stress and strain tensors,  $\psi$  the Helmholtz free energy,  $X_n$  the dissipation increment per unit volume of  $V_n$  (driving force of PT),  $k_n$  the threshold value of  $X_n$ , related to the actual dissipative processes in the course of PT (e.g. emission of acoustic waves, lattice friction, microplasticity); the indices 1 and 2 correspond to the value before and after PT. Eq.(1) means that the calculated value of dissipation increment in the course of PT reaches its actual value, and this equality will not be violated at the next time instant. Eq.(1)<sub>2</sub> is a counterpart of a consistency condition in plasticity theory. For macroscopically homogeneous boundary conditions on  $\Sigma$  the Mandel–Hill relation

$$\langle \tilde{\sigma} : \tilde{\epsilon} \rangle_n = \sigma_n : \epsilon_n, \quad \text{where} \quad \sigma_n = \langle \tilde{\sigma} \rangle_n, \quad \epsilon_n = \langle \tilde{\epsilon} \rangle_n, \quad \langle \dots \rangle_n = \frac{1}{V_n} \int_{V_n} (\dots) dV_n \quad (2)$$

is valid [2] and Eq.(1)<sub>1</sub> is equivalent to

$$X_n := \int_{\epsilon_1}^{\epsilon_2} \sigma_n : d\epsilon_n - (\psi_2 - \psi_1) = k_n. \quad (3)$$

Here  $\sigma_n$  and  $\epsilon_n$  are the mean stress and strain tensors in  $V_n$ . The rate of dissipation per unit volume of  $V$  due to PT is defined by  $D = X_n \dot{c}_n > 0$ , where  $\dot{c}_n = V_n / (\Delta t V)$ . For the determination of changes of  $\sigma_n$  and  $\epsilon_n$  in the course of PT due to nucleation, the method developed in [1, 2] is used. It allows us to determine explicitly stress and strain in each (isotropic or anisotropic) phase of  $n$ -phase material under the assumption of homogeneity of stress and strain in each phase. For compactness we shall consider phases with equal isotropic tensors of elastic moduli  $E_i = E$  and neglect the volumetric transformation strain. Assume that

$$\epsilon_n = \epsilon_n^e + \epsilon_n^t \quad \text{and} \quad \psi_i = \psi_i^\theta(\theta) + 0.5 \epsilon_i^e : E : \epsilon_i^e = \psi_i^\theta + \psi_i^e \quad (i = 1, 2), \quad (4)$$

where the superscripts  $e$  and  $t$  mean the “elastic” and “transformation” strains,  $\theta$  the tempera-

ture,  $\psi_i^\theta$  the thermal part of  $\psi_i$  (at  $\epsilon_i^e = 0$ ),  $\psi_i^e$  the elastic part of  $\psi_i$ . As

$$\int_{\epsilon_1^e}^{\epsilon_2^e} \sigma_n : d\epsilon_n^e = \mathbf{E} \cdots \int_{\epsilon_{n1}^e}^{\epsilon_{n2}^e} \epsilon_n^e d\epsilon_n^e = 0.5 \epsilon_{n2}^e : \mathbf{E} : \epsilon_{n2}^e - 0.5 \epsilon_{n1}^e : \mathbf{E} : \epsilon_{n1}^e = \psi_2^e - \psi_1^e, \quad (5)$$

then from Eq.(3) it follows

$$X_n = \int_{\epsilon_1^e}^{\epsilon_2^e} \mathbf{S}_n : d\epsilon_n^e - (\psi_2^\theta - \psi_1^\theta) = k_n, \quad (6)$$

where  $\mathbf{S}_n$  and  $\mathbf{e}_n^t$  are the deviators of  $\sigma_n$  and  $\epsilon_n^t (= \epsilon_n^t)$ . Using the results of [1, 2] we obtain

$$\mathbf{S}_A = \mathbf{S} + P \mathbf{e}^t; \quad \mathbf{S}_M = \mathbf{S} - P(1-c) \mathbf{e}_M^t; \quad \mathbf{S}_n = \mathbf{S}_A - P \mathbf{e}_n^t; \quad \mathbf{e}^t = c \mathbf{e}_M^t, \quad (7)$$

where  $\mathbf{S}$  and  $\mathbf{e}^t$  are the stress and transformation strain averaged over the mixture (Fig.2). The subscripts  $A$  and  $M$  mean averaged over  $A$  and  $M$  values,  $c$  the volume fraction of  $M$ ,  $P$  a constant depending on elastic moduli. Note that  $\mathbf{e}_A^t \equiv 0$ .

