Phase Transitions in Elastoplastic Materials: Thermodynamical Theory and Numerical Simulation

V.I. Levitas, E. Stein and A.V. Idesman*

*University of Hannover, Institute of Structural and Computational Mechanics, Appelstrasse 9A,
30167 Hannover, Germany*

** Institute for Superhard Materials, Avtozavodska 2, 254153 Kiev, Ukraine*

ABSTRACT

A general condition of nucleation in elastoplastic materials is derived and specified for dilatational phase transitions (PT). The work integral in the nucleation criterion is calculated numerically after solution of a set of boundary-value problems using finite elements method. The example of the relation between applied axial stress, volumetric transformation strain and PT temperature is determined numerically. Effect of superimposed hydrostatic pressure is taking into account analytically.

INTRODUCTION

Phase transitions in elastoplastic materials play a significant role for a lot of advanced technical problems, e.g. for thermomechanical treatment of metals, for transformation induced plasticity (TRIP) phenomenon and for activation of phase transitions by large plastic shear straining in combination with high pressure. A knowledge of the influence of plastic strain, applied and local stress fields of phase transitions is very important for understanding, simulation and improvement of the above processes. Due to weak mobility of interfaces in elastoplastic materials the main mechanism of PT is a permanent appearance of new martensitic particles in austenitic matrix (nucleation). Only recently a noncontradictory nucleation criterion in elastoplastic materials was suggested^{1,2}, which, due to its local character, can be easily applied for analytical and numerical studies. Some analytical results are obtained in papers^{1,2}. In the present paper, after short derivation and simplification of nucleation criterion, the first numerical study of dilatational PT in elastoplastic medium based on it will be presented.

CONDITION OF NUCLEATION IN ELASTOPLASTIC MATERIALS

Consider a volume V of austenite + martensite mixture with a boundary S . Assume that on one part of surface S the stress vector $\mathbf{p}$ is prescribed and on the other part the velocity vector $\mathbf{v}$ is given, but mixed boundary conditions (BC) are also possible. Assume that in some volume V_n with the fixed boundary Σ_n , due to PT during the time Δt , the new nuclei appeared. For isothermal processes the dissipation increment N_n in the volume V_n during the time Δt can be defined, using the second law of thermodynamics

$$N_n := \int_t^{t+\Delta t} \int_{\Sigma_n} \mathbf{p} \cdot \mathbf{v} d\Sigma_n dt - \int_t^{t+\Delta t} \frac{d}{dt} \int_{V_n} \psi dV_n dt \geq 0, \quad (1)$$

where ψ is the Helmholtz free energy per unit volume, $\mathbf{v}$ is the velocity on Σ_n from the side of the nucleus. For elastic materials without dissipation, condition $N_n = 0$ can be considered as equilibrium nucleation criterion, because it describes PT at zero dissipation. For PT in elastoplastic materials and in elastic materials with hysteresis this condition can not be applied, because finite dissipation occurs in the course of PT.

Let us assume that we can determine the actual value of dissipation increment N_n^a in course of PT in V_n as $N_n^a = \int (k_n^f + k_n^p) dV_n$, where $k_n^p = \int \boldsymbol{\sigma} : d\boldsymbol{\varepsilon}^p$ and k_n^f are the plastic dissipation increment

and the dissipation increment due to phase transition in a unit volume, ϵ^p the plastic strain. The term k_n^f is related to the emission of acoustic waves and lattice friction, and it is responsible for the hysteresis at PT in elastic materials.

Both N_n and N_n^a depend on the BC. If at given BC $N_n < N_n^a$, then PT will not take place, because for actually occurring PT $N_n = N_n^a$, as N_n^a is by definition the actual value of dissipation increment. Consequently, the necessary condition of nucleation is $N_n = N_n^a$, i.e.

$$\int_t^{t+\Delta t} \int_{\Sigma_n} \mathbf{p} \cdot \mathbf{v} d\Sigma_n dt - \int_{V_n} (\psi_2 - \psi_1) dV_n = \int_{V_n} (k_n^f + k_n^p) dV_n > 0, \quad (2)$$

$$\text{or} \quad \int_{\epsilon_1}^{\epsilon_2} \int_{V_n} \boldsymbol{\sigma} : d\boldsymbol{\epsilon} dV_n - \int_{V_n} (\psi_2 - \psi_1) dV_n = \int_{V_n} (k_n^f + k_n^p) dV_n > 0, \quad (3)$$

where subscripts 1 and 2 denote the phase before and after PT. Note that Gauss theorem was used. If we decompose for linear kinematics

