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A nanoscale model of the transformation-induced plasticity

In this paper a nanoscale model of the transformation-induced plasticity in a single crystal is introduced. Scale of averaging of physical phenomena is considered between 10^{-9} m and 10^{-8} m. Then, single martensite variants and interfaces are distinguished in description of the martensitic transformation. Furthermore, single slip surfaces are introduced for the description of plasticity. Modelling of these phenomena in such a small scale allows taking into account precise interactions between them. The central part of the discussed model is the free energy. Form of this function is introduced by means of a set of geometrical objects distinguished within the crystal structure. Conditions for slip initiation and martensitic transformation are defined with the aid of free energy. Qualitative role of shuffles in the transformation-induced plasticity is discussed.

1. Introduction

Inelastic behaviour of materials is usually connected with complex physical phenomena, frequently involved in the atomic scale. Modelling behaviour of such materials can be realized by means of phenomenological assumptions in an averaged way. On the other hand we could try to describe some distinguished elementary processes responsible for the inelastic deformation. This leads to complicated models with considerable number of variables and complex form of constitutive equations. Such models are characterized by a small scale of averaging.

State of theory describing the transformation-induced plasticity could be recognized with the aid of papers [1-7]. Dominant approach is related to a larger scale of averaging characterized by volume fraction of martensite as a variable. Description of evolution of this variable is frequently supported by methods of micromechanics.

In this paper we tend towards modelling the most elementary mechanisms related to the transformation-induced plasticity. Let us notice that motion of an interface separating various martensite variants is associated with transformation of one martensite variant into another. Then, the slip systems are also

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transformed. Therefore, in order to describe elementary mechanisms related to discussed phenomena, single martensite variants and single slip surfaces should be distinguished in the framework of the model. Furthermore, modelling of interactions between martensitic transformation and slips needs option of common scale appropriate for both phenomena described separately.

Let us note that usual crystal plasticity is related to a scale about of 10^{-6} m. Then, the deformation induced by slips on various slip surfaces can be viewed as approximately homogeneous and the gradient of deformation associated with plastic slips is applied in description [9, 10, 11, 8].

Elementary units which define martensite variants have sometimes eighteen atomic layers [12]. In the case of CuAl alloy, considered in the paper, there are nine atomic layers [13]. As a result, lower bound related to the linear size of averaging has to exceed distance defining the martensite unit. On the other hand distances between single slip surfaces are of the order of 10^{-8} m [8]. Accordingly, linear size related to volume of averaging connected with the model discussed should fall between 10^{-9} m and 10^{-8} m. This justifies the nanoscale model name.

The aim of this paper is to provide a nanoscale model of the transformation induced plasticity in a single crystal for which interactions between systems of separate martensite variants and slips on distinguished slip surfaces are considered.

The small scale model of the martensitic transformation which consider separate martensite variants has already been discussed in [19]. A model of plasticity with distinguished slip surfaces has been considered in [15]. In this paper a modification of discussed models is carried out in order to join them into one description of the transformation-induced plasticity.

2. Kinematical considerations

Nanoscale modelling induces a kind of kinematics which is convenient for description of single martensite variants, evolution of interfaces as well as displacements on the slip surfaces.

The dominant feature which characterizes the martensitic transformation is a shear strain [16]. Martensitic transformation is initiated when a corresponding critical shear stress is exceeded. In order to distinguish the characteristic shear strain, we introduce here shear systems in the austenitic state of material. The I-th shear system is represented by a pair of orthonormal vectors $\mathbf{d}_{I\alpha}$, $\alpha = 1, 2$, $I \in I_{SH}$. The set I_{SH} consists of indexes which determine all distinguished shear systems related to all variants of martensite.

We denote by E the set of all Lagrangean strain tensors $\mathbf{e}$ expressed in a given base $\mathbf{b} = \{\mathbf{b}_1,\ \mathbf{b}_2,\ \mathbf{b}_3\}$. Measure of the shear strain in I-th shear system is given by

$$e_{I12} = \mathbf{d}_{I1}\mathbf{e}\mathbf{d}_{I2}\ . \tag{1}$$

Let us notice that a critical parameter for initiation of slip is also a shear strain. Therefore, we introduce additionally the slip systems determined by a pair of unit and orthogonal vectors $\{\mathbf{m}_\alpha,\ \mathbf{n}_\alpha\}$, $\alpha \in I_{SL}$. Then, the shear strain related to the slip system is given by

$$e_{\alpha mn} = \mathbf{m}_\alpha \mathbf{e} \mathbf{n}_\alpha\ . \tag{2}$$

Difference between the shear system and the slip system rests on interpretation of phenomena after exceeding the critical strain. The martensite appears in I-th shear systems after exceeding a critical shear strain e^*_{I12} and the strain e_{I12} is further developed. The strain $e_{\alpha mn}$ is determined in an elastic region only. After exceeding a critical strain of this kind, the situation changes qualitatively since the slip appears. Slip on a slip surface is connected with displacements defined on a discontinuity surface. This is entirely different kind of deformation measure. Then, the measure of strain $e_{\alpha mn}$ is not interpreted in the slip system $\{\mathbf{m}_\alpha,\ \mathbf{n}_\alpha\}$ if exceeds the elastic region of austenite.

Summing up these considerations, we see that the Lagrangean strain tensor is a convenient deformation measure in elastic domain of austenite. Then, we are able to express characteristic strains corresponding to initiation of the martensitic transformation or plastic slip. Elastic domain for austenite is expressed as a subset $A \subset E$ and is characterized by property that boundary ∂A determines conditions for initiation of the inelastic phenomena. Furthermore, we introduce elastic domains of martensite $M_K \subset E$ in a similar way as A, and the spinodal region $S \subset E$ placed between elastic regions.

The tensor $\mathbf{e}$ is not considered as a full measure of deformation associated with the martensitic transformation. Next components have to be adjoined. In order to justify this point of view let us consider the behaviour of CuAl alloy structure during the martensitic transformation. This alloy has representative properties corresponding to a large class of shape memory alloys. In particular, it is shown that shuffles [17, 16] which are small and usually are neglected, have a qualitative meaning in the description of TRIP.

The martensitic transformation in CuAl alloy is realized in three stages [18]. Extension along the Bain axis allows attaining the Bain strain which gives conditions for activation of micro nonhomogeneous shear. The shear occurs on one of four base planes and is connected with nonhomogeneous shifts of atoms from positions predicted by $\mathbf{e}$. We obtain then four kinds of structures. Each of them can, subsequently, rotate towards two possible habit planes. Thus, the Bain strain, micrononhomogeneous shear and internal rotation create three stages realized within each shear system.

Directions of micro nonhomogeneous shear for this structure are defined by $\mathbf{d}_{I\alpha}$, where $I = (ij)$, $\alpha = 1, 2$. (ij) define plane spanned on $\mathbf{b}_i$, $\mathbf{b}_j$ in which the shear takes place. The vectors $\mathbf{d}_{I\alpha}$ are defined by the formula $\mathbf{d}_{(ij)\alpha} = \frac{\sqrt{2}}{2}(\mathbf{b}_i + (-1)^\alpha \mathbf{b}_j)$.