Let us analyze expressions (7). Stresses in  $\mathbf{S}_A$  and  $\mathbf{S}_M$  consist of two parts: the external stresses  $\mathbf{S}$  and internal stresses. If  $\mathbf{e}_M^t = 0$ , no residual stresses exist in  $A$  and  $M$ . Consequently, the internal stresses must be proportional to  $\mathbf{e}_M^t$ , and  $P$  is a coefficient which transforms inelastic strain into stresses and characterizes elastic properties of a system. If there is no  $M$ ,  $c = 0$  and  $\mathbf{S}_A = \mathbf{S}$ ; if there is no  $A$ , then  $c = 1$  and  $\mathbf{S}_M = \mathbf{S}$ . The averaged value of internal stresses over the representative volume must be zero. As  $(1-c)cP\mathbf{e}_M^t - c(1-c)P\mathbf{e}_M^t = 0$ , we fulfill this requirement. As  $c_n \rightarrow 0$ , the nucleus does not affect the averaged stresses  $\mathbf{S}_A$  and  $\mathbf{S}_M$ . The expression for  $\mathbf{S}_n$  has also no qualitative contradictions. Thus, if  $\mathbf{e}_n^t = 0$  and the nucleus is austenitic, then  $\mathbf{S}_n = \mathbf{S}_A$ . If  $\mathbf{e}_n^t = \mathbf{e}_M^t$  and the nucleus is martensitic, then

$$\mathbf{S}_n = \mathbf{S}_A - P \mathbf{e}_M^t = \mathbf{S} - (1-c)P \mathbf{e}_M^t = \mathbf{S}_M. \quad (8)$$

There is one problem, related to a value of the constant  $P$ . Analytical expression obtained for  $P$  in [2] and similar expression in [4] give  $P \simeq \mu$ , where  $\mu$  is a shear modulus. At  $c \simeq 0$  or  $c \simeq 1$  the maximal internal stresses  $\mathbf{S}_{i_n}$  in  $M$  or  $A$  can be estimated as

$$\mathbf{S}_{i_n} = \mu \mathbf{e}_M^t = 2\mu e_Y \frac{\mathbf{e}_M^t}{2e_Y} = \tau_Y \frac{\mathbf{e}_M^t}{2e_Y}, \quad (9)$$

where  $\tau_Y = 2\mu e_Y$  and  $e_Y$  are a yield stress and an elastic strain at yielding in shear. If  $e_Y \simeq 10^{-3}$  for steel and  $e_Y \simeq 10^{-2}$  for shape memory alloys,  $|\mathbf{e}_M^t| \simeq 10^{-1}$ , then  $|\mathbf{S}_{i_n}| \simeq 0.5(10 \div 100)\tau_Y$ , which is impossible ( $|\mathbf{A}| := (\mathbf{A}:\mathbf{A})^{1/2}$ ). The reason of the contradiction lies in the fact, that simplified estimations for  $P$  do not take into account the anisotropic (plate-like) form of martensitic particles and the specific character of transformation strain distribution. E.g., at transformation strain with invariant plane and formation of fine microstructure the internal stresses are zero, but  $\mathbf{e}_M^t \neq 0$  [11]. It is in principle possible, but extremely difficult, to derive correct expression for  $P$ . That is why we shall determine the constant  $P$  from simple experiments.

After substituting  $\mathbf{S}_n$  from Eq.(7) into Eq.(6) and integrating we obtain

$$X_n = \mathbf{S}_A : (\mathbf{e}_2^t - \mathbf{e}_1^t) - 0.5P(|\mathbf{e}_2^t|^2 - |\mathbf{e}_1^t|^2) - (\psi_2^\theta - \psi_1^\theta) = k_n. \quad (10)$$

Using the postulate of realizability [5]-[7] the extremum principle can be derived

$$X_n(\mathbf{e}_2^{t*}, \mathbf{e}_1^{t*}) - k_n(\mathbf{e}_2^{t*}, \mathbf{e}_1^{t*}) \leq 0 = X_n(\mathbf{e}_2^t, \mathbf{e}_1^t) - k_n(\mathbf{e}_2^t, \mathbf{e}_1^t), \quad (11)$$

i.e. the real values of  $\mathbf{e}_i^t$  maximize  $X_n - k_n$  in comparison with all possible  $\mathbf{e}_i^{t*}$ . Tensors  $\mathbf{e}_i^t$  meet some additional constraints, which depend on the type of PT. If  $k_n$  is independent of  $\mathbf{e}_i^t$  then from

the principle (11) we obtain

$$S_A : (e_2^{i*} - e_1^{i*}) - 0.5 P (|e_2^{i*}|^2 - |e_1^{i*}|^2) \leq S_A : (e_2^t - e_1^t) - 0.5 (|e_2^t|^2 - |e_1^t|^2). \quad (12)$$