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^e + \boldsymbol{\epsilon}^p + \boldsymbol{\epsilon}^f, \quad (4)$$

where $\boldsymbol{\epsilon}^e$ and $\boldsymbol{\epsilon}^f$ are elastic and transformation strains, then terms $\boldsymbol{\sigma} : d\boldsymbol{\epsilon}^p$ in the left and right parts of Eq. (3) eliminate each other, and we obtain

$$\int_{\epsilon_1}^{\epsilon_2} \int_{V_n} \boldsymbol{\sigma} : d(\boldsymbol{\epsilon}^e + \boldsymbol{\epsilon}^f) dV_n - \int_{V_n} (\psi_2 - \psi_1) dV_n - \int_{V_n} k_n^f dV_n = 0. \quad (5)$$

Formally Eq. (5) has the same form as for PT in elastic materials; plasticity effects implicit on a variation of $\boldsymbol{\sigma}$ in the course of PT and on the value k_n^f .

There is one general problem: for calculation of work integral in Eq. (5) it is necessary to determine the stress variation during PU (variation of $\boldsymbol{\epsilon}^f$).

We assume that after nucleation the interfaces Σ_n are fixed, and propagation and nondisappearance conditions^{1,2} are not important.

If $\psi_i = 1/2 \boldsymbol{\epsilon}_i^e : \mathbf{E}_i : \boldsymbol{\epsilon}_i^e + \psi_i^\theta$, $i = 1, 2$ and $\mathbf{E}_1 = \mathbf{E}_2$, where $\mathbf{E}_i$ are the tensors of elastic moduli of i -phase, ψ_i^θ the thermal part of the free energy, then

$$\int_{\epsilon_1^f}^{\epsilon_2^f} \int_{V_n} \boldsymbol{\sigma} : d\boldsymbol{\epsilon}^f dV_n - \int_{V_n} (\psi_2^\theta - \psi_1^\theta) dV_n - \int_{V_n} k_n^f dV_n = 0, \quad (6)$$

i.e. the elastic strains also disappear. A pure deviatoric transformation strain is considered analytically in paper³ for elastic and in papers^{1,2} for elastoplastic materials. Here we examine the opposite situation with pure dilatational transformation strain $\boldsymbol{\epsilon}^f = 1/3 \epsilon_o^f \mathbf{I}$, where $\mathbf{I}$ is a unit tensor, ϵ_o^f is a volumetric transformation strain. In this case $\boldsymbol{\sigma} : d\boldsymbol{\epsilon}^f = \bar{\sigma}_o d\epsilon_o^f$, where $\bar{\sigma}_o$ is a hydrostatic pressure. As the volumetric transformation strain is distributed homogeneously in the nucleus, Eq. (6) can be transformed into the following form

$$\int_{\epsilon_o^f}^{\epsilon_o^f} \bar{\sigma}_o d\epsilon_o^f - (\psi_2^\theta - \psi_1^\theta) - k_n^f = 0, \quad \bar{\sigma}_o = \frac{1}{V_n} \int_{V_n} \sigma_o dV_n, \quad (7)$$

where $\bar{\sigma}_o$ is the averaged over the nucleus pressure. It is assumed that temperature and k_n^f are distributed uniformly in the nucleus. Eq. (7) is a final form of phase transformation criterion which is used in the present paper. The integral in Eq. (7) is calculated numerically after solution of a set of boundary-value problems using finite elements method. The explicit expressions for ψ_i^θ can be adopted in the following form⁴

$$\begin{aligned} \psi_1^\theta &= \psi_{o1} - s_{o1} (\theta - \theta_o) - \nu_1 \theta \left(\ln \frac{\theta}{\theta_o} - 1 \right) - \nu_1 \theta_o, \\ \psi_2^\theta &= \psi_{o2} - s_{o2} (\theta - \theta_o) - \nu_2 \theta \left(\ln \frac{\theta}{\theta_o} - 1 \right) - \nu_2 \theta_o. \end{aligned} \quad (8)$$

Here $\nu_1 > 0$ and $\nu_2 > 0$ are specific heats, s_{o1} , s_{o2} , ψ_{o1} , ψ_{o2} are constants, θ_o is a reference temperature.