We have introduced a system of multiindices associated with stages of development of the martensitic transformation. The first one is $I = (ij)$, next ones are $J = (I, \alpha)$ related to directions of micro nonhomogeneous shear and $K = (J, \beta) = (I, \alpha, \beta)$ related to internal rotations. I is defined by $i, j = 1, 2, 3$ $i \neq j$, $\alpha, \beta = 1, 2$. The set I_K contains all multiindices K which define all martensite variants [19].

Two different micro nonhomogeneous shears in the same shear system have the same strain expressed by the strain tensor. They differ by small displacements of atoms called shuffles. Shuffles are associated with a complex crystal lattice. Discussed here CuAl alloy has a complex crystal lattice. This gives an opportunity for using a description characteristic for a multicomponent body and to obtain by this shuffles.

Modelling of multicomponent body requires several deformation functions. In our case these functions are associated with sub-lattices. Thus, let $\mathbf{x}$, $\mathbf{y}_\lambda$, $\lambda \in \Lambda$ be the deformation functions accompanied by separate sub-lattices. They are related by the formula

$$\mathbf{y}_\lambda = \mathbf{x} + \boldsymbol{\xi}_\lambda , \tag{3}$$

where $\mathbf{x}$ corresponds to a specific sub-lattice and $\boldsymbol{\xi}_\lambda$ are relative displacement vectors considered as independent variables.

Shuffles accompanied by micro nonhomogeneous shear are observed to appear in $\mathbf{d}_{I1}$ or $\mathbf{d}_{I2}$ direction in the I-th shear system. The vectors $\mathbf{d}_{I1}$, $\mathbf{d}_{I2}$ can also be considered as material directors which deform as $\mathbf{d}'_{I\alpha} = \mathbf{F}\mathbf{d}_{I\alpha}$ for $\alpha = 1, 2$, where $\mathbf{F}$ is the gradient of deformation related to $\mathbf{x}$. We assume that $\boldsymbol{\xi}_\lambda = w_\lambda \mathbf{d}'_{I1}$ or $\boldsymbol{\xi}_\lambda = w_\lambda \mathbf{d}'_{I2}$. Then, for instance for $\alpha = 1$, we obtain $\boldsymbol{\xi}_\lambda = w_\lambda \mathbf{F}\mathbf{d}_{I1}$. Putting $\mathbf{w}_\lambda = w_\lambda \mathbf{d}_{I1}$ we have $\boldsymbol{\xi}_\lambda = \mathbf{F}\mathbf{w}_\lambda$.

The gradient of deformation transforms orthonormal vectors $\mathbf{d}_{I\alpha}$ into $\mathbf{d}'_{I\alpha}$ which are usually not orthonormal. In some cases, it is convenient to assume approximately that $\mathbf{d}'_\alpha = \mathbf{R}\mathbf{d}_{I\alpha}$, where $\mathbf{R}$ is a rotation tensor which appears in the polar decomposition $\mathbf{F} = \mathbf{V}\mathbf{R}$ [23]. Taking into consideration (3), we can also write that $\mathbf{y}_\lambda = \mathbf{x} + \mathbf{F}\mathbf{w}_\lambda \approx \mathbf{x} + \mathbf{R}\mathbf{w}_\lambda$. Let us notice that the approximation $\mathbf{F}\mathbf{w}_\lambda \approx \mathbf{R}\mathbf{w}_\lambda$ is not a constraint imposed on the gradient of deformation but on the relative displacement vector $\boldsymbol{\xi}_\lambda$.

Finally, we have introduced components of deformation measure represented by vectors $\mathbf{w}_\lambda$ which describe shuffles related to micro nonhomogeneous shear. Then, we use one deformation function $\mathbf{x}$ only and $\mathbf{w}_\lambda$.

Next components of deformation measure are related to rotation towards the habit plane. This rotation is caused by forces in the material, which act in order to fit together the austenite and creating martensite variant. The habit plane is a plane where the mentioned structures are fitted together and which is undeformed. We may say that the austenite attracts a creating martensite variant until this variant takes appropriate, energetically most advantageous position in the crystal. This attraction is accompanied by two habit planes related to determined hitherto two first stages of martensitic transformation in CuAl structure. Thus, a bifurcation process related to the internal rotation has to be modelled.

Special variables $\mathbf{a}_\beta$, $\beta = 1, 2$ based on material directors, are introduced in order to describe internal rotations. Let $\mathbf{p}_1$ and $\mathbf{p}_2$ be a pair of material directors which lie on a habit plane. They are transforming as $\mathbf{p}'_\beta = \mathbf{F}\mathbf{p}_\beta$, $\beta = 1,2$ in accordance with acting of the gradient of deformation.

Considered variables are defined by means of expression

$$\mathbf{a}_\beta = \mathbf{R}^{-1}(\mathbf{F} - \mathbf{R})\mathbf{p}_\beta = (\mathbf{R}^{-1}\mathbf{F} - \mathbf{1})\mathbf{p}_\beta\,, \tag{4}$$

where $\mathbf{R}$ is an external rotation.

Internal rotation is introduced as a part of $\mathbf{F}$. The gradient of deformation can be expressed as $\mathbf{F} = \mathbf{F}^{em}\mathbf{F}^s\mathbf{F}^{ea}$, where $\mathbf{F}^{ea}$ corresponds to attaining ∂A, $\mathbf{F}^s$ and $\mathbf{F}^{em}$ are realized in the spinodal region and in domain of elastic martensite correspondingly. Let $\mathbf{F}^{ea} = \mathbf{V}\mathbf{R}$ and $\mathbf{F}^s = \mathbf{R}^s\mathbf{U}^s$. If deformation is in S domain then $\mathbf{a}_\beta$ is expressed as

$$\mathbf{a}_\beta = \mathbf{R}^{-1}(\mathbf{R}^s\mathbf{U}^s\mathbf{V}\mathbf{R} - \mathbf{R})\mathbf{p}_\beta\,. \tag{5}$$

It is assumed that the internal rotation $\mathbf{R}^I$ is identified with $\mathbf{R}^s$. It means that this rotation appears in the S domain only. However, precise definition of internal rotation is possible if we know the form of free energy exactly.

Let us note that the definition of variables $\mathbf{a}_\beta$ depends on the selection of vectors $\mathbf{p}_\beta$. In the simplified case it is possible to take into account one director lying on the rotation axis of the martensitic structure. This axis can be approximately considered as unchanged with respect to austenite. In this case, behaviour of the second director describes rotation and hence the number of variables is reduced.

Kinematics introduced above is in accordance with the well known in material sciences, WLR theory [20]. Theory which considers separate martensite variants is also discussed in mechanics in [21, 22].