### 3. Phase transition austenite $\rightarrow$ martensite due to nucleation

At  $A \rightarrow M$  PT,  $e_1^t = e_A^t = 0$ ,  $\dot{c} = \dot{c}_n$ . Let the transformed particle consist of several variants of  $M$ . Then  $|e_2^t|$  could not exceed its maximal value  $a(c)$ , but due to, e.g., twinning it is possible that  $|e_2^t| \leq a$ . Consequently it follows from the principle (12)

$$S_A : e_2^{i*} - 0.5 P |e_2^{i*}|^2 \leq S_A : e_2^t - 0.5 P |e_2^t|^2 \quad \text{at} \quad |e_2^t| \leq a; \quad (13)$$

$$e_2^t = (1/P) S_A \quad \text{at} \quad |e_2^t| < a; \quad e_2^t = a S_A / |S_A| \quad \text{at} \quad |e_2^t| = a. \quad (14)$$

Substituting Eq.(14) in Eq.(10) we obtain an explicit expression of  $A \rightarrow M$  PT criterion in stress space

$$0.5 P^{-1} |S_A|^2 = (\psi_M^\theta - \psi_A^\theta) + k_{A \rightarrow M} \quad \text{at} \quad |S_A| < P a; \quad (15)$$

$$a |S_A| = a^2 P/2 + (\psi_M^\theta - \psi_A^\theta) + k_{A \rightarrow M} \quad \text{at} \quad |S_A| \geq P a. \quad (16)$$

If we assume as usual that  $\psi_M^\theta - \psi_A^\theta$  is a linear function of  $\theta$  and  $k_{A \rightarrow M}$ ,  $P$  and  $a$  are temperature independent, then Eqs.(16) and (15) exhibit linear and quadratic dependence between PT temperature and stress respectively. Linear dependence is observed in the most of experiments, quadratic one can be found in [12] for  $\beta$ -Cu Zn.

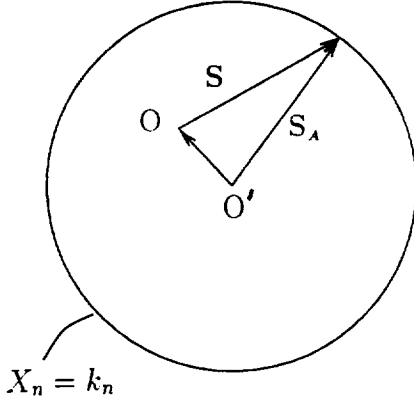


FIG. 3. PT surface in deviatoric space  $S$ .

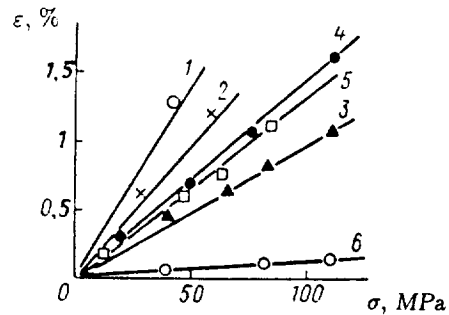


FIG. 4. Experimentally determined dependence of transformation strain on stress at cooling of various alloys [14].

Note that  $k_{A \rightarrow M}$  is an increasing function of  $c$  [3, 13]. In the space of deviatoric stress in  $A$ , PT criterion (15), (16) represents a *sphere* with growing radius. As  $S_A = S + P e^t$ , this sphere is *shifted* on vector  $-P e^t$  (Fig.3) in the space of deviatoric macroscopic stress  $S$ . The modulus  $|e^t|$  grows when  $c$  grows, and at a radial loading the center of sphere moves in direction opposite to  $S$ . Consequently (using similarity with plasticity theory) in space  $S$  material exhibits *isotropic hardening and kinematic softening*.

Note, that if we neglect dissipation,  $k_{A \rightarrow M} = 0$ , then only kinematic softening occurs, and at prescribed stress two-phase equilibrium is unstable and consequently impossible. The same conclusion was made in [1, 2] and this was a reason for the introduction of a dissipative threshold.

After substitution of  $e_2^t$  from Eq.(14)<sub>1</sub> (for  $|e_2^t| < a$ ) in Eq.(7)<sub>3</sub> we obtain  $S_n = 0$ , i.e. the deviatoric stress in nucleus after PT is zero. This result can be important to generalize the mathematical theory of formation of fine microstructure in single crystals [11] for the stress induced PT in polycrystals. Let us determine  $e^t$ . By definition

$$e^t(t) = c(t) e_M^t(t), \quad \text{and} \quad e^t(t + \Delta t) = c(t) e_M^t(t + \Delta t) + c_n(t) e_2^t(t), \quad (17)$$

If  $e_M^t$  in previously formed  $M$  is not changed, then  $\dot{e}^t = e_2^t \dot{c}$ ,

$$\frac{de^t}{dc} - e^t = \frac{1}{P} S, \quad e^t = \exp c \int_0^c \frac{1}{P} S(x) \exp(-x) dx \quad \text{at} \quad |e_2^t| < a; \quad (18)$$

$$\frac{de^t}{dc} = a \frac{S_A}{|S_A|} \quad \text{at} \quad |e_2^t| = a. \quad (19)$$

