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Critical thought experiment to choose the driving force for interface propagation in inelastic materials

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Abstract

The problem of defining the driving force for interface propagation in inelastic materials is discussed. In most publications, the driving force coincides with the Eshelby driving force, i.e. it represents a total dissipation increment on the moving interface due to all the dissipative processes (phase transition (PT) and plasticity). Recently (Levitas, V.I., 1992a. Post-bifurcation Behaviour in Finite Elastoplasticity. Applications to Strain Localization and Phase Transitions. Universität Hannover. Insititut für Baumecharik and Numerische Mechanik, [BNM-Bencht 1JP 585-LC, 92/5, Hannover; Int. J. Eng. Sci. 33 (1995) 921; Mech. Res. Commun. 22 (1995) 87; J. de Physique III 5 (1995) 173; J. De Physique III 5 (1995) 41; Int. J. Solids Struct. 35 (1998) 889], an alternative approach was developed in which the driving force represents the dissipation increment due to PT only, i.e. total dissipation minus plastic dissipation. The aim of this paper is to prove the contradictory character of application of the Eshelby driving force to inelastic materials. For this purposes, a problem on the interface propagation in a rigid–plastic half-space under homogeneous normal and shear stresses is solved using both definitions, along with the principle of the maximum the driving force. Finite strain theory is used. It appears that the first approach exhibits some qualitative contradictions, which are not observed in our approach. In particular, even for shape memory alloys, when transformation strain can be accommodated elastically (or even without internal stresses), maximization of the Eshelby driving force requires as much plasticity as possible. When applied shear stress tends to the yield stress in shear of a new phase, the driving force tends to infinity, i.e. PT has to always occur at the beginning of plastic flow. Note that in this paper plasticity means dislocation plasticity rather than plasticity due to twinning. Twinning during martensitic PT is the appearance of several martensitic variants which are in twin

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relation to each other. Consequently, for twinned martensite one has microheterogeneous transformation strain without plastic dissipation term, i.e. both approaches coincide.

Keywords: Phase transformation; Elastic–plastic materials; Finite strain; Constitutive behaviour

1. Introduction

The interaction between PT and plastic deformation attracts the attention of material scientists, physicists, and mechanicians. The practical significance of this interaction is connected to such phenomena as plastic accommodation during the heat treatment of steels, transformation-induced plasticity (TRIP), strain-induced PT, morphological transition from plate to lath martensite in steels, high pressure PT, and plastic shear-induced PT under high pressure. Despite the significant amount of papers devoted to the thermodynamic description of PT in plastic materials, some questions remain open. One of these questions is the definition of the driving force for interface propagation in plastic material.

Martensitic PT represents a special type of deformation of a crystal lattice from the parent phase (austenite) into a crystal lattice of the product phase (martensite) without diffusion, see Fig. 1, which is accompanied by a jump in all the thermomechanical properties. This deformation is described by the transformation deformation gradient $\mathbf{F}_t$ (Bain strain). For martensitic PT, the transformation deformation gradient cannot be arbitrary (as elastic or plastic strain). For each PT, the right stretch transformation tensor $\mathbf{U}_t$ is some fixed tensor to within symmetry operations. Due to the symmetry, there is a finite number (e.g. 6 for the PT from a cubic to orthorhombic lattices) of crystallographically equivalent variants of martensite with the same (to within symmetry operations) $\mathbf{U}_t$. Tensors $\mathbf{U}_t$ for different martensitic variants have the same components in different crystallographically equivalent vector basises which are related by symmetry operations of the austenitic crystal lattice. Note that by variants we mean the "lattice correspondence variants" or Bain strain variants which are associated with changes in the crystal structure,

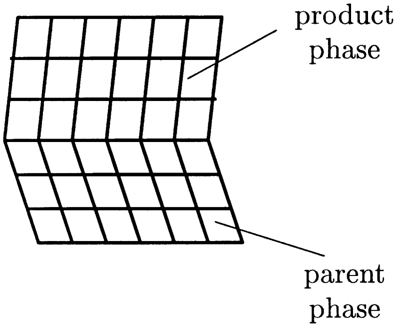

Fig. 1. Deformation of crystal lattice during martensitic PT.

not the "habit-plane variants" or "plate variants" (see also Bhattacharyya and Kohn, 1996).

For elastic materials and isothermal conditions, the well-known Eshelby driving force

$$X_E := \frac{1}{\rho_0}\mathbf{P}^t : [\mathbf{F}] - [\psi] \tag{1}$$

is used as the driving force for interface motion (Eshelby, 1970; Grinfeld, 1991; Kaganova and Roitburd, 1988 and references herein). Here **P** is the first Piola–Kirchoff nonsymmetric stress tensor with respect to reference (nondeformed) configuration V_0, **F** is the deformation gradient, ρ_0 is the mass density in V_0, and ψ is the Helmholtz free energy per unit mass, superscript t denotes transposition, and [**a**] means the jump of function **a** across the interface. The dissipation rate due to interface motion per unit area in the reference configuration is defined as

$$\mathcal{D}_E := \rho_0 X_E \upsilon_n, \tag{2}$$

where υ_n is the interface velocity with respect to material points in the reference configuration. It follows from thermodynamics and the universal relation across the discontinuity surfaces (Truesdell and Toupin, 1960) that Eq. (2) for the dissipation rate due to interface motion with the Eshelby driving force Eq. (1) is valid for any inelastic material as well. As for elastic materials, there are no other sources of dissipation than PT, dissipation across the interface occurs due to PT only. For inelastic materials (elastoplastic, viscoelastic, viscoplastic), dissipation due to inelastic deformation jump across the moving interface contributes to the total dissipation rate in Eqs. (1) and (2). That is why a doubt arises whether X_E characterizes the driving force for PT in inelastic materials.

Let us discuss various thermodynamic approaches to interface propagation in plastic materials. In material science literature (Olson and Cohen, 1986, Haezebrouck, 1987) various contributions to the driving force for interface propagation were analyzed and the growth of ellipsoidal nucleus in a viscoplastic material was approximately modeled. In physical literature, Roitburd and Temkin (1986) solved the problem of growth of a spherical inclusion in a spherical elastoplastic matrix; Kaganova and Roitburd (1987, 1989) studied the same problem by allowing for defect heredity, as well as another problem on the interface equilibrium of elastoplastic ellipsoidal inclusion in elastic space. However, a general equation for interface propagation was not formulated explicitly in the above papers. This was done for finite strain formulation by Kondaurov and Nikitin (1986); however the equation was derived under the assumption of an absence of a jump of plastic strain at the interface. Under such an assumption, the dissipation due to plastic flow across the interface is absent, and the driving force coincides with the Eshelby driving force, i.e. as for elastic materials.

Levitas (1992b) and independently Fischer et al. (1994) and Marketz and Fischer (1994a,b) suggested using the Eshelby driving force for interface propagation condition in elastoplastic materials. In this work, the numerous papers devoted to the generalization of Eq. (1) for the dynamic case and finding equivalent expressions for X_E will not be discussed, if they are not related explicitly to the description of interface propagation in inelastic materials.

Levitas (1992a, 1995a,b,c,d, 1998) developed an approach in which the driving force for nucleation and interface propagation represents the dissipation increment due to PT only, i.e. excluding all other types of dissipation, in particular plastic dissipation. For interface propagation, the driving force and the dissipation rate due to PT only are given by the formulas

$$X := X_E - A_p = \frac{1}{\rho_0}\mathbf{P}^t : [\mathbf{F}] - [\psi] - A_p; \tag{3}$$

$$\mathcal{D} := \rho_0 X v_n. \tag{4}$$

Here A_p is the dissipation across the interface due to a jump of plastic deformation across the interface (for simplicity we neglect the dissipation contribution due to the jump in internal variables).

So, now two different approaches are used for different problem formulations: based on the Eshelby driving force (Fischer and Reisner, 1998; Fischer et al., 2000; Cherkaoui et al., 1998; Cherkaoui and Berveiller, 2000) and based on the dissipation increment due to PT only (Levitas, 2000; Levitas et al., 1998c, 2001; Idesman et al., 1999, 2000). The question is which driving force is the proper one in the most general problem formulation?

The goal of this paper is *to demonstrate a conceptual contradiction which arises when the Eshelby driving force is applied for the description of interface propagation in plastic materials*. An approach using a driving force based on the dissipation increment due to PT only does not exhibit this type of contradiction.

In Section 2, derivations leading to the Eshelby driving force X_E and to the driving force based on dissipation due to PT only X are outlined and critically compared. The actual multivariant martensitic microstructure is determined by the principle of the maximum corresponding driving force. To prove that the contradiction exists, it is sufficient to demonstrate it for the simplified theory and problem. The simplest version of the theory is considered, and only information necessary for the comparison of the two approaches and the solution of the model problem in Section 3 is presented. A comparison of derivation procedures shows the advantage of using X rather than X_E for interface propagation in plastic materials. However, stronger arguments are needed.

In Section 3, a model problem on interface propagation through rigid-plastic material is solved at finite strains using both types of driving force. It is shown that the application of the Eshelby driving force leads to conceptual contradictions. In particular, even when complete compatibility of martensitic variants at the austenite-martensite interface is possible [e.g. for some shape memory alloys (SMA)], maximization of the Eshelby driving force requires as much plasticity as possible.

This result is in qualitative disagreement with reality and means that shape memory effect could not exist.

In Section 4, further analysis of possible limitations of the solution obtained is made and further arguments supporting the contradiction are given. A connection with similar problems for other types of structural changes (fracture, chemical reactions) is outlined.