Shuffles introduced by means of the relative displacement vectors are usually neglected as small in description of the martensitic transformation. However, they have qualitative meaning in description of TRIP. Firstly, they undergo bifurcation $\mathbf{w} \to \mathbf{w}'$ or $\mathbf{w} \to \mathbf{w}''$. Secondly, positions of habit planes depend on kind of $\mathbf{w}$ developed. Thus, we have two possible habit planes after the bifurcation for structure determined by $\{e_{I12},\ \mathbf{w}'\}$ and two other habit planes for $\{e_{I12},\ \mathbf{w}''\}$. It means that the internal rotation $\mathbf{R}^I$ depends on $\mathbf{w}_\lambda$. In particular, slip systems defined in martensitic structure depend on $\mathbf{R}^I$ and finally on $\mathbf{w}_\lambda$. This induces qualitative role of shuffles for TRIP.

We assume for simplicity that $\mathbf{w}_\lambda$ and internal rotation $\mathbf{R}^I$ are developed in the spinodal region S. After exceeding some critical shear strain in austenite, the deformation is continued through S and finally the elastic domain M_K of martensite is attained. We assume general form of decomposition of domain of the free energy into disjoint sets as $D = A \cup S \cup \bigcup_K M_K \subset E$, where A stands for elastic domain for austenite, M_K is elastic domain for K-th martensite variant and S is the spinodal region. They will be defined more precisely in the next section.

The set S plays a special role. Its boundary ∂S determines critical conditions for initiation of martensitic transformation or slip. Thus, we distinguish some subsets $\partial S = \partial S_A \cup \bigcup_K \partial S_K$, where $\partial S_A = \partial A$, $\partial S_K = \partial M_K$. Furthermore, ∂S_A consists of the following parts

$$\partial S_A = \bigcup_I \partial S_I \cup \bigcup_\alpha \partial S_\alpha \,, \tag{6}$$

∂S_I is a criterion for initiation of martensitic transformation in I-th shear system and ∂S_α is responsible for initiation of slip in the α-th slip system. Similarly, we introduce also a partition

$$\partial S_K = \bigcup_{K'} \partial S_{KK'} \cup \partial S_{KA} \cup \bigcup_\beta \partial S_{K\beta} \,, \tag{7}$$

where $\partial S_{KK'}$ determines conditions for initiation of transformation of K-th into K'-th martensite variant, ∂S_{KA} determines initiation of K-th martensite variant into austenite and $\partial S_{K\beta}$ initiation of slip in β-slip system determined in K-th martensite variant.

At this moment we consider also additional elastic regions M_K. As a result we have to define slip systems and critical strains for slip initiation in this part of domain.

Let $\mathbf{e}_K = \frac{1}{2}(\mathbf{F}_K^T\mathbf{F}_K - \mathbf{1})$ stand for the strain tensor corresponding to equilibrium of K-th variant of martensite. The strain tensor $\mathbf{e}$ is defined with respect to undeformed austenite configuration. Slip systems in K-th martensite variant corresponds to strains $\tilde{\mathbf{e}}_K = \frac{1}{2}(\tilde{\mathbf{F}}_K^T\tilde{\mathbf{F}}_K - \mathbf{1})$ defined with respect to undeformed martensite. On the other hand we would like to consider common strain measure $\mathbf{e}$ on the whole domain. Let

$$\begin{aligned}\mathbf{e} &= \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{1}) = \frac{1}{2}(\mathbf{F}_K^T\tilde{\mathbf{F}}_K^T\tilde{\mathbf{F}}_K\mathbf{F}_K - \mathbf{1}) = \\ &= \mathbf{F}_K^T\frac{1}{2}(\tilde{\mathbf{F}}_K^T\tilde{\mathbf{F}}_K - \mathbf{1})\mathbf{F}_K + \frac{1}{2}(\mathbf{F}_K^T\mathbf{F}_K - \mathbf{1}) = \mathbf{F}_K^T\tilde{\mathbf{e}}_K\mathbf{F}_K + \mathbf{e}_K \,.\end{aligned} \tag{8}$$

Consequently,

$$\tilde{\mathbf{e}}_K = (\mathbf{F}_K^T)^{-1}(\mathbf{e} - \mathbf{e}_K)\mathbf{F}_K^{-1} \tag{9}$$

expresses $\tilde{\mathbf{e}}_K$ with the help of known $\mathbf{e}_K$ and varying $\mathbf{e}$ referred to equilibrium state of austenite.

Let $\{\mathbf{m}_{K\beta},\ \mathbf{n}_{K\beta}\}$, $\beta \in I_{SLK}$ represents set of slip systems defined in M_K. With the help of (9) we define shear strain in the β-th slip system as

$$e_{K\beta mn} = \mathbf{m}_{K\beta}((\mathbf{F}_K^T)^{-1}(\mathbf{e} - \mathbf{e}_K)\mathbf{F}_K^{-1})\mathbf{n}_{K\beta} \,. \tag{10}$$

Thus, we are able to define the critical strain condition for initiation of slip by means of (10) which is expressed with the help of strain tensor $\mathbf{e}$ considered with respect to undeformed austenite. Then, $\partial S_{K\beta}$ can be determined.

Transformation of K-th martensite variant into K'-th one is connected with several shear systems. Therefore $\partial S_{KK'}$ cannot be expressed with the help of one shear system. As a result, a more general situation should be considered. Let us notice that shear system generate a one-dimensional path parameterized by e_{I12} in E. We could generalize this fact into more general one dimensional path.

Let $G(K, K') \subset E$ be discussed path which join equilibrium states of K-th and K'-th martensite variants. Then, the critical condition related to $\partial S_{KK'}$ would be defined by means of $G(K, K')$. This will be discussed in the next section in more detail.

Kinematics related to slip has different character. Measure of slip is connected with discontinuity of deformation function χ on the slip surface within this model.

The slip surface $\mathcal{S}$ consists of two material surfaces $\mathcal{S}^+$, $\mathcal{S}^-$ of two parts of the body which are in contact on $\mathcal{S}$. Consequently, two deformation functions χ^+ and χ^-related to parts of the body on the "+" and on the "−" sides of $\mathcal{S}$ are considered.