If PT occurs during cooling at  $S = \text{const}$  ( $|e_2^t| < a$ ), then

$$e^t(c) = (1/P) S (\exp c - 1), \quad e^t(1) = (1.78/P) S, \quad (20)$$

i.e.,  $e^t$  and  $S$  are related linearly, as in experiments for TRIP steels (Fig.4) [14]. Comparing of Eq.(20)<sub>2</sub> with experiments (Fig.4), we can determine constant  $P$  for a number of materials. For example, for negligible elastic strains and one dimensional tension Eq.(20)<sub>2</sub> reads as  $\varepsilon = (1.19/P) \sigma$ , where  $\sigma$  and  $\varepsilon$  are the stress and strain. Then  $P = 4377 \text{ MPa}$  for *Cu 88% Mn* (material 1 in Fig.4) and  $P = 99167 \text{ MPa}$  for *Cu 52% Mn* (material 6 in Fig.4).

If PT proceeds under  $S = S_o = \text{const}$  at  $0 < c \leq c_o$  and  $S = 0$  at  $c_o < c$ , then

$$e^t = (1/P) S_o \exp c (1 - \exp(-c_o)), \quad (21)$$

i.e. at  $S = 0$ , strain  $e^t$  continues to grow which also corresponds to experiments (Fig.5) [15].

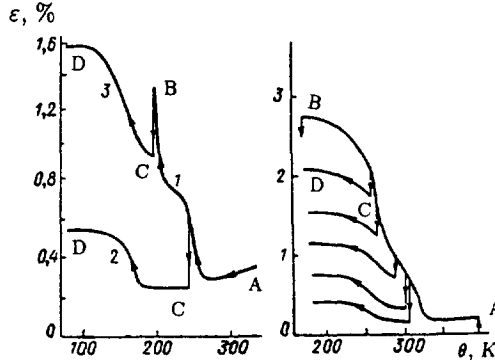


FIG. 5. Experimentally determined dependence of strain  $\varepsilon$  on temperature at  $S \neq 0$  (A - B) and  $S = 0$  (CD) [15]. Strain grows with decreasing temperature at  $S = 0$  as well.

Let us designate the PT surface (15), (16) with equation  $\phi(S + P e^t) = K(c, \theta)$ . Then we can represent the constitutive Eqs.(18) and (19) in the form of associated flow rule

$$\dot{e}^t = \dot{c} \frac{\partial \phi}{\partial S}. \quad (22)$$

A kinetic equation for  $\dot{c}$  coincides with the consistency condition  $\dot{\phi}(\mathbf{S} + P\mathbf{e}^t) = \dot{K}(c, \theta)$ , i.e.

$$\dot{c} = \left( \frac{\partial \phi}{\partial \mathbf{S}} : \dot{\mathbf{S}} - \frac{\partial K}{\partial \theta} \dot{\theta} \right) \left( \frac{\partial K}{\partial c} - P \frac{\partial \phi}{\partial \mathbf{S}} : \frac{\partial \phi}{\partial \mathbf{S}} \right)^{-1}. \quad (23)$$

**4. Phase transition  $M \rightarrow A$  due to nucleation and reorientation process**

At  $M \rightarrow A$  PT, transformation strain accumulated during  $A \rightarrow M$  PT is recovered, i.e. in Eqs.(10) and (12)  $\mathbf{e}_2^t = 0$ . As  $D = X_n \dot{c}_n = X_c \dot{c}$  and  $\dot{c} = -\dot{c}_n$ , then  $X_c = -X_n$  and Eq.(10) results in

$$X_c = \mathbf{S}_A : \mathbf{e}_1^t - 0.5 P | \mathbf{e}_1^t |^2 - (\psi_M^\theta - \psi_A^\theta) = k_{M \rightarrow A} < 0, \quad (24)$$

where  $\mathbf{e}_1^t$  now is the transformation strain in particle of  $M$  undergoing PT. Let us redesignate  $\mathbf{e}_d^t(\xi) = \mathbf{e}_2^t(c)$ ,  $\xi = c$ , the transformation strain at  $A \rightarrow M$  PT, which occurs at fraction  $c$ . For the definition  $\mathbf{e}_1^t$  let us further assume that  $\mathbf{e}_1^t = \mathbf{e}_d^t(\xi)$  for some  $\xi$ , and let us use the principle (12) for choosing  $\xi$ :

$$\mathbf{S}_A : \mathbf{e}_1^{t*} - 0.5 P | \mathbf{e}_1^{t*} |^2 \geq \mathbf{S}_A : \mathbf{e}_1^t - 0.5 P | \mathbf{e}_1^t |^2 \quad \text{at} \quad \mathbf{e}_1^{t*} \in \mathbf{e}_d^t(\xi). \quad (25)$$

According to Eqs.(24) and (25) the following procedure for definition of reverse PT surface is valid. For each  $\mathbf{e}_1^t \in \mathbf{e}_d^t(\xi)$ , condition (24) defines the plane which is orthogonal to  $\mathbf{e}_1^t$ . According to principle (25), the resulting surface of reverse PT is formed by points of these planes, which are the closest to end of the vector  $\mathbf{S}_A$  during or after the direct PT (Figs. 6 and 7).