FORMULATION OF PROBLEM

To determine the regularities of martensitic PT in elastoplastic materials we solve the simplest boundary-value problem. Let us consider a two phase material consisting of a matrix with periodic arrangement of embedded spherical particles. Assume that at the given temperature and applied external stresses the spherical particles undergo the dilatational martensitic transformation. Transformation of graphite particles, embedded in an iron matrix (cast iron), into diamond can be considered as possible example.

Consider axisymmetric formulation of the problem for a unit cell, i.e. spherical inclusion into cylindrical matrix (Fig. 1). Because of symmetry, Fig. 1 shows a quarter of the unit cell of the composite, where X_1 is the axis of revolution and X_2 is the horizontal axis of symmetry, respectively. A coherent interface between the particle and the matrix was assumed, i.e. the displacements were taken to be continuous across the interface. Both, matrix and inclusion are isotropic with equal elastic properties, i.e. Hooke's law is valid

$$\sigma = E : \epsilon^e = \lambda \epsilon^e : II + 2\mu \epsilon^e, \quad (9)$$

where λ , μ are the Lamé coefficients.

The inclusion is elastic, the matrix is elastic-perfectly-plastic with von Mises yield condition

$$f(\sigma) = \sigma_i - \sigma_y = 0, \quad (10)$$

where $\sigma_i = (3/2 S : S)^{1/2}$ is the stress intensity; $S = \text{dev } \sigma$ is the deviatoric stress tensor; σ_y is the yield limit. In the elastic region it holds $f < 0$, or $f = 0$ and $\frac{\partial f}{\partial \sigma} : d\sigma < 0$. In an elastoplastic region we have $f = 0$, $\frac{\partial f}{\partial \sigma} : d\sigma = 0$, and the associated plastic flow rule reads

$$\dot{\epsilon}^p = \lambda S; \quad \lambda \geq 0. \quad (11)$$

The kinematic additive decomposition (4) is used, for inclusion $\epsilon^p = 0$, for matrix $\epsilon^f = 0$.

In the general case for the local stress tensor the following formula is valid⁵

$$\sigma(\mathbf{r}) = \mathbf{A}(\mathbf{r}) : \Sigma + \sigma_r(\mathbf{r}), \quad \Sigma := \frac{1}{V} \int_S \mathbf{r} \sigma \cdot \mathbf{n} dS = \frac{1}{V} \int_V \sigma dV = \langle \sigma \rangle, \quad (12)$$

where Σ is a mean (external) stress tensor, $\sigma_r(\mathbf{r})$ the field of residual stresses at $\Sigma = 0$ (i.e. $\langle \sigma_r \rangle = 0$), $\mathbf{r}$ the position vector, $\mathbf{A}$ the localization (concentration) fourth order tensor, $\mathbf{n}$ the external unit normal to the boundary S . In the case of homogeneous elastic properties $\mathbf{A}$ is an identity tensor, i.e.

$$\sigma(\mathbf{r}) = \Sigma + \sigma_r(\mathbf{r}). \quad (13)$$

A superposition of an additional pure hydrostatic pressure in the above boundary-value problem does not influence on plastic strain and consequently on σ_r . The additional hydrostatic pressure contributes additively to Σ ; according to Eq. (13) it contributes also additively to σ and consequently to $\bar{\sigma}_o$ and can be taken into account analytically. That is why it is sufficient to consider macroscopically one-dimensional loading in our two dimensional problem.

The following properties are used in calculations: Young modulus $E = 2 \cdot 10^6$, Poisson ratio $\mu = 0.3$, yield limit $\sigma_y = 2 \cdot 10^3$. Volume fraction of nucleus is $c = 0.28$. The following boundary conditions are applied: along ABC and AKE boundaries $u_n = 0$, $\tau_n = 0$ (from symmetry condition); along DE boundary $\sigma_n = \tau_n = 0$ (free surface); along CD boundary $\sigma_n = P$, $\tau_n = 0$ (prescribed normal compressive stress P). Here u_n is the normal displacement, τ_n is the tangential stress, σ_n is the normal stress.