Let us introduce a point $\mathbf{x}_{\mathcal{S}}^-(t) = \chi^-(\mathbf{X}^-,\ t) \in \mathcal{S}^-$ for which displacements related to slip will be discussed. With the help of the introduced relation we obtain $\mathbf{X}^- = (\chi_t^-)^{-1}(\mathbf{x}_{\mathcal{S}}^-)$. We assume that the reference configuration is chosen in order to fulfill the condition $\chi^+(\mathbf{X}^-, t) = \chi^-(\mathbf{X}^-, t)$. Then, the slip displacement is defined as

$$\mathbf{u}_{\mathcal{S}}(\mathbf{x}_{\mathcal{S}}^-(t+s)) = \chi^+(\mathbf{X}^-,\ t+s) - \chi^-(\mathbf{X}^-,\ t+s)\,. \tag{11}$$

Above introduced assumptions follow that $\mathbf{u}_{\mathcal{S}}(\mathbf{x}_{\mathcal{S}}^-(t)) = 0$. Let us note also that

$$d\mathbf{u}_{\mathcal{S}} = \chi^+(\mathbf{X}^-,\ t+ds) - \chi^-(\mathbf{X}^-,\ t+ds) =$$

$$= \frac{\partial \chi^+}{dt}ds - \frac{\partial \chi^-}{dt}ds = (\mathbf{v}^+(\mathbf{X}^-,\ t) - \mathbf{v}^-(\mathbf{X}^-,\ t))ds\,. \tag{12}$$

Consequently, we have

$$\frac{d\mathbf{u}_{\mathcal{S}}}{dt} = \mathbf{v}^+(\mathbf{X}^-,\ t) - \mathbf{v}^-(\mathbf{X}^-,\ t) = \mathbf{s}(\mathbf{x}_{\mathcal{S}})\,. \tag{13}$$

Thus, $\mathbf{s}(\mathbf{x}_{\mathcal{S}})$ stands for the velocity of slip in the point $\mathbf{x}_{\mathcal{S}}$.

3. Free energy

Presented in the paper model of the transformation-induced plasticity is characterized by possible existence of slip surfaces $\mathcal{S}$. Discontinuity of deformation function is the main feature of these surfaces. The three dimensional Lebesque measure $\mu(\bigcup_{\mathcal{B}}(\mathcal{S}))$ of all surfaces in $\mathcal{B}$ is equal to zero. It means that almost whole body is considered as a material, in which no slips occur. Then, the physical role of slips is transmitted to parts of the body without any slips, by surface conditions as a kind of the boundary conditions. Such a situation brings about the treatment of description of the martensitic transformation as of the first rank. Slips are viewed to be higher stadium of deformation. Then, for this small scale approach, the free energy F has to comprise conditions for which slips are initiated.

Role of defects and dislocations are taken into considerations in the free energy in an averaged form by appropriate densities considered as internal state variables. They can affect realization of slip process. Consequently, the whole approach to TRIP is concentrated around the free energy formulation.

The free energy function related to discussed small scale of averaging will be introduced with the help of the following program:

1. The skeleton of the free energy is based on geometrical objects distinguished in the crystal structure of austenite and martensite.

   Geometrical objects related to the structure of austenite are:
   – Bain axes,
   – six different base planes in undeformed state of austenite,
   – twenty four habit planes,
   – directions of micro nonhomogeneous shear which define a set of shear systems,
   – a set of slip systems.

   Geometrical objects related to the structure of martensite are:
   – slip systems,
   – paths of martensite-martensite transformation, habit and twin type interfaces.

2. It is assumed that elastic properties of austenite and martensite are known. The free energy is defined in the neighbourhood of equilibrium of austenite and martensite as a positive definite quadratic form with appropriate symmetry properties.

3. The boundary of elastic range for austenite and martensite are given as five-dimensional hypersurfaces in the space of strain E. On these hypersurfaces the phase transformation is initiated. Determination of these surfaces is introduced with the aid of shear systems, slip systems and paths of martensite-martensite transformation.

4. The main idea of shaping of the free energy relies on the expression of the graph of free energy as a fiber bundle spanned on the geometrical skeleton introduced.

5. The first stage of construction of free energy consists in defining its part which depends mainly on the strain tensor.

6. The second stage is connected with introducing relative displacement vectors in order to describe evolution of shuffles.

7. The third stage consists in taking into account internal rotations towards possible habit planes.
8. The last stage consists in introducing higher gradients of deformation based on hierarchy of distinguished directions in the crystal structure.
9. Dependence of free energy on temperature and densities of inhomogeneities is introduced by plotting separate elements which define graph of free energy with these variables.

We have discussed miscellaneous components of the deformation measure. The Lagrangean strain tensor $\mathbf{e}$ is the main part of it. This measure is considered within domain divided on parts $E = A \cup S \cup \bigcup_K M_K$.

Let

$$F_{ijkl}(\mathbf{e}) = \frac{\partial^2 F}{\partial e_{ij} \partial e_{kl}}(\mathbf{e}).$$

We define domain of elastic austenite as

$$A = \{\mathbf{e} : \ F_{ijkl}(\mathbf{e}) > 0, \ l(\mathbf{0}, \ \mathbf{e}) \subset A\} , \tag{14}$$

where $F_{ijkl}(\mathbf{e}) > 0$ means that the matrix F_{ijkl} represents a positive definite quadratic form and $l(\mathbf{0}, \ \mathbf{e})$ stands for segment with ends $\mathbf{0}$ and $\mathbf{e}$.

The domain of elastic martensite M_K is defined as

$$M_K = \{\mathbf{e} : \ F_{ijkl}(\mathbf{e}) > 0, \ l(\mathbf{e}_K, \ \mathbf{e}) \subset M_K\} , \tag{15}$$

where $\mathbf{e}_K$ is the strain tensor corresponding to equilibrium martensite. Accordingly, the set S is related to non-positive definite quadratic form F_{ijkl}.

The starting point for determination of the free energy on the domain A is the positive definite function

$$\bar{F}_A = c_{ijkl} e_{ij} e_{kl} \ . \tag{16}$$

This function describes elastic properties of austenite in the neighbourhood U_A of $\mathbf{0} \in E, U_A \subset intA$. Function of this kind cannot be valid on the whole domain A since the quadratic form represented by $\bar{F}_{ijkl}$ has to be semipositive definite on $\partial A = \partial S_A$. It follows that $\bar{F}_A$ should be modified on the domain $A - U_A$ in order to change continuously its properties.

Thus, we have shown that there exists necessity of defining ∂S_A in the first place, as an important element of the geometrical skeleton of free energy constructed.

Let us introduce the set of hypersurfaces $\mathcal{P}_I \subset E$ defined by the following formula

$$\mathcal{P}_I = \{\mathbf{e} : \frac{\partial}{\partial e_{I12}} (\mathbf{d}_{I1} \frac{\partial F}{\partial \mathbf{e}} \mathbf{d}_{I2}) = 0\} \tag{17}$$

and $\mathcal{P}_\alpha \subset E$ defined by

$$\mathcal{P}_\alpha = \{\mathbf{e} : \frac{\partial}{\partial e_{\alpha mn}}(\mathbf{m}_\alpha \frac{\partial F}{\partial \mathbf{e}} \mathbf{n}_\alpha) = 0\} \,. \tag{18}$$

We define the set

$$L_c = \{\mathbf{e} : \mathbf{e}_B = \{e_{Bij}\} = \{p\delta_{ij}\},\ \mathbf{e} = k\mathbf{e}_B,\ k \in R,\ p \neq 0\}\,, \tag{19}$$

where p is a constant.