Direct tensor notations are used throughout this paper. Vectors and tensors are denoted in boldface type; $\mathbf{m}\,\mathbf{n}=\{m_i n_j\}$ is the dyadic product of vectors **m** and **n** and $\mathbf{A}\cdot\mathbf{B}=\{A_{ik}B_{kj}\}$ and $\mathbf{A}{:}\mathbf{B}=A_{ik}\ B_{ki}$ are the contraction of tensors over one and two indices. Superscripts t and -1 denote the transposition and inverse operation, subscript s symmetrization of the tensors, $[\mathbf{a}]=\mathbf{a}_2-\mathbf{a}_1$ the jump of value **a** across the interface, $\Delta\mathbf{a}=\mathbf{a}_2-\mathbf{a}_1$ the differences in **a**, **I** the unit tensor second order, $:=$ means equals per definition, the indices 1 and 2 denote the values before and after PT.

2. General problem formulations for interface propagation in inelastic material

2.1. Formulation based on the Eshelby driving force

Let the motion of the inelastic material with PT occupying the volume υ and bounded by the surface S in the reference configuration V_0 be described by the function $\mathbf{r}=\mathbf{r}(\mathbf{r}_0,t)$ where **r** and $\mathbf{r}_0$ are the positions of points in the actual V_t and reference V_0 configuration, and t is the time. We define the deformation gradient as $F=\frac{\partial r}{\partial r_0}$ and particle velocity as $\boldsymbol{\upsilon}=\dot{\mathbf{r}}$.

For coherent interfaces, the function $\mathbf{r}(\mathbf{r}_0,\ t)$ is continuous, but the velocity vector $\mathbf{v}(\mathbf{r}_0,\mathrm{t})$ and the deformation gradient $\mathbf{F}(\mathbf{r}_0,t)$ have jumps across the interface Σ. In this case, the Hadamard compatibility conditions

$$[\mathbf{F}]=-\frac{1}{\upsilon_n}[\boldsymbol{\upsilon}]\mathbf{n}\cdot[\boldsymbol{\upsilon}]=-[\mathbf{F}]\cdot\mathbf{n}\upsilon_n;\ \ [\mathbf{F}]=\mathbf{n}\cdot\left[\mathbf{F}^t\right]\mathbf{n}=[\mathbf{F}]\cdot\mathbf{n}\mathbf{n} \tag{5}$$

are valid (Truesdell and Toupin, 1960), where **n** is the unit normal to the interface. the contraction of Eq. $(5)_1$ with the normal vector **n** gives Eq. $(5)_2$; the substitution of Eq. $(5)_2$ into Eq. $(5)_1$ results in Eq. $(5)_3$. The traction continuity condition at the neglected inertia term follows from the equilibrium condition

$$[\mathbf{p}]=[\mathbf{P}]\cdot\mathbf{n}=0. \tag{6}$$

According to the second law of thermodynamics at fixed temperature, the global rate of dissipation is

$$D:=\int_S\mathbf{p}\cdot\boldsymbol{\upsilon}\mathrm{d}S-\frac{\mathrm{d}}{\mathrm{d}t}\int_\upsilon\rho_0\psi\mathrm{d}\upsilon\geqslant 0. \tag{7}$$

To pass from the integral form of Eq. (7) to the local one, it is necessary to use the Gauss theorem for a volume with discontinuity surfaces.

The general scheme to apply the Gauss theorem is the following one. The volume υ is divided by surfaces Σ and S into a finite number of volumes. In each of them all functions are continuous and, using the Gauss theorem, we obtain some equations. After summing up all of these equations, we obtain an integral over the volume $\bar{\upsilon} = \upsilon - \Sigma$ at one side and on the other side an integral over S and an integral over Σ of the jumps of the functions (because the integration on Σ is fulfilled two times for two volumes, divided by Σ). Thus we derive

$$\int_S \mathbf{p}\cdot\boldsymbol{\upsilon}\,\mathrm{d}S = \int_{\bar{\upsilon}} \mathbf{P}^t : \dot{\mathbf{F}}\,\mathrm{d}\bar{\upsilon} - \int_\Sigma \mathbf{p}\cdot[\boldsymbol{\upsilon}]\,\mathrm{d}\Sigma \tag{8}$$

[Eq. (6) was applied]. Using the known formula for differentiating we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\upsilon \rho_0\psi\,\mathrm{d}\upsilon = \int_{\bar{\upsilon}} \rho_0\dot{\psi}\,\mathrm{d}\bar{\upsilon} + \int_\Sigma \rho_0[\psi]\upsilon_n d\Sigma. \tag{9}$$

From Eqs. (7)–(9) it follows

$$D = \int_\upsilon \left(\mathbf{P}^t : \dot{\mathbf{F}}\right)\mathrm{d}\upsilon + \int_\Sigma \mathcal{D}_E\,\mathrm{d}\Sigma \geqslant 0, \tag{10}$$

where

$$\mathcal{D}_E = -\mathbf{p}\cdot[\boldsymbol{\upsilon}] - \rho_0[\psi]\upsilon_n \tag{11}$$

is the rate of dissipation per unit area of the interface. Using Eqs. $(5)_2$ and $(5)_3$ we get

$$-\mathbf{p}\cdot[\boldsymbol{\upsilon}] = \mathbf{n}\cdot\mathbf{P}^t\cdot[\mathbf{F}]\cdot\mathbf{n}\upsilon_n = \mathbf{P}^t : ([\mathbf{F}]\cdot\mathbf{nn})\upsilon_n = \mathbf{P}^t : [\mathbf{F}]\upsilon_n. \tag{12}$$

Substituting Eq. (12) into Eq. (13) we obtain

$$\mathcal{D}_E = \rho_0 X_E \upsilon_n; \;\; \rho_0 X_E := \mathbf{P}^t : [\mathbf{F}] - \rho_0[\psi]. \tag{13}$$

As constitutive equations were not used, Eq. (13) is valid for any material. As for elastic materials, where there are no other sources of dissipation than PT, $\mathcal{D}_E$ represents the dissipation due to PT only. For inelastic materials, dissipation due to the inelastic deformation jump across the moving interface contributes to $\mathcal{D}_E$.

As is usual in nonequilibrium thermodynamics, the kinetic equation between rate and force $\rho_0\upsilon_n = f_0(X_E)$ or force and rate $X_E = F_0(\rho_0\upsilon_n)$ has to be formulated. It is also usually assumed that interface starts its motion when $X_E \geqslant K$, where K is the threshold value of dissipation. This condition is similar to the condition that the applied force has to exceed friction force at rest for motion with dry friction, or stress intensity has to reach or exceed the yield stress for plastic flow. In most cases (Fischer and Reisner, 1998; Fischer et al., 2000; Cherkaoui et al., 1998; Cherkaoui and Berveiller, 2000), the instantaneous rate independent kinetics is considered, i.e. interface moves when

$$X_E = K. \tag{14}$$

For elastic materials, K represents the dissipation due to PT which can be considered as material constant. Contributions to K due to the Peierls barrier and the interaction of the interface with various defects can be estimated using corresponding microscopic models (see e.g. Olson and Cohen, 1986, Ghosh and Olson, 1994).

As for inelastic materials, if X_E includes the dissipation due to PT and plastic deformation at the moving interface then K has to include both contributions as well. However, plastic dissipation depends strongly on applied stress and can be calculated if the corresponding stress history is given. Examples of the calculation of plastic dissipation at the moving interface are given in (Levitas, 1998, Levitas et al., 1998c, 2002; Idesman et al., 1999, 2000) and in the example in Section 3. The stress dependence of plastic dissipation can be very strong and plastic dissipation can tend to infinity under some conditions (see Section 3). In all known approaches based on the Eshelby driving force (Fischer et al., 1994, 2000; Fischer and Reisner, 1998; Cherkaoui et al., 1998; Cherkaoui and Berveiller, 2000), the threshold value K is considered as a material constant.

2.2. Formulation based on the dissipation increment due to PT only

We will derive all the necessary equations for interface propagation in the reference configuration, because it is much simpler than in the actual configuration. However, in Section 3 we will need expressions for X and X_E in terms of stress and deformation rate measures determined in the actual configuration. It is related to the fact that the equations of flow theory of plasticity look much simpler in the actual configuration. That is why in Section 2.2.2. we transform equations for X and X_E obtained to the current configuration.

2.2.1. Derivation in the reference configuration

Recognizing the above contradictions Levitas (1992b, 1995a,b,c,d) added actual plastic dissipation A_p during the PT to the right-hand side of Eq. (14), i.e.

$$X_E = K + A_p. \tag{15}$$

However, even such a simple step requires a completely different problem formulation. To calculate X_E, it is necessary to know the current values of stresses and strains from both sides of an interface, without knowledge of the detailed process in the transforming region. Due to the history-dependent character of plastic flow equations, calculation of A_p requires the consideration of the whole history of stress and strain variation during the transformation process, rather than a jump of parameters. Consequently, we have to make an infinitesimal interface advance $v_n\,\mathrm{d}t$ and consider a smooth deformation process in a volume $\Sigma v_n\,\mathrm{d}t$ covered by the moving interface (Fig. 2). During this process, a transformation deformation gradient $\mathbf{F}_t$ grows from the unit tensor $\mathbf{I}$ to a final value $\mathbf{F}_{t2}$ determined by crystallography, and all mechanical and thermal material properties of austenite transform to properties of martensite. However, similar consideration can be done for martensite nucleation, i.e. when a similar process is considered in a small volume V_n surrounded by austenite (Fig. 2). Consequently, the description of interface propagation and nucleation can be unified.