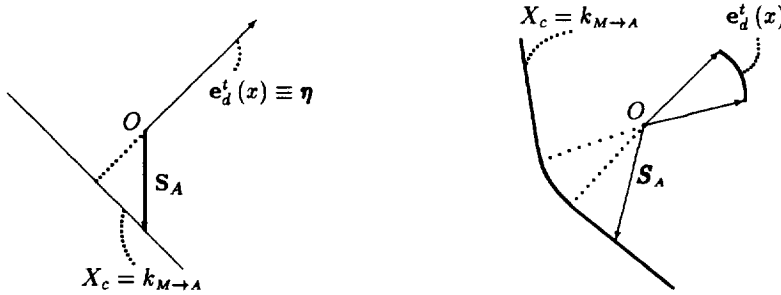


FIG. 6. Surface of reverse PT at  $\mathbf{S}_A : \mathbf{e}_1^t < 0$  (pseudoplasticity).

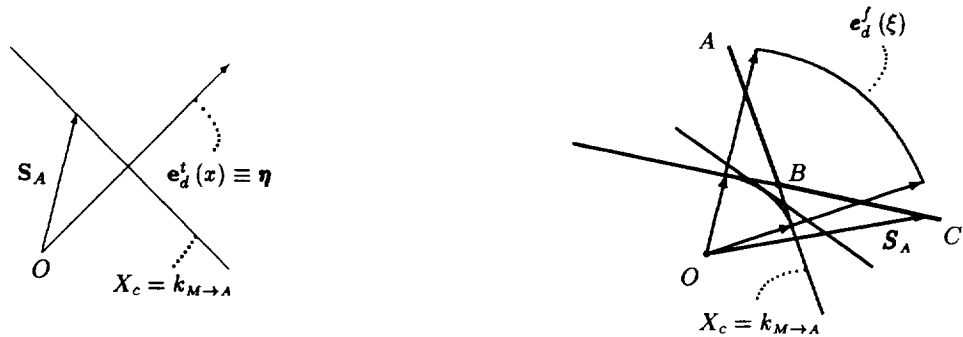


FIG. 7. Surface of reverse PT  $ABC$  at  $\mathbf{S}_A : \mathbf{e}_{t1} > 0$  (pseudoelasticity).

$$\text{If } \mathbf{e}_d^t(\xi) = \boldsymbol{\eta} = \text{const}, \quad \text{then } \mathbf{e}_1^t = \boldsymbol{\eta} \quad \text{and} \\ X_c = \mathbf{S} : \boldsymbol{\eta} + P |\boldsymbol{\eta}|^2 (c - 0.5) - (\psi_M^\theta - \psi_A^\theta) \quad (26)$$

has the same expression for  $A \rightarrow M$  and  $M \rightarrow A$  PT. Such situation at unidimensional tension was considered in [13, 16] for the description of experiments [16] with pseudoelastic CuZnAl single crystal. It was shown [13] that in this case  $k = B(c - c_0)$ , where  $B = 2P|\boldsymbol{\eta}|^2$  is constant,  $c_0$  the volume fraction of  $M$  at the beginning of the last type of PT ( $A \rightarrow M$  or  $M \rightarrow A$ ). Knowing constants  $B$  and  $|\boldsymbol{\eta}|$  [16], we can determine  $P$ . Thus, at  $B = 635090 \text{ J/m}^2$  [13] and  $\eta \simeq 0.06$  [16]  $P = 88206944 \text{ J/m}^3$ .

Let tensors  $\mathbf{e}_d^t(\xi)$  describe some continuous line in  $R^5$ . If at  $M \rightarrow A$  PT tensor  $\mathbf{S}_A$  also describes a continuous line in  $R^5$  then a number of variants are possible. Let us enumerate two of them.

1. The maximum in Eq.(25) is reached at one of the ends of line  $\mathbf{e}_d^t(\xi)$ . Due to the exclusion the tensors  $\mathbf{e}_d^t$ , which were recovered at  $M \rightarrow A$  PT, the line  $\mathbf{e}_d^t(\xi)$  will contract and disappear after completing of  $M \rightarrow A$  PT. For complex loading jumps from one end of the line  $\mathbf{e}_d^t(\xi)$  to the other are possible.

2. If the maximum in Eq.(25) is reached in some internal point of the line  $\mathbf{e}_d^t(\xi)$ , then after excluding this tensor we obtain two lines, and maximum in Eq.(25) will be reached at one of the ends of one of the lines. In the course of PT jumps between the ends are possible.