We assume that $\mathcal{P}_I \cap L_c = \emptyset$, $\mathcal{P}_\alpha \cap L_c = \emptyset$ for each I and α. Formulas (17) and (18) define the set of conditions imposed on the free energy. In general we assume that the form of $\mathcal{P}_I$ and $\mathcal{P}_\alpha$ is known or postulated. Let us also introduce the set

$$\mathcal{P}_A = \bigcup_I \mathcal{P}_I \cup \bigcup_\alpha \mathcal{P}_\alpha.$$

Let

$$\mathbf{e}_D \in E \text{ and } ||\mathbf{e}_D||_E = 1$$

determine a direction in the space E. Let us also define the set

$$[\mathbf{e}_D] = \{\mathbf{e} : \mathbf{e} = a\mathbf{e}_D,\ a \in R_+\}.$$

The set of all $[\mathbf{e}_D]$ is denoted by K_D. With the help of above defined sets we introduce functions

$$\alpha_a : [\mathbf{e}_D] \to R_+$$

defined by

$$\alpha_a(\mathbf{e}) = a,\quad \mathbf{e} \in [\mathbf{e}_D],\quad \mathbf{e} = a\mathbf{e}_D$$

and $a_A : K_D \to R_+$ defined with the help of the formula

$$a_A([\mathbf{e}_D]) = \inf_a \{\alpha_a([\mathbf{e}_D] \cap \mathcal{P}_A)\}\,. \tag{20}$$

By means of the last function we define ∂S_A as

$$\partial S_A = \{\mathbf{e} : \mathbf{e} = a\mathbf{e}_D,\ a = a_A([\mathbf{e}_D]),\ ||\mathbf{e}_D|| = 1\}\,. \tag{21}$$

Consequently, the remaining sets distinguished in the framework of ∂S_A are defined as follows

$$\partial S_I = \partial S_A \cap \mathcal{P}_I,\quad \partial S_\alpha = \partial S_A \cap \mathcal{P}_\alpha\,. \tag{22}$$

We assume furthermore that there is an accordance between definition of the slip system and postulated ∂S_α. This accordance is expressed by the fact that ∂S_α are defined exactly by slip systems $\{\mathbf{m}_\alpha,\ \mathbf{n}_\alpha\}$ which are present in (18). Similar remark is valid for shear systems and ∂S_I.

Form of the free energy corresponding to discussed here martensitic transformation is introduced usually by means of polynomial expansion [24]. In this paper we try to concentrate on characteristic features of this function, responsible for important physical effects. This is done by means of introduced geometrical skeleton. The set ∂S_A, for instance, is an element of this skeleton which expresses physically important aspect of initiation of transformation. Therefore, ∂S_A should be postulated. Then, approach which uses polynomial expansions should approximate precisely form of ∂S_A. This leads usually to very high degree of these polynomials. In order to escape this difficulty we use fiber bundles as a generalization of the Cartesian product [25]. Consequently, the graph of free energy is considered as a fiber bundle spanned on the geometrical skeleton. We discuss one coordinate representation. Then, the structural group consists of one element only.

First we will express the domain A as a fiber bundle. Let $A_I : E \to E_I$ be mapping which transforms the strain tensor $\mathbf{e}$ in a given basis $\mathbf{b}$ into the strain tensor $\mathbf{e}_I$ expressed in the basis

$$\mathbf{d}_I = \{\mathbf{d}_{I\alpha},\ \mathbf{d}_{I1} \times \mathbf{d}_{I2}\}$$

and $A_\alpha : E \to E_\alpha$ transforms the strain tensors into $\mathbf{e}_\alpha$ expressed in the basis

$$\{\mathbf{m}_\alpha,\ \mathbf{n}_\alpha,\ \mathbf{m}_\alpha \times \mathbf{n}_\alpha\}.$$

Let us introduce sets

$$N_{IA} = \{\mathbf{e} : 0 \le e_{I12} \le e^*_{I12},\ e_{Ikl} = 0\},$$

$$N_{IS} = \{\mathbf{e} : e^*_{I12} \le e_{I12} \le e^{**}_{I12},\ e_{Ikl} = 0\},$$

$$N_{IM} = \{\mathbf{e} : e^{**}_{I12} \le e_{I12} \le e_{K12},\ e_{Ikl} = 0\},$$

$$N_I = N_{IA} \cup N_{IS} \cup N_{IM}.$$

We introduce also the set

$$N_\alpha = \{\mathbf{e} :\ 0 \le e_{\alpha mn} \le e^*_{\alpha mn},\ e_{\alpha ij} = 0\}.$$

as a result we define

$$\mathbf{e}^*_I = A_I(N_I \cap \partial S_A),$$

$$\mathbf{e}^{**}_I = A_I(N_I \cap \partial S_K),$$

$$\mathbf{e}^*_\alpha = A_\alpha(N_\alpha \cap \partial S_A).$$

Let

$$h_{AI}(e_{I12}) :\ \partial S_A \to f(e_{I12}),\quad e_{I12} \in T_{IAo} = \{e_{I12} :\ 0 \le e_{I12} \le e^*_{I12}\}$$

be a family of homeomorphisms. The set

$$\bigcup_{e_{I12} \in T_{IAo}} f(e_{I12}) \cup \{\mathbf{0}\} = A$$

represents decomposition of the domain A, and the following condition is satisfied

$$f(e'_{I12}) \cap f(e''_{I12}) = \emptyset \text{ for } e'_{I12} \neq e''_{I12} \in T_{IAo}.$$

Then, $N_o = N_{IA} - \{\mathbf{0}\}$ can be viewed as a basis of the fiber bundle and $f(e_{I12})$ are viewed to be fibers. Finally, the domain

$$A = \bigcup_{e_{I12} \in T_{IAo}} f(e_{I12}) \cup \{\mathbf{0}\} = N_o \times \partial S_A \cup \{\mathbf{0}\}$$

is expressed as the fiber bundle or generalized Cartesian product of N_o and ∂S_A.

The graph of the function F is considered in the space $E \times R$. Let us introduce the following sets in this space

$$\bar{B}_{IA} = \{\bar{b}_{IA} : \bar{b}_{IA} = \{\mathbf{e},\ \bar{F}_A(\mathbf{e})\},\ \mathbf{e} \in N_{IA}\},$$

$$\bar{B}_{\alpha A} = \{\bar{b}_{\alpha A} : \bar{b}_{\alpha A} = \{\mathbf{e},\ \bar{F}_A(\mathbf{e})\},\ \mathbf{e} \in N_{\alpha A}\}$$

and

$$\bar{F}_{\partial S_A} = \{\{\mathbf{e},\ \bar{F}_A(\mathbf{e})\} : \mathbf{e} \in \partial S_A = f(e^*_{I12})\},$$

$$\bar{F}_{f(e_{I12})} = \{\{\mathbf{e},\ \bar{F}_A(\mathbf{e})\} : \mathbf{e} \in f(e_{I12})\}.$$

At this stage of considerations we express the graph of the function $\bar{F}$ as a fiber bundle. Thus, we have

$$Gr\bar{F}_A = \bigcup_{\mathbf{e} \in N_o} \bar{F}_{f(e_{I12})} = \bar{B}_{IA} \times \bar{F}_{\partial S_A} \tag{23}$$

with projection in the bundle

$$\pi(\bar{F}_{f(e_{I12})}) = \{\mathbf{e},\ \bar{F}_A(\mathbf{e})\} \in \bar{B}_{IA},$$

$$(A_I(\mathbf{e}))_{12} = e_{I12}.$$

$\bar{F}_A$ can be expressed alternatively by $Gr\bar{F}_A = \bar{B}_{\alpha A} \times \bar{F}_{\partial S_A}$ by assumption.