Such a new approach based on local consideration of transformation process in each transforming point was developed in Levitas (1996a, 1998) for small strain and in Levitas (1996b, 1998) at large strain. Further development of this idea starting with the global rather than the local form of the thermodynamic laws is made in Levitas (2000). This approach allowed us to try to apply standard thermodynamic procedure to derive constitutive relations for PT, to demonstrate the limitation of standard procedure, and to find a new correct description. The main outcome of this approach is the separation of dissipation due to PT from other dissipation sources (e.g. due to plasticity) and the strict and explicit determination of the driving force and rate for PT.

We use a multiplicative decomposition of the total deformation gradient $\mathbf{F}$ into elastic $\mathbf{F}_e$, transformational $\mathbf{F}_t$, and plastic $\mathbf{F}_p$ parts

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_t \cdot \mathbf{F}_p \tag{16}$$

Then we introduce the dimensionless order parameter $\xi (0 \leqslant \xi \leqslant 1)$ which is related to $\mathbf{F}_t$ and has the following properties: PT starts at $\xi = 0$ and finishes at $\xi = 1$ and when ξ varies between 0 and 1, the transformation deformation gradient grows from $\mathbf{I}$ to a final maximum value $\mathbf{F}_{t2}$ determined by crystallography. It is possible to define the order parameter ξ e.g. as $\xi := \frac{|\mathbf{F}_t - \mathbf{I}|}{|\mathbf{F}_{t2} - \mathbf{I}|}$. Using Eq. (16) the deformation rate $\mathbf{d}$ is

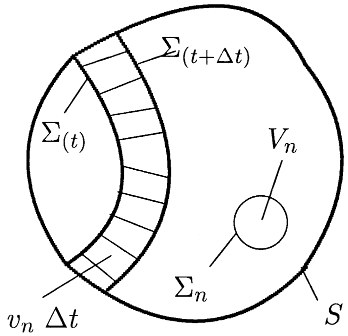

Fig. 2. Volume v with moving interface Σ and new nucleus V_n.

decomposed as follows

$$\mathbf{d} := \left(\frac{\partial \boldsymbol{\upsilon}}{\partial \mathbf{r}}\right)_s = \left(\dot{\mathbf{F}}\cdot\mathbf{F}^{-1}\right)_s = \mathbf{d}_e + \mathbf{d}_t + \mathbf{d}_p, \tag{17}$$

$$\mathbf{d}_e := \left(\dot{\mathbf{F}}_e\cdot\mathbf{F}_e^{-1}\right)_s, \ \mathbf{d}_t := \left(\mathbf{F}_e\cdot\dot{\mathbf{F}}_t\cdot\mathbf{F}_t^{-1}, \mathbf{F}_e^{-1}\right)_s, \tag{18}$$

$$\mathbf{d}_p := \left(\mathbf{F}_e\cdot\mathbf{F}_t\cdot\dot{\mathbf{F}}_p\cdot\mathbf{F}_p^{-1}\cdot\mathbf{F}_t^{-1}\cdot\mathbf{F}_e^{-1}\right)_s = \left(\mathbf{F}_e\cdot\mathbf{F}_t\cdot\dot{\mathbf{F}}_p\cdot\mathbf{F}^{-1}\right)_s \tag{19}$$

where $\mathbf{d}_e$, $\mathbf{d}_t$, and $\mathbf{d}_p$ are elastic, transformational, and plastic parts of the deformation rate.

Using a thermodynamic approach, it is shown (Levitas, 1998) that the total local dissipation rate per unit mass in the transforming material point is equal to

$$D_t = \mathbf{X}_p : \dot{\mathbf{F}}_p + X_\xi \dot{\xi} \geqslant 0, \tag{20}$$

where

$$X_p = \frac{1}{\rho_0}\mathbf{P}^t\cdot\mathbf{F}_e\cdot\mathbf{F}_t; \tag{21}$$

$$X_\xi = \frac{1}{\rho_0}\mathbf{P}^t\cdot\mathbf{F}_e : \frac{\partial \mathbf{F}_t}{\partial \xi}\cdot\mathbf{F}_p - \frac{\partial \psi}{\partial \xi} \tag{22}$$

are dissipative forces conjugated to dissipative rates $\dot{\mathbf{F}}_p$ and $\dot{\xi}$ respectively. Eqs. (20), (21), and (22) are simplified version of Eqs. (36)–(38) in Levitas (1998). In particular, a stored energy of plastic deformation is neglected here. The simplest assumption that each rate depends on the conjugate force only leads to the flow rule $\dot{\mathbf{F}}_p = \mathbf{f}_p(\mathbf{X}_p)$, the evolution equation $\dot{\xi} = f_\xi(X_\xi, \xi)$, and to the decoupling of plastic dissipation and dissipation due to PT. Key point of this result is that *PT has to be described in terms of a dissipative force due to PT only rather than dissipative force due to all dissipative processes.*

As the next step, it was demonstrated (Levitas, 1996a,b, 1998) that the description $f_\xi(X_\xi, \xi)$ is contradictory. To avoid contradiction, it is necessary to average the dissipation rate $X_\xi \dot{\xi}$ over the whole transformation process (or time of transformation event t_p), i.e to introduce the averaged dissipation rate due to PT

$$\mathcal{D}_\xi := \frac{1}{t_p}\int_0^{t_p} X_\xi \dot{\xi}\,\mathrm{d}t = \frac{1}{t_p}\int_0^1 X_\xi \mathrm{d}\xi = \frac{X}{t_p} = X\dot{\chi} \tag{23}$$

$$\text{where } X := \int_0^1 X_\xi \mathrm{d}\xi \text{ and } \dot{\chi} := \frac{1}{t_p} \tag{24}$$

are the averaged dissipative force and rate [see Eq. (14) in Levitas, 1998]. The definition of dissipative rate is logical, because a variation of the parameter ξ during the time t_p is one. The dissipative force is defined as a conjugate variable in the expression for the rate of dissipation. An alternative expression for the driving force X,

$$X = \int_{\mathbf{F}_1}^{\mathbf{F}_2} \frac{1}{\rho_0} \mathbf{P}^t : \mathrm{d}\mathbf{F} - [\psi] - \int_{\theta_1}^{\theta_2} s \mathrm{d}\theta - \int_{\mathbf{F}_{p1}}^{\mathbf{F}_{p2}} \mathbf{X}_p : \mathrm{d}\mathbf{F}_p \tag{25}$$

[see Eq.(42) in Levitas, 1998] leads to the conclusion that the driving force for PT X represents the difference between the total dissipation increment due to all dissipative processes [the first three terms in Eq. (25)] minus the plastic dissipation increment, i.e. it is in fact the dissipation increment due to PT only. Here s is specific (per unit mass) entropy and the third term takes into account temperature θ change.

After integration over the transforming volume V_n and allowing the surface energy [or using more strict approach based on the global form of thermodynamic laws (Levitas, 2000)] one obtains the dissipation rate due to PT only in the transforming volume

$$\mathcal{D}_\upsilon := X_\upsilon \dot{\chi}; \qquad X_\upsilon := \int_{V_n} \rho_0 X \mathrm{d}V_n - \Delta\Gamma, \tag{26}$$

where $\Delta\Gamma$ is the change in surface energy. Eq. (26) is valid both for nucleation and interface propagation. For nucleation, equations $X_\upsilon \geqslant K_n m_n$ and $\dot{\chi} = f(X_\upsilon)$ represent nucleation criterion and the kinetic equation, where K_n is the dissipative barrier for nucleation and m_n is the mass of the transforming volume V_n.

For the interface propagation, further simplifications are possible. Assume that the volume V_n is obtained by the interface Σ propagation with a normal velocity υ_n in time Δt, 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 $\upsilon_n \Delta t$ (Fig. 2). Let us fix the surface $\Sigma_{(t+\Delta t)}$ and consider the PT process in a fixed volume $\mathrm{d}V_n = \upsilon_n \Delta t \mathrm{d}\Sigma_{(t)}$. It appears that due to the infinitesimal height $\upsilon_n \Delta t$; the results are independent of the details of the process inhomogeneity along the height. At the same time, due to the history-dependent character of the constitutive equations for inelastic materials, we must in any case consider the transformation process in the transforming points. Let us transform the stress work integral in expressions for X_υ Eqs. (25) and (26). Using the Gauss theorem and taking into account the Hadamard compatibility condition Eq. (5) and traction continuity condition Eq. (6), as well as Eq. (12) and neglecting all the terms of order Δt^2 one obtains

$$\begin{aligned}\int_{V_n}\int_{\mathbf{F}_1}^{\mathbf{F}_2}\mathbf{P}^t:\mathrm{d}\mathbf{F}\,\mathrm{d}V_n&=\int_t^{t+\Delta t}\int_{V_n}\mathbf{P}^t:\dot{\mathbf{F}}\mathrm{d}V_n\mathrm{d}t=\int_t^{t+\Delta t}\int_{\Sigma_n}\mathbf{p}\cdot\boldsymbol{\upsilon}\mathrm{d}\ \Sigma\ \mathrm{d}t\\&=\left(\int_{\Sigma(t+\Delta t)}\mathbf{p}_1\cdot\boldsymbol{\upsilon}_1\mathrm{d}\Sigma_{(t+\Delta t)}-\int_{\Sigma(t)}\mathbf{p}_2\cdot\boldsymbol{\upsilon}_2\mathrm{d}\Sigma_{(t)}\right)\Delta t=-\int_{\Sigma(t)}[\mathbf{p}\cdot\boldsymbol{\upsilon}]\Delta t\mathrm{d}\Sigma_{(t)}\\&=\int_{\Sigma(t)}\mathbf{P}^t:[\mathbf{F}]\upsilon_n\Delta t\mathrm{d}\Sigma_{(t)}=\int_{V_n}\mathbf{P}^t:[\mathbf{F}]\mathrm{d}V_n.\end{aligned}\tag{27}$$