Usually  $M$  particle consists of several martensitic variants with various orientations. Transformation of one  $M$  variant into another (reorientation) changes the mean transformation strain in the particle. If  $M$  particle with transformation strain  $\mathbf{e}_1^t$  transforms to  $M$  particle with transformation strain  $\mathbf{e}_2^t$ , then in Eq.(10)  $\psi_2^\theta = \psi_1^\theta$ ,  $\mathbf{e}_2^t$  is determined with Eq.(14),  $\mathbf{e}_1^t$  is defined by principle (25) and

$$0.5P^{-1} |\mathbf{S}_A|^2 - \mathbf{S}_A : \mathbf{e}_1^t + 0.5P |\mathbf{e}_1^t|^2 = k_r \quad \text{at} \quad |\mathbf{e}_2^t| \leq a; \quad (27)$$

$$a |\mathbf{S}_A| - \mathbf{S}_A : \mathbf{e}_1^t - 0.5P (a^2 - |\mathbf{e}_1^t|^2) = k_r \quad \text{at} \quad |\mathbf{e}_2^t| = a. \quad (28)$$

At  $|\mathbf{e}_1^t| = a$ , Eq.(28) results in  $a |\mathbf{S}_A| - \mathbf{S}_A : \mathbf{e}_1^t = k_r$ . At  $\mathbf{e}_1^t = 0$  Eqs.(27), (28) describe the reorientation of completely twinned (self-accommodated)  $M$ .

## 5. Phase transition due to interface motion

Assume that the volume  $V_n$  is obtained by interface  $\Sigma$  propagation with a normal velocity  $v_n$  during time  $\Delta t$ , i.e. it is bounded by surfaces  $\Sigma_t$  and  $\Sigma_{t+\Delta t}$  at time  $t$  and  $t + \Delta t$  respectively, as well as by two lateral infinitesimal surfaces with the heights  $v_n \Delta t$  (Fig.1),  $V_n = v_n d\Sigma_t \Delta t$ . Let us transform the stress work integral in Eq.(1).

Across the moving coherent interface the position vector and the traction vector  $\mathbf{p}$  are continuous,  $\mathbf{p}_2 = \mathbf{p}_1$ , and due to compatibility condition [7]

$$[\mathbf{F}] = -[\mathbf{v}] \mathbf{n} / v_n, \quad \text{whence} \quad [\mathbf{v}] = -[\mathbf{F}] \cdot \mathbf{n} v_n \quad \text{and} \quad [\mathbf{F}] = [\mathbf{F}] \cdot \mathbf{n} \mathbf{n}. \quad (29)$$

Here  $\mathbf{n}$  is the unit normal to the interface,  $\mathbf{F} = \mathbf{I} + \boldsymbol{\varepsilon} + \boldsymbol{\omega}$ ,  $\boldsymbol{\omega}$  the rotation tensor,  $\mathbf{I}$  the unit tensor,  $[\mathbf{a}] := \mathbf{a}_2 - \mathbf{a}_1$ . Then neglecting all the terms higher than  $O(\Delta t)$  we obtain

$$\int_{V_n} \int_{\tilde{\mathbf{e}}_1}^{\tilde{\mathbf{e}}_2} \tilde{\boldsymbol{\sigma}} : d\tilde{\boldsymbol{\varepsilon}} dV_n = \int_t^{t+\Delta t} \int_{\Sigma} \mathbf{p} \cdot \mathbf{v} d\Sigma dt = \\ = \left( \int_{\Sigma_{t+\Delta t}} \mathbf{p}_1 \cdot \mathbf{v}_1 d\Sigma_{t+\Delta t} - \int_{\Sigma_t} \mathbf{p}_2 \cdot \mathbf{v}_2 d\Sigma_t \right) \Delta t = - \int_{\Sigma_t} [\mathbf{p} \cdot \mathbf{v}] \Delta t d\Sigma_t,$$

$$-[\mathbf{p} \cdot \mathbf{v}] = -\mathbf{p} \cdot [\mathbf{v}] = \mathbf{n} \cdot \bar{\boldsymbol{\sigma}} \cdot [\tilde{\mathbf{F}}] \cdot \mathbf{n} v_n = \bar{\boldsymbol{\sigma}} : [\tilde{\mathbf{F}}] \cdot \mathbf{n} \mathbf{n} v_n = \bar{\boldsymbol{\sigma}} : [\tilde{\boldsymbol{\varepsilon}}] v_n. \quad (30)$$

Due to the compatibility condition only the normal to the interface components of the stress and the strain jump tensors produce work. Due to traction continuity across the interface the work-producing components of stress tensor are fixed in the course of PT ( $\boldsymbol{\varepsilon}^t$  variation).