The function $\bar{F}_A$ expresses elastic properties of austenite for $\mathbf{e} \in U_A$ and has to be modified on $A - U_A$ in order to gradually attain appropriate properties on ∂S_A. Concept of this modification consists in adding a correction function C determined on $A - U_A$. Accordingly, the modified function F_A takes the form

$$F_A = \begin{cases} \bar{F}_A, & \mathbf{e} \in U_A \\ \bar{F}_A + C, & \mathbf{e} \in A - U_A \end{cases}. \tag{24}$$

The graph of the function C is defined as follows

$$GrC = \begin{cases} \{\mathbf{e},\ 0\}, & \mathbf{e} \in U_A,\ e_{I12} \leq \bar{e}_{I12} = A_I(N_{IA} \cap \partial U_A)_{12} \\ \{\mathbf{e},\ C_{e_{I12}}(\mathbf{e})\}, & \mathbf{e} \in f(e_{I12}),\ \bar{e}_{I12} < e_{I12} < e^*_{I12} \end{cases} . \tag{25}$$

We assume that the following conditions are fulfilled by the modified function

$$\frac{\partial^2(\bar{F}_A + C)}{\partial \mathbf{n}^2(e_{I12})}(\mathbf{e}) = 0\,,\quad \mathbf{e} \in \partial S_A \cap N_{IA}\,, \tag{26}$$

$$\frac{\partial^2(\bar{F}_A + C)}{\partial \mathbf{n}^2(e_{\alpha mn})}(\mathbf{e}) = 0\,,\quad \mathbf{e} \in \partial S_A \cap N_\alpha\,, \tag{27}$$

where $\frac{\partial^2}{\partial \mathbf{n}^2(e_{I12})}$, $\frac{\partial^2}{\partial \mathbf{n}^2(e_{\alpha mn})}$ represent differentiation in tangent to N_{IA} and N_α directions in the given point $\mathbf{e} \in \partial S_A \cap N_{IA}$ or $\mathbf{e} \in \partial S_A \cap N_\alpha$ respectively. Furthermore, F_{Aijkl} is semipositive definite on the whole ∂S_A.

Let

$$B_{IA} = \{b_{IA} :\ b_{IA} = \{\mathbf{e}, F_A(\mathbf{e})\} :\ \mathbf{e} \in N_{IA}\},$$

$$F_{f(e_{I12})} = \{\{\mathbf{e}, (\bar{F}_A + C)(\mathbf{e})\} :\ \mathbf{e} \in f(e_{I12})\},$$

$$F_{\partial S_A} = \{\{\mathbf{e}, (\bar{F}_A + C)(\mathbf{e})\} :\ \mathbf{e} \in \partial S_A\}.$$

Then, the graph of the function F_A can be expressed as

$$GrF_A = B_{IA} \times F_{\partial S_A} = \bigcup_{\mathbf{e} \in N_o} F_{f(e_{I12})}.$$

Similar construction will be carried out for free energy function determined on the domain M_K. Situation becomes more complicated since criteria of determination of ∂S_K are not so clear. We have assumed that ∂S_K is determined with the help of its general form given by (7).

We define the set L_{Kc} accompanied by isotropic part of strain of K-th martensite variant as follows

$$L_{Kc} = \{\mathbf{e} :\ \tilde{e}_{BKij} = p\delta_{ij},\ \tilde{\mathbf{e}}_K = k\tilde{\mathbf{e}}_{BK},\ p \neq 0\}\,. \tag{28}$$

Determination of $\mathcal{P}_{K\beta}$ is related to slip systems $\{\mathbf{m}_{K\beta},\ \mathbf{n}_{K\beta}\}$ introduced for K-th variant of martensite and the strain $\tilde{\mathbf{e}}_K$ defined by (9). Consequently, we introduce the following definition

$$\mathcal{P}_{K\beta} = \{\mathbf{e} :\ \frac{\partial}{\partial e_{K\beta mn}}(\mathbf{m}_\beta \frac{\partial F}{\partial \tilde{\mathbf{e}}_K}\mathbf{n}_\beta) = 0\}\,. \tag{29}$$

The hypersurface $\mathcal{P}_{KA}$ related to path connected with K-th martensite variant to austenite transformation is defined with the help of shear systems introduced for austenite as

$$\mathcal{P}_{KA} = \{\mathbf{e}:\ \frac{\partial}{\partial e_{I12}}(\mathbf{d}_{I1}(\mathbf{R}_K)\frac{\partial F}{\partial \mathbf{e}}\mathbf{d}_{I2}(\mathbf{R}_K)) = 0\}\ , \tag{30}$$

where $\mathbf{R}_K$ is internal rotation accompanied by K-th martensite variant. Thereby, we have admitted that the shear system $\{\mathbf{d}_{I1},\ \mathbf{d}_{I2}\}$ undergo internal rotation for deformation exceeding range of elastic austenite.

Above discussed hypersurface is defined in the same way as (17). $\mathcal{P}_{KA}$ contains $A_I^{-1}(\mathbf{e}_I^{**})$ while $\mathcal{P}_I$ contains $A_I^{-1}(\mathbf{e}_I^{*})$ as critical values of strains.

As it was discussed previously, there is also possible transformation of K-th to K'-th martensite variant. However this does not happens in one slip system. Therefore, we define first a one dimensional path $G(K,K') \subset E$ which join equilibrium states of martensities determined by $\mathbf{e}_K$ and $\mathbf{e}_{K'}$. We try to define $\mathcal{P}_{KK'}$ with the help of $G(K,K')$. We introduce some simplified assumptions. First, $\mathcal{P}_{KK'}$ is flat and it is a five dimensional hyperplane.

In considered case $\mathcal{P}_{KK'}$ is expressed in a general form as follows

$$\mathcal{P}_{KK'} = \{\mathbf{e}:\ D_{ij}e_{ij} + D_o = 0\}\ . \tag{31}$$

We have to determine six coefficients D_{ij}. There are some premises in order to do it. First, $\mathcal{P}_{KK'} || L_{Kc}$ which gives one equation related to D_{ij}. It is expected that a value $\mathbf{e}^* \in G(K,K') \cap \partial S_K$ is attainable by experiments for well defined path $G(K,K')$. Other constants could be a result of analysis of transversality conditions between $G(K,K')$ and $\mathcal{P}_{KK'}$ in the point $\mathbf{e}^*$.