It is taken into account that the surface Σ_n of the volume V_n consists of surfaces $\Sigma_{(t)}$ and $\Sigma_{(t+\Delta t)}$ and two infinitesimal surfaces with heights $\upsilon_n\Delta t$ which we neglected. The minus sign before the integral $\int_{\Sigma(t)}\mathbf{p}_2\cdot\boldsymbol{\upsilon}_2\ \mathrm{d}\ \Sigma_{(t)}$ is because the external normal to surface Σ_n is directed opposite to direction of interface motion and normal **n** to the interface. Consequently, for points of the interface

$$\int_{\mathbf{F}_1}^{\mathbf{F}_2}\mathbf{P}^t:\mathrm{d}\mathbf{F}=\mathbf{P}^t:[\mathbf{F}].\tag{28}$$

Substituting Eq. (28) into Eq. (25), one obtains

$$X=\frac{1}{\rho_0}\mathbf{P}^t:[\mathbf{F}]-[\psi]-\int_{\theta_1}^{\theta_2}s\,\mathrm{d}\theta-\int_{\mathbf{F}_{p1}}^{\mathbf{F}_{p2}}\mathbf{X}_p:\mathrm{d}\mathbf{F}_p.\tag{29}$$

To find the physical meaning of parameter X for interface propagation, assume that each infinitesimal volume $\mathrm{d}V_n=\upsilon_n\Delta t\ \mathrm{d}\Sigma$ transforms independently of the other. Then we can study locally each point of the interface. Neglecting the surface energy in Eq. (26), the rate of dissipation due to PT per unit $\mathrm{d}\Sigma$ with allowance for $\Delta t=t_p$ has the form

$$\mathcal{D}:=\frac{\mathcal{D}_\upsilon}{\mathrm{d}\sum}=\frac{X_{p_0}\upsilon_n\mathrm{d}\sum t_p}{\mathrm{d}\sum t_p}=\rho_0\,X\,\upsilon_n.\tag{30}$$

Consequently, X and $\rho\upsilon_n$ are the driving force and rate for the interface propagation. Comparing Eqs. (29) and (13), we conclude that for elastic material and an isothermal process, X coincides with the Eshelby driving force. As follows from the above derivations, Eq. (29) [and Eq. (25)] represents the driving force for interface propagation for inelastic material and nonisothermal conditions.

2.2.2. Relations in the actual configuration

Using the relation between the Piola-Kirchhoff stress tensor **P** and the true Cauchy stress **T**

$$\mathbf{P}=\frac{\rho_0}{\rho}\mathbf{T}\cdot\mathbf{F}^{-1t};\ \mathbf{P}^t=\frac{\rho_0}{\rho}\mathbf{F}^{-1}\cdot\mathbf{T},\tag{31}$$

one obtains

$$\frac{1}{\rho_0}\mathbf{P}^t:\dot{\mathbf{F}}=\frac{1}{\rho}\mathbf{F}^{-1}\cdot\mathbf{T}:\dot{\mathbf{F}}=\frac{1}{\rho}\mathbf{T}:\dot{\mathbf{F}}\cdot\mathbf{F}^{-1}=\frac{1}{\rho}\mathbf{T}:\mathbf{d}; \tag{32}$$

$$\begin{aligned}\mathbf{X}_p:\dot{\mathbf{F}}_p&=\frac{1}{\rho_0}\mathbf{P}^t\cdot\mathbf{F}_e\cdot\mathbf{F}_t\cdot\dot{\mathbf{F}}_p=\frac{1}{\rho}\mathbf{F}^{-1}\cdot\mathbf{T}\cdot\mathbf{F}_e\cdot\mathbf{F}_t:\dot{\mathbf{F}}_p=\\&=\frac{1}{\rho}\mathbf{T}\cdot\mathbf{F}_e\cdot\mathbf{F}_t\cdot\dot{\mathbf{F}}_p\cdot\mathbf{F}^{-1}=\frac{1}{\rho}\mathbf{T}:\left(\mathbf{F}_e\cdot\mathbf{F}_t\cdot\dot{\mathbf{F}}_p\cdot\mathbf{F}^{-1}\right)_s=\frac{1}{\rho}\mathbf{T}:\mathbf{d}_p.\end{aligned} \tag{33}$$

Here ρ is the mass density in the actual configuration. The symmetry of the Cauchy stress $\mathbf{T}$ and the possibility of permutation of tensors in a scalar product are taken into account. Substituting Eqs. (32) and (33) into Eq. (25), we obtain an expression for the driving force X in terms of tensors defined in the actual configuration

$$X=\int_0^{t_p}\frac{1}{\rho}\mathbf{T}:\mathbf{d}\,\mathrm{d}t-[\psi]-\int_0^{t_p}\frac{1}{\rho}\mathbf{T}:\mathbf{d}_p\mathrm{d}t. \tag{34}$$

It is evident that neglecting the plastic work in Eq. (34) will give us a generalization of the Eshelby driving force for anisothermal processes written in the current configuration

$$X_E=\int_0^{t_p}\frac{1}{\rho}\mathbf{T}:\mathbf{d}\,\mathrm{d}t-[\psi]-\int_{\theta_1}^{\theta_p}s\mathrm{d}\theta \tag{35}$$

which will be used in Section 3. It is possible (Levitas, 1998) to express the stress work integral in Eqs. (35) and (37) in a form independent of the transformation process; however, we will not need this expression. The first and the last term in Eq. (34) can be transformed using the equation

$$\mathbf{T}:\mathbf{d}-\mathbf{T}:\mathbf{d}_p=\mathbf{T}:(\mathbf{d}_t+\mathbf{d}_e), \tag{36}$$

where Eq. (17) was used. Then, we obtain

$$X=\int_0^{t_p}\frac{1}{\rho}\mathbf{T}:(\mathbf{d}_t+\mathbf{d}_e)\mathrm{d}t-[\psi]-\int_{\theta_1}^{\theta_2}s\mathrm{d}\theta. \tag{37}$$

This transformation is reasonable in view of $\mathbf{d}_e=0$ for the rigid-plastic materials considered in Section 3. Similar to Eq. (30), one can define the rate of dissipation due to PT per unit interface area in the actual configuration $\mathrm{d}\Sigma_t$

$$\mathcal{D}_t := \frac{\mathcal{D}_v}{\mathrm{d}\ \Sigma_t} = \frac{X\rho_1 v_{n1}\mathrm{d}\Sigma_t t_p}{\mathrm{d}\ \Sigma_t t_p} = X\rho_1 v_{n1} = X\rho_2 v_{n2}. \tag{38}$$

Here v_1 and v_2 designate the interface velocity with respect to the particle of phase 1 and 2. In transformations, we used the mass balance $\rho_0 v_n \mathrm{d}\Sigma = \rho_1 v_{n1}\mathrm{d}\Sigma_t = \rho_2 v_{n2}\mathrm{d}\Sigma_t$ and $\rho_1 v_{n1} = \rho_2 v_{n2}$.

The interface propagation criterion has the form

$$X \geqslant K \tag{39}$$

in any configuration, because X is defined per unit mass and is independent of the configuration. Kinetic equations in the actual configuration take a form $\rho_1 v_{n1} = f(X)$ or $X = F(\rho_1 v_{n1})$ (or similar expressions in terms of $\rho_2 v_{n2}$). As $\rho_1 v_{n1} = \rho_0 v_n \frac{\mathrm{d}\ \Sigma}{\mathrm{d}\ \Sigma_t}$ the corresponding function $X = F_0(\rho_0 v_n)$ in reference configuration can be found from the relation $X = F_0(\rho_0 v_n) = F\left(\rho_0 v_n \frac{\mathrm{d}\ \Sigma}{\mathrm{d}\ \Sigma_t}\right)$.