The PT is simulated by growing of compressive transformation strain ϵ_o^f from 0 till 0.005 under fixed P . The elastoplastic problems are solved using step by step method with transformation strain increment $\Delta \epsilon_o^f = 0.0005$. The transformation strain was taken into account as a fictitious thermal strain. Five different values of P were considered, $P = 0; 500; 1000; 1500; 1950$.

Fig. 1. Cross section of quarter of cylindrical matrix with spherical nucleus.

NODES NP= 1627 ELEMENTS NE= 3136

Fig. 2. Finite element mesh.

a

b

Fig. 3. Isolines of stress intensity σ_i (a) and accumulated plastic strain q (b) distribution at $\varepsilon = 0.005$ and $P = 0$.

NUMERICAL RESULTS AND THEIR ANALYSIS

Some information on macroscopic stresses Σ may be obtained without solving the problem. With due account of boundary conditions and definition (12)₂ we have

$$\Sigma_{11} = P; \quad \Sigma_{22} = \Sigma_{12} = 0. \quad (14)$$

To solve the problems, the finite element technique and a computer code for solving thermo-elastoplastic problems^{6,7} were used. The finite element mesh (Fig.2) contains about 3000 linear triangular elements with the mesh refinement near interface, where large gradients of plastic strain occur. Local fields of stresses, total and plastic deformations were determined. Isolines of stress intensity and accumulated plastic strain $q = \int (2/3 d\epsilon^p : d\epsilon^p)^{1/2}$ at $\epsilon_o^f = 0.005$ are shown in Fig. 3 at $P = 0$ and in Fig. 4 at $P = 1500$. At $P = 0$ the plastic region covers almost whole cross section of matrix (excluding upper right corner), and stress intensity is distributed uniformly in this region (material is perfectly plastic). At $P = 1500$ the plastic strain is concentrated near the interface, the maximal value of q is more than three times the maximal value of q at $P = 0$. Such a concentration of plastic strain can lead to noncoherency (discontinuity of the displacements) at the interface. Fig. 5 and Fig. 6 give the relationships between averaged (over the nucleus) hydrostatic pressure $\bar{\sigma}_o$, the work integral

$\varphi := \int_0^{\epsilon_o^f} \bar{\sigma}_o d\epsilon_o^f$ and transformation volumetric strain ϵ_o^f for five different values of macroscopic axial stress P . There is an evident saturation of values $\bar{\sigma}_o$ with the growth of ϵ_o^f for each P , which is related to a limit plastic equilibrium state.

The most informative for the analysis of PT conditions is shown in Fig. 6. Practically linear dependence of φ from ϵ_o^f at $\epsilon_o^f > 0.001$ for each P allows to use a simple analytical approximation of the obtained numerical results.

It is evident that at $\sigma_y = 0$ we have $\bar{\sigma}_o = 0$. Assume that additionally $k_n^f = P = 0$. Then condition (7) results in ordinary PT criterion of chemical thermodynamics $\psi_2^\theta - \psi_1^\theta = 0$, which determines a phase equilibrium temperature θ_e . If in a thought experiment at $\sigma_y = 0$, $P = 0$, PT starts at temperature θ_s , then $k_n^f := \psi_2^\theta(\theta_s) - \psi_1^\theta(\theta_s)$. If k_n^f is a given function of θ then Eq. (7) determines the PT temperature; the value of the work integral φ at the given transformation volumetric strain ϵ_o^f and axial stress P is determined from Fig. 6. In particular, at $P = 0$, Eq. (7) should give an experimentally observed martensitic start temperature M_s . If the PT temperature and transformation volumetric strain ϵ_o^f are given, then Eq. (7) determines the value of the work integral φ and axial stress P is determined from Fig. 6.

CONCLUDING REMARKS

In the paper a general thermodynamical approach for the description of PT, due to nucleation in elastoplastic materials, is suggested, and an example of dilatational PT is considered. It is remarkable that in the presented formulation a standard computer code for solving thermo-elastoplastic problems was used. The planned further work will be related to deviatoric components of transformation strain tensor, variation of volume fraction of nucleus, elastic and plastic properties and to an analytical approximation of obtained results.