Assume that on the interface it holds  $\bar{\boldsymbol{\sigma}} \cdot \mathbf{n} = \bar{\boldsymbol{\sigma}} \cdot \mathbf{n}$ , where  $\bar{\boldsymbol{\sigma}}$  is some constant stress tensor. Then

$$\begin{aligned} \int_{V_n} \int_{\tilde{\boldsymbol{\varepsilon}}_1}^{\tilde{\boldsymbol{\varepsilon}}_2} \bar{\boldsymbol{\sigma}} : d\tilde{\boldsymbol{\varepsilon}} dV_n &= \int_{V_n} \mathbf{n} \cdot \bar{\boldsymbol{\sigma}} \cdot (\tilde{\mathbf{F}}_2 - \tilde{\mathbf{F}}_1) \cdot \mathbf{n} v_n d\Sigma dt = \\ &= \bar{\boldsymbol{\sigma}} : \int_{V_n} ((\tilde{\mathbf{F}}_2 - \tilde{\mathbf{F}}_1) \cdot \mathbf{n}) \mathbf{n} v_n d\Sigma dt = \bar{\boldsymbol{\sigma}} : \int_{V_n} (\tilde{\boldsymbol{\varepsilon}}_2 - \tilde{\boldsymbol{\varepsilon}}_1) dV_n = \bar{\boldsymbol{\sigma}} : (\boldsymbol{\varepsilon}_2 - \boldsymbol{\varepsilon}_1) V_n. \end{aligned} \quad (31)$$

Consider two specific cases. In the first one we assume, that the particles of  $A$  are imbedded in a martensitic matrix, and  $\Sigma$  is an external surface of  $A$ . Then  $\boldsymbol{\sigma}_A := V_n^{-1} \int_{\Sigma} \mathbf{r} \bar{\boldsymbol{\sigma}} \cdot \mathbf{n} d\Sigma = \bar{\boldsymbol{\sigma}}$ , where  $\mathbf{r}$  is a position vector. In the second case, when the particles of  $M$  are imbedded in an austenitic matrix and  $\Sigma$  is an external surface of  $M$ , we obtain  $\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}_M$ . In the intermediate situation, when it is impossible to distinguish uniquely which phase is the matrix and which is the inclusion, we assume that  $\bar{\boldsymbol{\sigma}} = x \boldsymbol{\sigma}_A + (1-x) \boldsymbol{\sigma}_M$ , where  $0 \leq x \leq 1$  is some function of  $c$  and the geometry of  $A + M$  mixture. The PT criterion (1) reads

$$X_{\Sigma} = \bar{\boldsymbol{\sigma}} : (\boldsymbol{\varepsilon}_2 - \boldsymbol{\varepsilon}_1) - (\psi_2 - \psi_1) = k_{\Sigma}, \quad (32)$$

where  $k_{\Sigma}$  is related to the actual dissipative processes in the transforming volume and to intersection of interface with various defects (grains and subgrains boundary, dislocations, and so on). For the isotropic phases with equal elastic moduli and pure deviatoric transformation strain, Eq.(32) can be reduced to

$$X_{\Sigma} = \bar{\mathbf{S}} : (\mathbf{e}_2^t - \mathbf{e}_1^t) - (\psi_2^{\theta} - \psi_1^{\theta}) = k_{\Sigma}. \quad (33)$$

For PT  $A \rightarrow M$  we have  $\mathbf{e}_1^t = 0$ . Using the postulate of realizability the extremum principle – similar to Eq.(11) – can be obtained. Application of this principle together with the constraint  $|\mathbf{e}_2^t| \leq a$  yields

$$\mathbf{e}_2^t = a \frac{\bar{\mathbf{S}}}{|\bar{\mathbf{S}}|} \quad \text{and} \quad a |\bar{\mathbf{S}}| = (\psi_M^{\theta} - \psi_A^{\theta}) + k_{\Sigma A \rightarrow M}. \quad (34)$$

PT criterion (34) represents the sphere in a space  $\bar{\mathbf{S}}$ , in particularly, in the space  $\mathbf{S}_M$  at relatively small  $c$  and in the space  $\mathbf{S}_A$  at relatively small  $(1-c)$ . For PT  $M \rightarrow A$ ,

$$\mathbf{e}_2^t = 0, \quad X_{c\Sigma} = -X_{\Sigma} = \bar{\mathbf{S}} : \mathbf{e}_1^t - (\psi_M^{\theta} - \psi_A^{\theta}) = k_{\Sigma M \rightarrow A} < 0. \quad (35)$$

The method of determination of  $\mathbf{e}_1^t$  is similar to that proposed for PT due to nucleation.

## 6. A similarity between the theories of phase transition and plasticity

Constitutive equations of the theories of  $A \rightarrow M$  PT and plasticity are summarized in a Box. Parameters  $c$  and  $\lambda$  represent corresponding internal variables in the expression for the free energy. In the special case when a time derivative of a plastic internal variable  $\lambda$  coincides with the plastic parameter in the flow rule, there is a complete similarity between these theories. One not important difference consists in the fact, that in the theory of PT a kinematical softening occurs, but in the plasticity theory kinematical hardening takes place.



The above similarity allows the application of numerical algorithms – which were developed for the solution of elastoplastic boundary-value problems – for the solution of boundary-value problems for materials with PT.