For small strain and rotation, the reference and current configurations approximately coincide, and all the above equations are simplified significantly:

$$\mathbf{F} = \mathbf{I} + \boldsymbol{\varepsilon};\quad \mathbf{F}_e = \mathbf{I} + \boldsymbol{\varepsilon}_e;\quad \mathbf{F}_t = \mathbf{I} + \boldsymbol{\varepsilon}_t;\quad \mathbf{F}_p = \mathbf{I} + \boldsymbol{\varepsilon}_p;\quad \boldsymbol{\varepsilon},\ \boldsymbol{\varepsilon}_e,\ \boldsymbol{\varepsilon}_p,\ \boldsymbol{\varepsilon}_t \ll \mathbf{I}; \tag{40}$$

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p + \boldsymbol{\varepsilon}_t;\quad d = \dot{\boldsymbol{\varepsilon}};\quad \mathbf{d}_e = \dot{\boldsymbol{\varepsilon}}_e;\quad \mathbf{d}_p = \dot{\boldsymbol{\varepsilon}}_p;\quad \mathbf{d}_t = \dot{\boldsymbol{\varepsilon}}_p; \tag{41}$$

$$\rho_0 = \rho;\quad \mathbf{P} = \mathbf{T};\quad v_n = v_{n1} = v_{n2}; \tag{42}$$

$$\begin{aligned} X &= \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \frac{1}{\rho}\mathbf{T} : \mathrm{d}\boldsymbol{\varepsilon} - [\psi] - \int_{\theta_1}^{\theta_2} s\mathrm{d}\theta - \int_{\varepsilon_{p1}}^{\varepsilon_{p2}} \frac{1}{\rho}\mathbf{T} : \mathrm{d}\varepsilon_p \\ &= \int_{\boldsymbol{\varepsilon}_{t1}}^{\boldsymbol{\varepsilon}_{t2}} \frac{1}{\rho}\mathbf{T} : \mathrm{d}\boldsymbol{\varepsilon}_t + \int_{\varepsilon_{e1}}^{\varepsilon_{e2}} \frac{1}{\rho}\mathbf{T} : \mathrm{d}\boldsymbol{\varepsilon}_e - [\psi] - \int_{\theta_1}^{\theta_2} s\mathrm{d}\theta; \end{aligned} \tag{43}$$

$$X_E = \int_{\boldsymbol{\varepsilon}_1}^{\boldsymbol{\varepsilon}_2} \frac{1}{\rho}\mathbf{T} : \mathrm{d}\boldsymbol{\varepsilon} - [\psi] - \int_{\theta_1}^{\theta_2} s\mathrm{d}\theta. \tag{44}$$

2.3. Extremum principle

In addition to the interface propagation equation, an extremum principle is needed to determine the multivariant structure of martensite. For elastic materials, the principle of the minimum of Gibbs energy is usually used which results in the principle of the maximum driving force. For inelastic materials, Patel and Cohen (1953) suggested maximizing the mechanical work in order to choose proper habit-plane variant (or invariant plane strain). This in fact is equivalent to the maximization of the Eshelby driving force (if interface propagation is considered), because invariant plane strain includes plastic shear in addition to transformation (Bain) strain and rigid-body rotation. Fischer et al. (1994), Marketz and Fischer (1994a,b), Fischer and Reisner (1998), Cherkaoui et al. (1998), and Cherkaoui and Berveiller (2000) also maximized the Eshelby driving force with respect to the proper habit-plane variant.

Levitas (1992b, 1995a,b,c,d, 1998) formulated a plausible assumption called the postulate of the realizability, which results in the maximization of the difference $X - K$ both for nucleation and interface propagation. At constant K, this principle reduces to a maximization of X. In Levitas (2000) the more general extremum principle is derived based on the kinetic consideration; however, it will not be used here. Consequently, for both definitions of the driving force, the principle of the maximum driving force

$$X_E \Rightarrow \max; \; X \Rightarrow \max \tag{45}$$

will be used.

A comparison of the derivation procedure for both driving forces, X_E and X, demonstrates advantages of using X rather than X_E. This follows directly from the thermodynamic procedure when the local transformation process is considered in a material point which belongs either to the nucleus or to the moving interface, see Eq. (20). This follows also from Eq. (15), if we can prove that A_p varies significantly with a change of external stresses. We will prove this in the next section, as well as demonstrate a conceptual contradiction in the application of the Eshelby driving force for interface propagation in plastic materials.

3. Analytical solution for interface propagation in rigid-plastic materials

3.1. Problem formulation

It is necessary to mention that by plasticity it is meant dislocation plasticity rather than plasticity due to twinning. Twinning during martensitic transformation means the appearance of several martensitic variants which are in twin relation to each other. Consequently, for twinned martensite, we have a microheterogeneous transformation deformation gradient without the plastic dissipation term, i.e. both approaches coincide.

To check which driving force has to be used for the description of the interface propagation in inelastic materials, we suggest the following critical thought experiment.

For a number of PT, e.g. for PT from cubic to tetragonal or orthorhombic phase, complete compatibility at the austenite—twinned martensite interface is possible without internal stresses and plasticity [e.g. for *Au–Cd* or *CuZnAl SMA* (Wayman, 1994; Ball and James, 1992)]. We will demonstrate the following contradictions.

Even in this case:

1. The maximization of the Eshelby driving force requires as much plasticity as possible.
2. When an applied shear stress reaches the yield stress in shear, the Eshelby driving force tends to infinity, i.e. PT has to always occur at the beginning of plastic flow.

We consider a simple scheme (Fig. 3): interface propagation inside of a rigid-plastic half-space with prescribed normal σ_n and shear τ component of Cauchy stress **T** under a plane strain condition. It is sufficient to consider an infinitesimal interface advance in order to calculate both driving forces. We assume that the total transformation and plastic deformation gradients are homogeneous in a layer covered by the moving interface and that the stress field is homogeneous and time independent. Plastic straining during PT in the layer ABCD is concentrated inside the layer while the remaining parts of half-space are rigid.

This assumption corresponds to reality when the yield stress of the new phase is smaller than the yield stress of the parent phase. Then, the part of the half-space above the transforming layer can be considered rigid. This is the case for PT austenite to martensite in SMA. For martensitic PT in steel, the yield stress of martensite is three times the yield stress of austenite, and solution obtained below is not applicable.

Transformed martensite (the part of the half-space below the transforming layer) has a higher yield stress than the transforming layer due to strain hardening during PT.

In most publications, plastic strain in the transforming region is determined using the crystallographic theory, i.e. as a lattice invariant shear which together with the

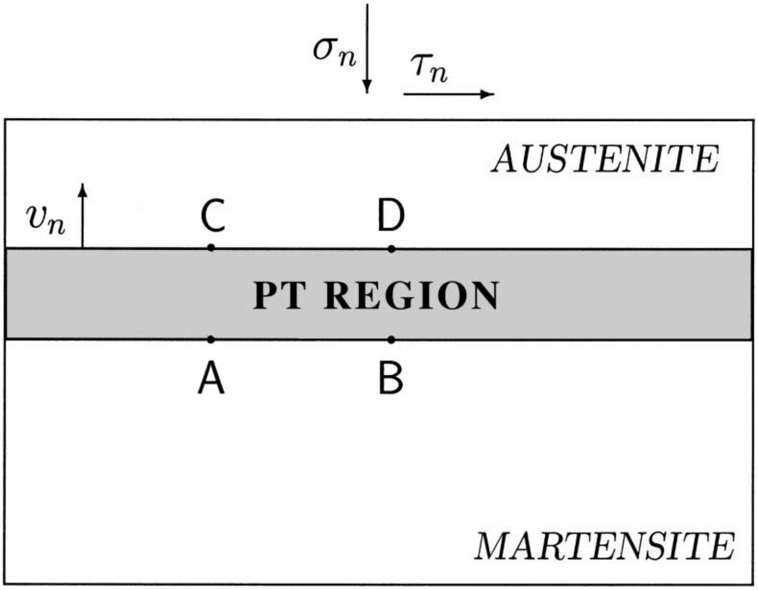

Fig. 3. Scheme of interface propagation in rigid–plastic half-space.

Bain strain and rotation provides compatibility across the interface. This assumption is a reasonable first approximation which allows use of invariant plane variants. However, the crystallographic theory is a purely geometric theory without any stresses, and it cannot be used as a general approach to find the jump in plastic strain. For superposition of an arbitrarily large plastic shear along an interface caused by shear stresses, the same compatibility condition is valid as for crystallographic theory. However, the Eshelby driving force varies significantly due to such additional shear strains. The only general way to determine the change in plastic strain is to integrate the proper flow rule under the prescribed transformation process.

For simplicity, phenomenological isotropic plasticity is used instead of phenomenological single crystal plasticity, or the theory of continuously distributed or discrete dislocations. This, however, does not change the main results and conclusions.

A complete system of equations in the actual configuration V_t is presented in Table 1. All terms related to elastic deformations are neglected. Due to homogeneity of all fields, the equilibrium equation and compatibility condition inside the layer are satisfied automatically. The Tresca yield condition (48) is assumed. Here σ_t is the tangential stress, σ_y the yield limit, $\mathbf{S}$ is the Cauchy stress deviator, d_{pn} and γ_p are the normal and shear component of the plastic strain rate. Plastic incompressibility, which follows from the flow rule associated with the Tresca yield condition, is taken into account.

The expression $\left(-[\psi]-\int_{\theta_1}^{\theta_2} s\mathrm{d}\theta\right)$ in Eqs. (35) and (37) are simplified in a similar way to the one described in Levitas et al. (1998a,b), see the expression for the driving force in Eq. (46) in Levitas et al. (1998a) or Eq. (8) in Levitas et al. (1998b). Simplifications include, in particular, the assumption on the same value ν of specific heats of both phases which is temperature independent. In Eqs. (52) and (53), ΔU_0 and Δs_0 designate a jump in internal energy and entropy due to the PT.

Under the same assumptions and in an adiabatic approximation, the temperature evolution equation has the form of Eqs. (55), see Eq. (45) in Levitas et al. (1998a).

We will consider two solutions. The first one corresponds to a complete compatibility of resulting transformation deformation gradient at the austenite – twinned martensite interface without plasticity, according to crystallographic theory and experiments. This solution follows in particular from the maximization of the driving force X, see below. In this case, crystallographic theory (Wayman, 1964, Ball and James, 1992) provides us with two martensitic variants involved in this solution, their orientation, and the resulting transformation deformation gradient (which is the volume averaged transformation deformation gradient of each variant). The resulting transformation deformation gradient describes the simple shear for the volume preserving case.