ACKNOWLEDGMENT

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REFERENCES

1. Levitas VI, Journal de Physique-Colloque, (1995), (in press).
2. Levitas VI, Mech. Res. Commun., 22 (1) (1995) 87-94.
3. Levitas VI and Stein E, ZAMM 75 (1995), S199-S200.
4. Fu S, Huo Y and Müller I, Acta Mechanica 99 (1993), 1-19.
5. Levitas VI, Thermomechanics of phase transformations and inelastic deformations in microinhomogeneous materials, Naukova Dumka, Kiev, (1992), 248.
6. Levitas VI and Idesman AV, Strength of Materials, 11 (1986), 1518-1525.
7. Idesman AV and Levitas VI, Comp. Methods Appl. Mech. Engineering (1995), (in press).

Fig. 4. Isolines of stress intensity σ_i (a) and accumulated plastic strain q (b) distribution at $\varepsilon = 0.005$ and $P = 1500$.

Fig. 5. Relationships between averaged over the nucleus hydrostatic pressure $\bar{\sigma}_0$ and transformation volumetric strain ε_0^f (1 - $P = 1950$; 2 - $P = 1500$; 3 - $P = 1000$; 4 - $P = 500$; 5 - $P = 0$).

Fig. 6. Relationships between the work integral φ and transformation volumetric strain ε_0^f (1 - $P = 1950$; 2 - $P = 1500$; 3 - $P = 1000$; 4 - $P = 500$; 5 - $P = 0$).

Opinion about the Paper "Simple Micromechanical Model of Thermoelastic Martensitic Transformations"

There are many goals of theoretical modelling of martensite phase transitions (m.p.t.) as observed at microscale. For example,

- to explain basic metallurgical phenomena using fundamental physical laws and well established physical principles and concepts,
- to determine the properties of an alloy undergoing m.p.t. using those principles,
- to give the advices as regards possible interrelations between an overall strain, stress and temperature of a macroscopic sample undergoing m.p.t.

The goal of this paper is not clearly stated. The paper does not contribute to the solutions of the existing problems, and I am afraid that it will be of the little interest to the readers of the Journal.

It seems that the considerations presented form the extract from the works already published by one of the Authors. An ambitious effort is undertaken to show that previous works contributed much to the field of mechanics of m. p.t. The result is poor and the paper, in fact, in some places is unreadable. It is bound to lead to superficial discussions of important issues and sometimes to incorrect statements that are based upon purely heuristic "assumptions". While heuristic postulates are admissible in phenomenological theories describing the overall behaviour, their number should be minimized when explaining the phenomena observed at microscale, because of they cannot be directly verified. I am sorry but I can't recommend this paper for publishing.

Examples (concerns Secs 2 and 3)

These Sections contain only 3 expressions that are based on the well-sound physical ground:

a) the left-hand side of Eq. (1)

- provided that: the temperature of R.V.E (volume V) is uniform at every time instant, the time Δt is greater than the relaxation time for the thermal equilibrium, preexisting mixture of A+M is in the peace and it is not influenced by the fields created in V_n .

b) The Equation (3)₂

- provided that at time period Δt the complete transition occurs in the considered subvolume V_n .

c) Equations (7)_{1,2}

- provided that P is the fourth rank tensor known in the literature as stress-concentration factor which depend strongly upon the micro-geometry

of A+M mixture and, of course, upon elasticity moduli. The term $\mathbf{Pe}_M^t$ vanishes when $\mathbf{e}_M^t$ is the compatible field. This fundamental facts are not mentioned in the paper. Instead, the artificial problem concerning the "value" of P is discussed.

The other formula are the unjustified assumptions, especially Eq (1) with unspecified function k_n , Eq. (7)₃ for average stress in the volume V_n , and Eq (15). The latter implies that $\mathbf{S}_n=0$ (average deviatoric stress vanishes in the nucleus) what contradicts the basic issue of the theory of the inclusions. According to A.L. Roitburd , for example, the stresses that are developed in the thin plate-like layer in the infinite crystal are responsible for the bifurcation of the equilibrium temperature into M_S and A_S .