Let us define the set

$$\mathcal{P}_K = \bigcup_\beta \mathcal{P}_{K\beta} \cup \mathcal{P}_{KA} \cup \bigcup_{K'} \mathcal{P}_{KK'}$$

by analogy to considerations related to austenite.

In order to define ∂S_K we introduce the function

$$a_K([\tilde{\mathbf{e}}_{KD}]) = \inf_a\{\alpha_a([\tilde{\mathbf{e}}_{KD}] \cap \mathcal{P}_K)\}\ . \tag{32}$$

Finally

$$\partial S_K = \{\mathbf{e}:\ \tilde{\mathbf{e}}_K = a\tilde{\mathbf{e}}_{KD},\ a = a_K([\tilde{\mathbf{e}}_{KD}]),\ ||\tilde{\mathbf{e}}_{KD}|| = 1\} \tag{33}$$

and

$$\partial S_{K\beta} = \partial S_K \cap \mathcal{P}_{K\beta}\ ,\ \partial S_{KA} = \partial S_K \cap \mathcal{P}_{KA}\ ,\ \partial S_{KK'} = \partial S_K \cap \mathcal{P}_{KK'}\ . \tag{34}$$

At this moment we are able to introduce procedure of defining graph of free energy on M_K domain by means of fiber bundles. Let

$$N_{\beta K} = \{\mathbf{e}:\ 0 \le e_{K\beta mn} \le e^*_{K\beta mn}\},$$

$$h_K(e_{K\beta mn}) : \partial S_K \to f(e_{K\beta mn}),\ e_{K\beta mn} \in T_{Ko}$$

be family of homeomorphisms and

$$N_{Ko} = N_{\beta K} - \{\mathbf{0}_K\}.$$

Then,

$$M_K = \bigcup_{e_{K\beta mn} \in T_{Ko}} f(e_{K\beta mn}) \cup \{\mathbf{0}_K\} = N_{Ko} \times \partial S_K \cup \{\mathbf{0}_K\}$$

is expressed as a generalization of Cartesian product of N_{Ko} and ∂S_K.

We introduce the function $\bar{F}_K = c_{Kijkl}\tilde{e}_{Kij}\tilde{e}_{Kkl}$ which describe elastic properties of K-th variant of martensite in the domain U_K, $\mathbf{0}_K \in U_K \subset intM_K$.

$$\bar{B}_{\beta K} = \{\bar{b}_K : \bar{b}_K = \{\mathbf{e},\ \bar{F}_K(\mathbf{e})\},\ \mathbf{e} \in N_{\beta K}\}\ ,$$

$$\bar{F}_{\partial S_K} = \{\{\mathbf{e},\ \bar{F}_K(\mathbf{e})\} : \mathbf{e} \in \partial S_K\}\ ,$$

$$\bar{F}_{f(e_{K\beta mn})} = \{\{\mathbf{e},\ \bar{F}_K(\mathbf{e})\} : \mathbf{e} \in f(e_{K\beta mn})\}\ .$$

With the help of these sets we define the graph of $\bar{F}_K$ as follows

$$Gr\bar{F}_K = \bigcup_{\mathbf{e} \in N_{Ko}} \bar{F}_{f(e_{K\beta mn})} = \bar{B}_{\beta K} \times \bar{F}_{\partial S_K}\ . \tag{35}$$

Next stage of defining of F_K consists in modification $\bar{F}_K$ on the domain $M_K - U_K$. This is carried out in similar way as for austenite by

$$F_K = \begin{cases} \bar{F}_K, & \mathbf{e} \in U_K \\ \bar{F}_K + C_K, & \mathbf{e} \in M_K - U_K \end{cases}\ , \tag{36}$$

where the graph of the function C_K is defined by

$$GrC_K = \begin{cases} \{\mathbf{e},\ 0\}, & \mathbf{e} \in U_K \\ \{\mathbf{e},\ C_K(\mathbf{e})\}, & \mathbf{e} \in f(e_{K\beta mn}),\ \bar{e}_{K\beta mn} \leq e_{K\beta mn} \leq e^*_{K\beta mn} \end{cases}\ . \tag{37}$$

We assume that F_K satisfies the following conditions on ∂S_K

$$\frac{\partial^2(\bar{F}_K + C_K)}{\partial \mathbf{n}^2(e_{K\beta mn})}(\mathbf{e}) = 0,\ \mathbf{e} \in \partial S_K \cap N_{\beta K}\ , \tag{38}$$

$$\frac{\partial^2(\bar{F}_K + C_K)}{\partial \mathbf{n}^2(e_{K12})}(\mathbf{e}) = 0,\ \mathbf{e} \in \partial S_K \cap N_{IM}\ , \tag{39}$$

$$\frac{\partial^2(\bar{F}_K + C_K)}{\partial \mathbf{n}^2(G(K,K'))}(\mathbf{e}) = 0, \ \mathbf{e} \in \partial S_K \cap G(K,K') \,. \tag{40}$$

Furthermore, the quadratic form F_{Kijkl} is semipositive definite on the whole domain ∂S_K.

Let

$$B_K = \{b_K : b_K = \{\mathbf{e}, F_K(\mathbf{e})\}, \ \mathbf{e} \in N_{\beta K}\},$$

$$F_{f(e_{K\beta mn})} = \{\{\mathbf{e}, (\bar{F}_K + C_K)(\mathbf{e})\} : \mathbf{e} \in f(e_{K\beta mn})\}$$

and

$$F_{\partial S_K} = \{\{\mathbf{e}, (\bar{F}_K + C_K)(\mathbf{e})\} : \mathbf{e} \in \partial S_K\}.$$

Finally, the graph of free energy F_K on the domain M_K is defined by

$$GrF_K = B_K \times F_{\partial S_K} = \bigcup_{\mathbf{e} \in N_{Ko}} F_{f(e_{K\beta mn})}.$$

The form of free energy function F_S defined on the domain S is less precisely determined. It follows from the fact that we have not too many detailed information on this subject. Therefore, we assume only general properties for this part of the free energy. Thus, we assume that the following conditions are fulfilled by this function:

$$F_S|_{N_{IS}} = B_{IS}, \ \ F_S|_{\partial S_A} = F_A|_{\partial S_A}, \ \ F_S|_{\partial S_K} = F_K|_{\partial S_K},$$

$$\frac{\partial F_S}{\partial \mathbf{e}}|_{\partial S_A} = \frac{\partial F_A}{\partial \mathbf{e}}|_{\partial S_A}, \ \ \frac{\partial F_S}{\partial \mathbf{e}}|_{\partial S_K} = \frac{\partial F_K}{\partial \mathbf{e}}|_{\partial S_K},$$

$$\frac{\partial^2 F_S}{\partial \mathbf{e}\partial \mathbf{e}}|_{\partial S_A} = \frac{\partial^2 F_A}{\partial \mathbf{e}\partial \mathbf{e}}|_{\partial S_A}, \ \ \frac{\partial^2 F_S}{\partial \mathbf{e}\partial \mathbf{e}}|_{\partial S_K} = \frac{\partial^2 F_K}{\partial \mathbf{e}\partial \mathbf{e}}|_{\partial S_K} \,, \tag{41}$$

where B_{IS} should be postulated.