The second solution corresponds to the incompatibility of the resulting transformation strain. In Fig. 4, a transformed particle is shown after transformation strain. In order to satisfy the displacement continuity across the interface AB additional plastic strain is needed (Fig. 4b).

We will show that such a solution corresponds to the maximization of the Eshelby driving force. To do this, it is not necessary to find the actual transformation strain

Table 1
Complete system of equations

Decomposition of deformation gradient

$$\mathbf{F} = \mathbf{F}_t \cdot \mathbf{F}_p. \tag{46}$$

Decomposition of deformation rate

$$\mathbf{d} : \left(\dot{\mathbf{F}} \cdot \mathbf{F}^{-1}\right)_s = \left(\dot{\mathbf{F}}_t \cdot \mathbf{F}_t^{-1}\right)_s + \mathbf{d}_p;\ \ \mathbf{d}_p := \left(\mathbf{F}_t \cdot \dot{\mathbf{F}}_p \cdot \mathbf{F}_p^{-1} \cdot \mathbf{F}_t^{-1}\right)_s. \tag{47}$$

Tresca yield condition for the transforming layer

$$\varphi(\mathbf{T}) = 2(\mathbf{S} : \mathbf{S}) - \sigma_y^2 = (\sigma_n - \sigma_t)^2 + 4\tau^2 - \sigma_y^2 = 0; \tag{48}$$

$$\mathbf{S} := \operatorname{dev}\mathbf{T} = 0.5(\sigma_n - \sigma_t)(\mathbf{nn} - \mathbf{tt}) + 2\tau(\mathbf{tn})_s. \tag{49}$$

Associated flow rule

$$\mathbf{d}_p = 0.5h\frac{\partial\varphi}{\partial\mathbf{S}} = 2h\mathbf{S};\ \ \mathbf{d}_p = d_{pn}(\mathbf{nn} - \mathbf{tt}) + \gamma_p(\mathbf{tn})_s; \tag{50}$$

$$d_{pn} = h(\sigma_n - \sigma_t);\ \ \gamma_p = 4h\tau. \tag{51}$$

Eshelby driving force

$$X_E = \int_0^{t_p} \frac{1}{\rho}\mathbf{T} : \mathbf{d}\,\mathrm{d}t - \Delta U_0 + \Delta s_0 \int_0^1 \theta\,\mathrm{d}\xi. \tag{52}$$

Driving force based on dissipation increment due to PT only

$$X = \int_0^{t_p} \frac{1}{\rho}\mathbf{T} : \mathbf{d}_t\,\mathrm{d}t - \Delta U_0 + \Delta s_0 \int_0^1 \theta\,\mathrm{d}\xi. \tag{53}$$

Extremum principle

$$X_E \Rightarrow \max;\ \ X \Rightarrow \max. \tag{54}$$

Temperature evolution equation

$$\nu\dot{\theta} = \frac{1}{\rho}\mathbf{T} : \mathbf{d} - \Delta U_0 \dot{\xi}. \tag{55}$$

and solution. It is sufficient to choose any transformation strain with incompatibility and to show that even for an arbitrary noncompatible transformation strain we can reach a higher driving force due to plastic strain than for a compatible one.

Remark. *There are discussions at various conferences related to the impossibility of the application of continuum mechanics to processes at a martensitic interface which has a typical width of few atomic distances. In particular, the difficulty to distinguish between displacements of atoms due to movement of dislocations and due to lattice rearrangement, and consequently the impossibility to split plastic and transformation strain at the moving interface is mentioned. Let us address these questions.*

Continuum mechanics operates with representative volumes which in plasticity theory have to include enough dislocations. So a typical size is of the order of magnitude of 0.1–10 μm depending on dislocation density. When we consider an interface, we consider two contacting representative volumes from both sides of an interface. In each of them, stresses, strains, transformation and plastic strains are defined in the same way, as far from the interface, because this is a representative volume. It is clear that the interface advance has to be greater than the size of the representative volume. Consequently, application of the continuum approach is noncontradictory for such characteristic sizes. The size of the representative volume can be reduced to the atomic scale if one uses discrete dislocation theory instead of continuum plasticity.

3.2. Solution and analysis

We choose one martensitic variant with transformation tensile strain $F_{tn}=a$ in **n**} direction and the compressive strain $F_{tt}=a^{-1}$ in **t** direction, i.e. $\mathbf{F}_t=a\mathbf{nn}+a^{-1}\,\mathbf{tt}$. Transformation, and consequently, total strains are volume preserving, i.e. $\rho=const$. Transformation shear is not included, i.e. we intentionally reduce the transformation work. We let a grow from 1 to a_2 under fixed external normal and shear stresses. Total deformation is simple shear, $\mathbf{F}=\mathbf{i}+\gamma\mathbf{tn}$. This is the only invariant plane solu-

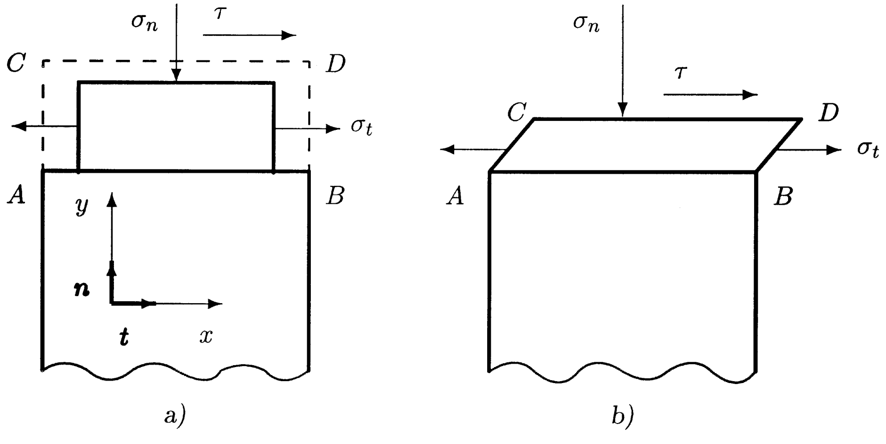

Fig. 4. Transformation (a) and plastic (b) strain in a thin layer covered by moving interface.

tion (i.e. deformation compatible with austenite along the plane CD and existing martensite along plane AB) for the volume preserving case. Here **i** is the two dimensional unit tensor.

Direct calculations of the rate of deformation gradient, inverse deformation gradient, velocity gradient and deformation rate result in

$$\dot{\mathbf{F}} = \dot{\gamma}\mathbf{tn};\ \ \mathbf{F}^{-1} = \mathbf{i} - \gamma\ \mathbf{tn}; \tag{56}$$

$$\mathbf{l} := \dot{\mathbf{F}}\cdot\mathbf{F}^{-1} = \dot{\gamma}\ \mathbf{tn}\cdot(\mathbf{i} - \gamma\ \mathbf{tn}) = \dot{\gamma}\ \mathbf{tn}; \tag{57}$$

$$\text{i.e. } \mathbf{l} = \dot{\mathbf{F}};\ \ \mathbf{d} := (\mathbf{l})_s = \dot{\gamma}(\mathbf{tn})_s. \tag{58}$$

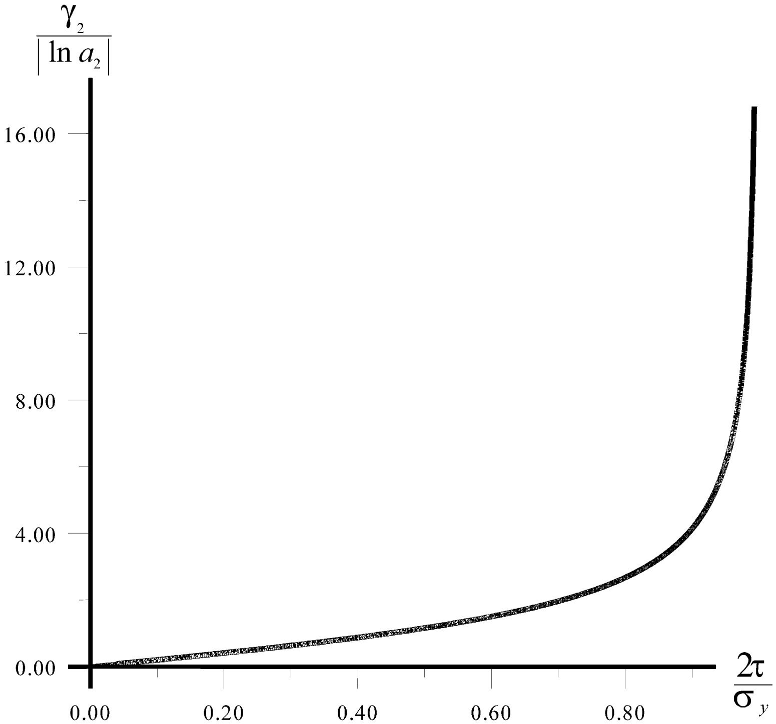

Fig. 5. Relationship between shear strain and stress in transforming layer.