Phase transition	Plasticity
Kinematical decomposition $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^t$	Kinematical decomposition $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p$
Free Energy $\psi = \frac{1}{2\rho} \boldsymbol{\varepsilon}^e : \mathbf{E} : \boldsymbol{\varepsilon}^e + \underbrace{(1-c)\psi_A^0 + c\psi_M^0}_{\psi_0(c)}$	Free Energy $\psi = \frac{1}{2\rho} \boldsymbol{\varepsilon}^e : \mathbf{E} : \boldsymbol{\varepsilon}^e + \psi_0(\lambda)$
Hooke's law $\boldsymbol{\sigma} = \mathbf{E} : \boldsymbol{\varepsilon}^e$	Hooke's law $\boldsymbol{\sigma} = \mathbf{E} : \boldsymbol{\varepsilon}^e$
PT criterion $\phi(\mathbf{S} + P\mathbf{e}^t) = K(c)$	Yield condition $\phi(\mathbf{S} - P\mathbf{e}^p) = K(\lambda)$
Associated flow rule $\dot{\mathbf{e}}^t = \dot{c} \frac{\partial \phi}{\partial \mathbf{S}} = \dot{c} \mathbf{n}$	Associated flow rule $\dot{\mathbf{e}}^p = \dot{\lambda} \frac{\partial \phi}{\partial \mathbf{S}} = \dot{\lambda} \mathbf{n}$
Evolution equation (Consistency condition) $\dot{c} = \mathbf{n} : \dot{\mathbf{S}} \left( \frac{\partial K}{\partial c} - P\mathbf{n} : \mathbf{n} \right)^{-1}$	Evolution equation (Consistency condition) $\dot{\lambda} = \mathbf{n} : \dot{\mathbf{S}} \left( \frac{\partial K}{\partial \lambda} + P\mathbf{n} : \mathbf{n} \right)^{-1}$

### 7. Concluding remarks

Comparing the obtained results with those, published in [4] we can state the following. In our criterion (1) based on consideration of transforming particle only, stress variation in transforming particle is taken into account in the course of transformation. The stress variation differs for different micromechanical mechanisms (nucleation, interface propagation or reorientation), and this fact is included in the description. In paper [4] (as well as in [1] – [3]) the derivation is based on the consideration of the whole representative volume. Difference between nucleation and interface propagation, as well as stress variation in the transforming particle, are not taken into account. It is necessary to mention that the results obtained in [4] are close to our results in the case of nucleation and  $|\mathbf{e}_2^t| = a$ .

One of the main assumption in [4] is a formula for transformation strain in nucleus (it coincides with Eq.(14)<sub>2</sub> at  $|\mathbf{e}_2^t| = a$ ) which was criticized in [17]. It is not clear why  $\mathbf{e}_2^t$  should be related to stress in A, even for reorientation of martensitic variants, and why  $|\mathbf{e}_2^t| = a$  has always maximum possible value.

In our paper an equation for  $\mathbf{e}_2^t$  is obtained, based on the postulate of realizability and corresponding extremum principles. In the particular cases of PT due to nucleation and reorientation of martensitic variants, at high stresses  $|\mathbf{S}_A| \geq Pa$ , we have obtained the same equation as accepted in [4], see Eq.(14)<sub>2</sub>. This equation is in agreement with some known experiments [4]. At the same

time Eq.(14)<sub>2</sub> can not describe the experiments [14] collected in Fig.4 which is done using our Eq.(14)<sub>1</sub> at  $|\mathbf{e}_2^t| < a$ .

Eq.(14)<sub>1</sub> at  $\mathcal{S}_A < Pa$  (for PT due to nucleation and reorientation) and Eq.(34) (for PT due to interface motion) differ from the postulated ones in [4]. This fact results in different PT criteria and kinetic equations.

As mentioned in Section 2, the constant  $P$  in Eq.(7)<sub>1</sub>, determined by formulas in [2, 4], is overestimated in one to two orders. We are determining this constant from simple experiments.

Thresholds  $k_n$  and  $k_r$  are constants in [4], but for the description of experiments, some constant is substituted there by a linear function of  $c$ . We have used variable  $k$ , which depends on  $c$  and the direct and reverse PT history, and is determined experimentally [13, 16].

For the reverse PT an application of the postulate of realizability allows to determine the  $M$  particle which is transformed in  $A$  in the given time instant. In [4] an empirical "forward transformation memory function" is used for this purpose.

In [3] transformation strain in  $M$   $\mathbf{e}_M^t$  is assumed to be collinear to total strain deviator  $\mathbf{e}$  and has a constant modulus. This means "instantaneous reorientation" and excludes any hysteresis and metastability in reorientation which contradicts to experiments at complex loading path [4]. A constant value of  $|\mathbf{e}_M^t|$  does not allow to describe the experiments in Fig.4. The description of reverse PT in [3] is also oversimplified in comparison with [4] and the present paper. The thermodynamical theory [3] is not based on specific micromechanical mechanisms of PT.

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