In the present paper one assumes $\mathbf{Pe}_M^t = \mathbf{S}$ when $c=0$. As a result there is no strain effect after the temperature induced p.t. at $S=0$. The well known phenomenon of the relief observed on the surface of a large crystal contradicts this assumption. The qualitative comparison with the experimental data shown in the Fig.4 are not adequate since the TRIP effect in steels strongly depend on the specific volume variation which has been neglected in the present paper. Moreover, TRIP effect is not associated with A-M transitions "due to nucleation". The Sec. 4 is hard to understand because of the underlying mathematics is not sufficiently rigorous.

The Section 5 contains an obvious error : $\mathbf{F} = \boldsymbol{\varepsilon} + \boldsymbol{\omega}$. The clear derivation of the thermodynamic driving force acting upon moving coherent interface may be found in the literature published much earlier than that quoted in this paper.

Response on the Reviewer's comments about the paper

Simple Micromechanical Model of Thermoelastic Martensitic Transformations

by V. Levitas and E. Stein

Goal of the paper. The goal is clear from the Introduction: analytical "description of PT in elastic materials under three-dimensional loading". It seems to us that this corresponds to the third example of admissible aims, declared by the reviewer: "To give the advices as regards possible interrelations between an overall strain, stress and temperature of a macroscopic sample undergoing m.p.t." The closest to the present work and widely cited papers in the literature [3-5] are mentioned, and the important distinguished features of our investigation are listed and evaluated in Section 1, Introduction. The scientific output consists in the combination of these points.

"The number of purely heuristic postulates (assumptions) should be minimized when explaining the phenomena observed at microscale".

That is exactly what we tried to do: to minimize the number of assumptions. The paper is based practically on three main points:

- PT criterion (1);
- formulas for the stresses in austenite, martensite and transforming particle (7);
- the extremum principle (12).

Eqs.(7) and (12) will be discussed later. The extremum principle (12) is a generalization of the generally recognized Patel-Cohen maximum work principle for the case of account for internal stresses and stress variation in the course of PT.

The principle (12) is derived using the postulate of realizability, suggested in [9]. This postulate was applied for the description of a number of different phenomena [6-9], especially PT. By the way, paper [9] has got the International Journal of Engineering Sciences Distinguished Paper Award (see enclosed letter). Sure that this is not the proof of validity of the extremum principle (12), we only would like to mention that there is an alternative opinion about "poor results".

Eq.(1). The PT criterion in most papers devoted to PT in dissipative materials has the following form (see practically all cited literature, and review articles by F.D. Fischer, M. Berveiller et. al. (Arch. Appl. Mech., 1994, Vol. 64, pp. 54-85); L. Delaey et.al. (J. Mater. Sci., 1974(!), Vol. 9, pp. 1521-1554): the calculated value of dissipation (driving force) reaches its actual value k_n (dissipative threshold). Eq.(1) has the same structure. Ironically, that the reviewer has recognized "the well-sound physical ground" (under some evident comment) of the left side of Eq.(1) (which seems to us new) and did not recognize the generally accepted concept of dissipative threshold. If the left side of Eq.(1) is good, what should stay on the right side? What does it mean that k_n is an unspecified function? Is the yield stress in plasticity theory specified better, which depends on the plastic strain, plastic strain history, temperature, temperature history, strain rate, grain size and so on? Function k_n should and can be determined experimentally, and even some

analytical approximations are known [3-5, 13].

Eq.(7). Again, Eqs.(7)_{1,2} are accepted, but Eq.(7)₃ not. Why? All these equations are derived under the same assumption of homogeneity of stresses or strains in austenite, martensite and transforming volume. This is a very strong assumption, but we do not see another way to develop an analytical solution. Eq.(7)₃ is even more strict than Eqs.(7)_{1,2}, because (due to infinitesimal size of nucleus) it can be derived considering infinitesimal spherical nucleus in austenitic matrix. As mentioned in the given paper, the expression for S_n has no qualitative contradictions: if $e_n^t = 0$ and the nucleus is austenitic, then $S_n = S_A$; if $e_n^t = e_M^t$, and the nucleus is martensitic, then $S_n = S_M$.