The expressions for the inverse transformation deformation gradient, the rate of transformation deformation gradient, and the deformation rate are:

$$\mathbf{F}_t^{-1} = \alpha^{-1}\mathbf{nn} + a\mathbf{tt};\;\; \dot{\mathbf{F}}_t = \dot{a}\mathbf{nn} - \frac{\dot{a}}{a^2}\mathbf{tt};$$

$$\dot{\mathbf{F}}_t\cdot\mathbf{F}_t^{-1} = \frac{\dot{a}}{a}(\mathbf{nn}-\mathbf{tt});\;\; \mathbf{d}_t = \frac{\dot{a}}{a}(\mathbf{nn}-\mathbf{tt}). \tag{59}$$

We can calculate the total work A per unit volume which is used in the Eshelby driving force and the transformation work A_t per unit volume which contributes to our driving force X. We have

$$\mathbf{T}{:}\mathbf{d} = \tau\dot{\gamma}_2;\;\; A := \int_0^{t_p}\mathbf{T}{:}\mathbf{d}\,\mathrm{d}t = \tau\gamma_2; \tag{60}$$

$$\mathbf{T}{:}\mathbf{d}_t = \mathbf{T}{:}\dot{\mathbf{F}}_t\cdot\mathbf{F}_t^{-1} = (\sigma_n - \sigma_t)\frac{\dot{a}}{a}; \tag{61}$$

$$\begin{aligned} A_t &:= \int_{\mathbf{i}}^{\mathbf{F}_2}\mathbf{T}{:}\mathrm{d}\mathbf{F}_t\cdot\mathbf{F}_t^{-1} = \int_1^{a_2}(\sigma_n-\sigma_t)\frac{\mathrm{d}a}{a} = (\sigma_n-\sigma_t)\ln a_2 \\ &= -\frac{\ln a_2}{|\ln a_2|}\sqrt{\sigma_y^2 - 4\tau^2}\ln a_2 = -\sqrt{\sigma_y^2-4\tau^2}|\ln a_2|. \end{aligned} \tag{62}$$

In Eq. (62), the yield condition $\sigma_n - \sigma_t = \pm\sqrt{\sigma_y^2 - 4\tau^2}$ is used to exclude tangential stress. The sign is chosen from the condition that at $\ln a_2 < 0$, the accommodation plastic tension in direction **n** has to occur, which is possible at $\sigma_n > \sigma_t$ only. At $\ln a_2 > 0$, plastic compression in direction **n** is possible at $\sigma_n < \sigma_t$ only. Consequently, transformation work in this problem is negative for a noncompatible transformation strain, independent of the applied stresses. It is apparent that the total work is not related to the transformation strain at all, because transformation strain does not contain shear. We will see that the total work is a part of the plastic work.

In order to derive the simple equations, we neglect the variation of the yield stress during the PT. To determine the total work A it is necessary to integrate the associated flow rule (51). The plastic deformation gradient can be calculated as

$$\mathbf{F}_p = \mathbf{F}_t^{-1}\cdot\mathbf{F} = \mathbf{F}_t^{-1}\cdot\mathbf{F} = a^{-1}\mathbf{nn} + a\;\mathbf{tt} + a\gamma\;\mathbf{tn}. \tag{63}$$

It is convenient to derive the expression for the plastic deformation rate as the difference between the total and the transformation deformation rates [see Eq. (47)]

$$\mathbf{d}_p = \left(\dot{\mathbf{F}}\cdot\mathbf{F}^{-1}\right)_s - \left(\dot{\mathbf{F}}_t\cdot\mathbf{F}_t^{-1}\right)_s = -\frac{\dot{a}}{a}(\mathbf{nn}-\mathbf{tt}) + \dot{\gamma}(\mathbf{tn})_s. \tag{64}$$

The associated flow rule (51) can be presented in the form

$$-\frac{\dot{a}}{a} = h(\sigma_n - \sigma_t);\quad \dot{\gamma} = 4h\tau. \tag{65}$$

Excluding h from Eq. $(65)_1$ and substituting it in Eq. $(65)_2$ we obtain

$$\dot{\gamma} = -4\frac{\dot{a}}{a}\frac{\tau}{(\sigma_n - \sigma_t)} = 4\left|\frac{\dot{a}}{a}\right|\frac{\tau}{\sqrt{\sigma_y^2 - 4\tau^2}} \tag{66}$$

and

$$\gamma_2 = |\ln a_2|\frac{4\tau}{\sqrt{\sigma_{y^2}^2 - 4\tau^2}}. \tag{67}$$

We took into account in Eq. (66) that the terms $\dot{a}$ and $\sigma_n - \sigma_t$ have opposite signs.

The relationship (67) is shown in Fig. 5. It is easy to see from Eq. (67) that plastic shear strain (as well as total shear strain) is due to the normal component of the transformation strain along the interface. The shear strain is proportional to the normal component of transformation strain along the interface and is independent of normal stresses. Plastic flow occurs at arbitrary (even at infinitesimal) shear stresses. External stresses τ and σ_n need not satisfy the yield condition. This result represents the well-known transformation-induced plasticity phenomenon or TRIP for martensitic and diffusive PT (Fischer et al., 1996, 2000; Padmanabhan and Davies, 1980; Mitter, 1987). This problem models the mechanism of TRIP similar to the Greenwood-Johnson (Greenwood and Johnson, 1965) effect, when at relative small external stresses (much less than the yield stresses), it is possible to obtain a very large value of macroscopic plastic strains due to martensitic or diffusive PT. The distinctive points of our consideration is related to the fact that (a) in the Greenwood–Johnson mechanism plastic flow occurs outside the transforming region, but in our problem the transforming particles deform plastically; (b) instead of a transformation volume change, the volume preserving case is considered here.

The important point of Eq. (67) is that shear strain can be very high. When shear stress tends to the yield stress in shear 0.5 σ_y, total (and plastic) shear strain tends to infinity. Plastic and total work tend to infinity as well.

Let us estimate the temperature change during an adiabatic transformation process. In Eq. (55), $\mathbf{T{:}d} = \tau\dot{\gamma}$. Combining Eqs. (66) and (67), we obtain

$$\dot{\gamma} = \gamma_2\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\ln a}{\ln a_2}\right). \tag{68}$$

If one chooses $\xi = \frac{\ln a}{\ln a_2}$, then Eq. (55) allows a simple integration:

$$\nu\dot{\theta} = \left(\frac{1}{\rho}\tau\gamma_2 - \Delta U_0\right)\dot{\xi};\ \ \theta = \theta_1 + \frac{\tau\gamma_2 - \rho\Delta U_0}{\rho\nu}\xi \tag{69}$$

and

$$\theta_2 := \theta(1) = \theta_1 + \frac{\tau\gamma_2 - \rho\Delta U_0}{\rho\nu}, \quad \int_0^1 \theta d\xi = \theta_1 + \frac{\tau\gamma_2 - \rho\Delta U_0}{2\rho\nu}. \tag{70}$$

Again, we choose the adiabatic approximation because this is the worst case for us. We took into account the transformation heat and plastic dissipation.

Now we can calculate driving forces for both approaches. Substituting Eqs. (60), (62) and (70) in Eqs. (52) and (53), one obtains

$$X_E = \frac{\tau\gamma_2}{\rho}\left(1 + \frac{\Delta s_0}{2\nu}\right) + \Delta s_0\theta_1 - \Delta U_0\left(1 + \frac{\Delta s_0}{2\nu}\right) \tag{71}$$

for the Eshelby driving force and

$$X = -\sqrt{\sigma_y^2 - 4\tau^2}\frac{|\ln a_2|}{\rho} + \frac{\tau\gamma_2}{\rho}\frac{\Delta s_0}{2\nu} + \Delta s_0\theta_1 - \Delta U_0\left(1 + \frac{\Delta s_0}{2\nu}\right) \tag{72}$$

for the driving force based on the dissipation increment due to PT only.

For compatible martensite, $A = A_t = \tau\gamma_{t2} \geqslant 0$ (because τ and γ_{t2} have the same sign), where γ_{t2} is the resulting transformation shear. The expressions for the Eshelby driving force and for the driving force based on the dissipation increment due to PT only coincide:

$$X_c = \frac{\tau\gamma_{t2}}{\rho}\left(1 + \frac{\Delta s_0}{2\nu}\right) + \Delta s_0\theta_1 - \Delta U_0\left(1 + \frac{\Delta s_0}{2\nu}\right). \tag{73}$$

The equations for the driving forces for isothermal processes can be obtained from Eqs. (71), (72), and (73) by putting $\nu \to \infty$:

$$X_E = \frac{\tau\gamma_2}{\rho} + \Delta s_0\theta_1 - \Delta U_0; \tag{74}$$

$$X = -\sqrt{\sigma_y^2 - 4\tau^2}\frac{|\ln a_2|}{\rho} + \Delta s_0\theta_1 - \Delta U_0; \tag{75}$$

$$X_c = \frac{\tau\gamma_{t2}}{\rho} + \Delta s_0\theta_1 - \Delta U_0. \tag{76}$$

For small strains and rotations

$$\mathbf{F} = \mathbf{i} + \boldsymbol{\varepsilon}; \quad \boldsymbol{\varepsilon} = \gamma(\mathbf{tn})_s; \quad \mathbf{d} = \dot{\boldsymbol{\varepsilon}} = \dot{\gamma}(\mathbf{tn})_s, \tag{77}$$

$$\mathbf{F}_t = \mathbf{i} + \boldsymbol{\varepsilon}_t; \quad \boldsymbol{\varepsilon}_t = (a-1)(\mathbf{nn} - \mathbf{tt}); \quad \mathbf{d}_t = \dot{\boldsymbol{\varepsilon}}_t = \dot{a}(\mathbf{nn} - \mathbf{tt}). \tag{78}$$

$$\mathbf{F}_p = \mathbf{i} + \boldsymbol{\varepsilon}_p; \quad \boldsymbol{\varepsilon}_p = -(a-1)(\mathbf{nn} - \mathbf{tt}) + \gamma(\mathbf{tn})_s \tag{79}$$

$$\gamma_p := \gamma; \quad \mathbf{d}_p = \dot{\varepsilon}_p = -\dot{a}(\mathbf{nn} - \mathbf{tt}) + \dot{\gamma}(\mathbf{tn})_s \quad 1\text{n}\ a_2 \simeq a_2. \tag{80}$$

It appears that the final Eqs. (71)–(76) are the same for the small and large strain. We needed, however, a large strain formulation, because our further conclusions will be based on the large plastic shear.

Let us analyze the results in Eqs.(71)–(76) for the driving forces for compatible and incompatible martensite for the isothermal case, which differ by the first terms only. It is evident that $X_c > X$ for any τ because the first term in the expression for X_c is positive for $\tau > 0$ or zero for $\tau = 0$, and in the expression for X, it is negative for $\tau < 0.5\ \sigma_y$ or zero for $\tau = 0.5\ \sigma_y$. This means that the maximization of the driving force in our theory leads to compatible martensite, which is correct.

Comparing X_E and X_c, we conclude that $X_E > X_c$ for $\gamma_2 > \gamma_{t2}$. The transformation shear is limited by crystallography and does not exceed 0.1–0.2. Plastic shear, according to Eq. (67) and Fig. 5, is unlimited. It can be 1 or 10 and tends to infinity when the shear stress tends to the yield stress in shear. Consequently, at relatively high shear stress $X_E > X_c$. This means that even when complete compatibility at the austenite—twinned martensite interface is possible without plasticity, the transformation with plasticity corresponds to a higher Eshelby driving force and has to occur according to the extremum principle Eq. (54). The larger the lattice incompatibility at the interface and plasticity is, the larger the driving force will be. This is an evident contradiction with reality, because it means that the elastic accommodation which is observed in SMA cannot exist according to the maximization of the Eshelby driving force.

Now let us consider the adiabatic approximation Eqs. (71)–(73) and check whether a temperature raise can change our conclusions. First, we estimate the term $\frac{\Delta s_0}{2\nu}$. For direct martensitic Δs_0 is negative. For *NiTi* $\rho\Delta s_0 = -0.46\ \frac{MJ}{m^3K}$, $\rho\nu = 2.12\ \frac{MJ}{m^3K}$ (Lagoudas and Bo, 1999) and $\frac{\Delta s_0}{2\nu} = -0.109$; for *FeNi* steel $\rho\Delta s_0 = -0.83\ \frac{MJ}{m^3K}$ (Kaufman and Cohen, 1958; Fischer et al., 1994), $\rho = 7800\ \frac{kg}{m^3}$, $\nu = 440\ \frac{Nm}{KgK}$, and $\frac{\Delta s_0}{2\nu} = -0.120$, and for *CuZnAl* SMA $\frac{\Delta s_0}{2\nu}$ has the same order of magnitude.

Then the first two terms in expression (72) for X are negative at any τ, and the first term in expression (73) for X_c is positive for $\tau > 0$ or zero for $\tau = 0$. Consequently $X_c > X$, the same as for an isothermal process.

Comparing X_E and X_c, we obtain the same result as for the isothermal process at $\frac{\Delta s_0}{2\nu} > -1$, which is the case for SMA. That is $X_E > X_c$ for $\gamma_2 > \gamma_{t2}$, and we have the same contradiction as in the isothermal case.

The same solution can be applied for the appearance of a new nucleus in the shape of a thin infinitesimally long layer, provided that the finite surface energy of the nucleus is added. At the deformation of a plastic material, the shear stress is equal to the yield stress in shear at the slip planes, both for single crystal and polycrystal obeying he Tresca yield condition. Then for the martensitic nucleus oriented along the slip plane, the Eshelby driving force tends to infinity (despite that the temperature tends to infinity as well). Thus, PT has to always occur at the beginning of plastic flow, independent of temperature.

Now it has to be clear why the consideration of adiabatic heating is important: for $\frac{\Delta s_0}{2\nu} < -1$ the first term in Eshelby driving force is negative, and the above contradictions do not exist. However, this is not the case. As a contradiction in the application of the Eshelby driving force is found for two limit cases, namely for isothermal and adiabatic processes, it has to exist for any intermediate case.

4. Concluding remarks

Let us discuss the details which are neglected in our model problem. The first limitation is related to a finite length of the transforming layer, which due to the elastic constraint of the parent phase limits the plastic shear strain. Plastic shear definitely cannot be infinite; however, it can be very high, namely 1–10 like on slip surfaces and micro shear bands.

Allowing for elastic strains and a change in the elastic modulus does not change the main conclusion. The variation of the yield stress due to hardening and PT is also not critical provided it is smaller than the yield stress of the parent phase.

For the reverse PT, $\Delta s_0 > 0$, and we have to check whether the second term in our driving force Eq. (72) is smaller than the first term in Eq. (73). Otherwise, $X > X_c$ and our approach has the same contradiction as the approach based on the Eshelby driving force. However, for SMA, the yield stress of martensite is smaller than the yield stress of austenite, i.e. our solution is not applicable, and large plastic strain cannot be reached. Even if we assume that it is applicable, then in contrast to the first term in Eq. (71), the term $\tau\gamma$ has a multiplyer of order 0.1. Allowing for the heat conduction may reduce this term by a factor of order 2, as well. So, it is very unprobable that $X > X_c$ for the reverse PT in SMA.

Moreover, as at direct PT a multivariant compatible multilayer martensite is formed, there is not any incompatibility if it returns strictly back during the reverse PT to austenite. Then plastic shear does not appear in Eq. (72). If, hypothetically, only one of the martensitic variant in each second layer undergoes the reverse PT, then incompatibility does exists. However, the above solution cannot be applied, because each second nontransforming layer constrains plastic flow and decreases γ significantly.

For the reverse martensite to austenite PT in steel (if it can be done fast enough to avoid alternative reactions), the yield stress decreases during the PT. Then the shear stress can be equal to the yield stress, and a very high driving force X according to Eqs. (67) and (72) is possible. Even if $X > X_c$, this is not a contradiction with reality, because for PT in steel, a huge plastic deformation is observed. The problem is that at very large plastic shear and consequently driving force X, the reverse PT has to start at the very beginning of the plastic deformation. However, plastic accommodation at direct PT creates a very heterogeneous defect structure and stress field, and our solution for the homogeneous stress and strain field in the infinite layer cannot be applied. For the case when shear localization may occur at $\Delta s_0 > 0$, the second term in X may in fact be a strong contribution (see similar analysis for strain-induced chemical reactions in Levitas et al., 1998a,b).

In the papers by Fischer et al. (1994), Marketz and Fischer (1994a,b), Fischer and Reisner (1998), Cherkaoui et al. (1998), and Cherkaoui and Berveiller (2000), $\boldsymbol{\varepsilon}_t$ represents a habit-plane variant or an invariant plane strain (rather than transformation (Bain) strain in our approach), and various habit-plane variants are compared in the extremum principle Eq. (54). As an invariant plane strain does not produce incompatibility, the above contradiction does not exist. Consequently, in the framework considered in the above papers, their results are self-consistent.

However, here we consider the more general problem formulation when the Bain strain is given and invariant plane strain has to be found. Such a formulation is used particularly in the crystallographic (Wayman, 1964; Christian, 1965) and mathematical theory of PT in elastic materials (Ball and James, 1992; Bhattacharyya and Kohn (1996)). Such a formulation is also the only reasonable one if we would like to study which mode of lattice invariant shear—slip or twinning—occurs. As it was shown, at such a more general problem formulation we do have a contradiction in application of Eshelby driving force for plastic materials.

Even when transformation strain represents invariant plane strain, but the stress–strain state in the transforming region is highly heterogeneous, large plastic strain can occur inside the transforming region (Idesman et al., 2000, Levitas et al., 2002). Our finite element solution for the martensitic plate growth in an austenitic matrix exhibits the following. Due to a very complex interaction between plastic and transformation strains due to previous and current transformation events, the accumulated plastic strain reaches 0.6 in some martensitic regions (despite the 3 times higher yield stress of martensite than of the austenite). If we add the corresponding plastic work to the driving force X, it will grow drastically during the plate growth. Instead of growth arrest due to plastic deformation, which is observed experimentally and can be described when X is used as the driving force, growth acceleration due to the accommodation plastic strain follows from the consideration based on the Eshelby driving force.

Summarizing, we can conclude that an approach based on the application of the Eshelby driving force for PT in plastic materials for the general problem formulation is conceptually contradictory. The reason for the contradiction is related to the fact that the Eshelby driving force includes plastic dissipation in addition to dissipation due to PT. Due to TRIP phenomenon inside the transforming region, plastic dissipation may be very significant. Maximization of the Eshelby driving force requires as much plasticity as possible. If it would be the case in reality, this could be easily achieved by choosing a combination of martensitic variants with maximum incompatibility across the interface. However, this would mean that elastic (or even stress-free) accommodation observed in SMA cannot exist, as well as the shape memory effect itself. The crystallographic theory of martensite, which is based on the zero incompatibility of the resulting transformation strain at the interface, would not be valid either. Our approach at least does not have any such contradictions.

Note that a similar driving force for some other structural changes (e.g. fracture and chemical reactions) in inelastic materials, based on the dissipation increment due to structural change only, was developed and used in Levitas (2000).

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