Concerning the compatibility of e_M^t and the artificial problem of the definition of the value P . In the paper it is written (before Eq.(11)): "at transformation strain with invariant plane and formation of fine microstructure the internal stresses are zero, but $e_M^t \neq 0$ ". It is impossible to take into account the possible compatibility of e_M^t into the simplified analytical model. This is one of the reasons why known theoretical formulas for the constant P [2, 5] overestimate it for one to two orders. How large should be an overestimation to be classified as not artificial, but real?

Eq.(15)₁. This equation is a direct consequence of Eqs.(7) and (12). Eq.(15)₂ coincides with the postulated in [4, 5] one. According to reviewer's comments, main drawback of Eq.(15)₂ is the fact, that it implies $S_n = 0$, which at his opinion contradicts the basic issue of the theory of the inclusions and the Roytburd's theory. We answer as follows:

The suggested theory assumes the possibility of self-accommodation of martensitic variants when it is energetically profitable (corresponds to principle (12)). This is not completely possible at $|S_A| \geq Pa$ and $S_n \neq 0$. At $|S_A| < Pa$ there is not any limitation on the value $|e_2^t|$, and complete self-accommodation is possible. In this case the obtained value of e_2^t implies $S_n = 0$. The same result can be obtained, when we use the theory of ellipsoidal inclusion. It is easy to show that result is independent of expressions for S_n and e_2^t . Actually, condition $X_n - k_n \rightarrow \max$ (when k_n is independent of e_i^t) results in $X_n \rightarrow \max$ and for the physically well-grounded expression (6) for X_n , we have $\frac{\partial X_n}{\partial e_2^t} = S_n = 0$.

There is also not any contradiction with Roytburd's theory. If self-accommodation is not possible, then the internal stresses are in fact (together with k_n) responsible for the shifting of the equilibrium temperature. Still, the main result of the Roytburd's theory is the energy minimization due to formation of self-accommodated polydomain phases. In case of complete self-accommodation the stress inside the inclusion is reduced to zero (A.L. Roytburd, Phase Transitions, 1993, Vol. 45, p. 12).

Consequently, equations for S_n and e_2^t are not responsible for the condition $S_n = 0$. It appears that the equation $S_n = 0$ is well motivated as well.

It follows from our theory that at $S = 0$ the *averaged* transformation strain over the representative volume is zero, $e^t = ce_M^t = 0$, which is in agreement with experiment. Why does this

contradict to the relief observed on the surface?

TRIP effect is related with two mechanisms: Magee mechanism due to preferable orientation of martensitic variants, which is considered in the given paper; Greenwood–Johnson mechanism related with the plastic flow due to rather high volumetric transformation strain, is neglected in our elastic model. In the cited books [14, 15] there is no information about volumetric transformation strain, but the theoretical model for the description of the experiments is based on the Magee mechanism. In a private talk Professor Likhachev confirmed the same.

By the way: some steels exhibit shape memory effect which is inconsistent with plastic straining (E. Hornbogen, *New Horizons for Materials* (Ed. R. Vincenzini), 1995, pp. 111–122), and some elastoplastic models of TRIP steels (J.M. Diani et.al., *Journal de Physique IV, Colloque C2*, Vol. 5, pp. 507–512), neglecting the volumetric transformation strain, describe satisfactory known experiments.

Section 4 is based on the same PT criterion (1) and extremum principle (12) and does not contain any new mathematics. We cannot understand the reviewer at all.

An obvious error $\mathbf{F} = \boldsymbol{\varepsilon} + \boldsymbol{\omega}$. Eq.(33) is valid when $[\mathbf{F}]$ is the jump of deformation gradient or jump of displacement gradient. We use the second possibility and definition $\mathbf{F} = \boldsymbol{\varepsilon} + \boldsymbol{\omega}$ is correct. But we agree that definition $\mathbf{F} = \mathbf{I} + \boldsymbol{\varepsilon} + \boldsymbol{\omega}$ suits better.

Expression for the driving force acting upon moving coherent interface is known starting from Eshelby. For us it is important to show, that our more general Eq.(1) for the transforming volume can be reduced to the known expression for the interface, as well as to develop an averaged description.

So according to our opinion we regret to state that the reviewer's comments are partly superficial and in some cases very surprising and even wrong. We suggest to publish our paper, and if not avoidable also reviewer's comments and our answers, and then the readers can decide who is right and who is wrong.

Valery Levitas

Erwin Stein