Finally, the part F_E of the free energy, which depends mainly on the strain tensor $\mathbf{e}$, has the form

$$F_E = \begin{cases} F_A, & \mathbf{e} \in A \\ F_K, & \mathbf{e} \in M_K \\ F_S, & \mathbf{e} \in S \end{cases} \tag{42}$$

The formula (42) determines form of the free energy which describes the case when austenite and martensite can coexist in equilibrium states. However, if temperature increases we obtain pseudo-elasticity phenomenon. Then, we have to maintain stress in order to observe stable martensite. It means also that no martensite exists if stress is equal to zero. Further increasing of temperature leads to elastic austenite only. On the other hand, decreasing of temperature brings about vanishing austenite state. Then, elastic martensite variants exist only. Dependence of the free energy on temperature should reflect above mentioned changes.

This discussion shows that temperature changes follow vanishing austenite states or martensite states. This induces, in turn, remark that behaviour of ∂S during temperature changes is of particular importance for modelling.

In general, dependence of F on temperature is introduced by $c_{ijkl}(T)$, $c_{Kjikl}(T)$, $C(T)$, $C_K(T)$, $U_A(T)$, $U_K(T)$ and $\partial S(T)$.

Let us discuss possible behaviour of ∂S during temperature changes with special regard to its decomposition on subsets. For stable austenite and martensite we have

$$\partial S_A = \bigcup_I \partial S_I \cup \bigcup_\alpha \partial S_\alpha$$

and

$$\partial S_K = \bigcup_\beta \partial S_{K\beta} \cup \partial S_{KA} \cup \bigcup_{K'} \partial S_{KK'}.$$

If temperature increases the free energy is transformed and describes pseudoelasticity. Then, ∂S_{KA}, $\partial S_{KK'}$ exist. However, there is no strain $\mathbf{e} \in M_K$ so that $\frac{\partial F}{\partial \mathbf{e}}(\mathbf{e}) = 0$. It means that there are no martensite in equilibrium. External stress is necessary in order to maintain martensite.

The question is what kind of changes is related to $\partial S_{K\beta}$. Martensite in pseudoelastic state, maintained by external stress differs to some degree from stable martensite. We could suppose, perhaps, that these differences change distribution of slip systems. We should admit possibility of slip for nonequilibrium martensite. Then, the stress should have two parts. The first one would maintain martensite and the second one would induce slips. Thus, $\partial S_{K\beta}$ has to be defined for stress-induced martensite.

Further increasing of temperature leads to vanishing ∂S_K and changing structure of ∂S_A. Then, we have $\partial S_K = \emptyset$ and $\partial S_A = \bigcup_{\alpha \in I_{ea}} \partial S_\alpha^{ea}$, where I_{ea} represents set of indexes defined for all slip systems of elastic austenite and ∂S_α^{ea} are domains on which initiation of α-th slip appear. No part of ∂S_A related to martensite exists.

If temperature decreases, the elastic domain A of austenite is gradually shrinked. This is connected with part of ∂S defined by $\bigcup_I \partial S_I$ mainly since decreasing of temperature makes easier martensitic transformation. Shrinking of $\mathcal{P}_I$ consists in their gradual approach. As a result, the domain A reduces to $\bigcap_I \mathcal{P}_I$. Then, metastable austenite appears. The shrinking is not connected with $\mathcal{P}_\alpha$. Finally, ∂S_A is transformed to the form $\partial S_A = \bigcap_I \mathcal{P}_I \cup \bigcup_\alpha \partial S_\alpha^{ma}$, where ∂S_α^{ma} represents critical condition for slip in α-th slip system for metastable austenite.

This kind of slips is not attainable physically. Metastable austenite is an atomic structure which have an excess of free space around atoms. Therefore it transforms to martensite. Generating of slips in such a structure destroy its metastable state immediately.

Slips do not affect directly the crystal structure by assumption. However, they generate inhomogeneities described by $\boldsymbol{\rho}$. The free energy is plotted with this variable by $c_{ijkl}(\boldsymbol{\rho})$, $c_{Kjikl}(\boldsymbol{\rho})$, $C(\boldsymbol{\rho})$, $C_K(\boldsymbol{\rho})$, $U_A(\boldsymbol{\rho})$, $U_K(\boldsymbol{\rho})$ and $\partial S(\boldsymbol{\rho})$. Precise model of these dependencies is much more complicated than dependence on temperature. In particular, by special modelling of ∂S possibility of realization of the martensitic transformation can be destroyed. It changes also slip systems.

Next stage of defining of the free energy consists in considering shuffles modelled by means of relative displacement vectors as independent variables.

Introduced here shuffles have qualitative meaning in description of the transformation induced plasticity. First, they can bifurcate. As a result various kinds of $\mathbf{w}_\lambda$ are active. Then, internal rotations dependent on $\mathbf{w}_\lambda$ create structures with considerable different slip systems. Consequently, the slip systems $\{\mathbf{m}_{K\beta},\ \mathbf{n}_{K\beta}\}(\mathbf{w}_\lambda)$ are dependent on shuffles.

There are also more complicated situations related to shuffles. With the help of vectors $\mathbf{w}_\lambda$, the two path martensitic transformation is described [14]. This transformation happens in *CuAlNi* alloy [12] and is accompanied by pseudo-elastic γ' martensite behaviour. During increasing of applied stress γ' martensite transforms to β' and further to α phase. If applied stress is decreased then the phase α returns to γ' through β'' type of martensite different than β'. Difference lies just in kind of shuffles which describe β' and β'' phases.

We have previously discussed possibility of slips in pseudo-elastic stress induced martensite. In the case of two-path martensitic transformation we have different stress-induced martensities. Then, history of applied stress can lead to different conditions for slips. They depend just on shuffles.

Our considerations connected with shuffles are based on CuAl structure. Then, the shuffles appear in two possible directions $\mathbf{d}_{I1}$ or $\mathbf{d}_{I2}$ in a given I-th shear system. As a result of this, a bifurcation process related to shuffles should be modelled.

Let $\mathbf{w}_\lambda$, $\lambda \in \Lambda$ be the λ-th relative displacement vector which can appear in the I-th shear system. Let us introduce also a function $C_\alpha(z)$, $\alpha = 1,\ 2$ which is symmetric, positive, and $C_\alpha(0) = 0$, $\frac{\partial C_\alpha}{\partial z}(0) = 0$ and $\frac{\partial^2 C_\alpha}{\partial z^2}(0) > 0$. This function has one minimum in $z = 0$ and for increasing z it increases up to a certain determined value.

Properties of the functions C_α allow to model the bifurcation of relative displacements. This is realized by means of the following function

$$M_{I\lambda} = C_1(\mathbf{w}_\lambda \mathbf{d}'_{I2})(\mathbf{w}_\lambda \mathbf{d}'_{I1})^2 + C_2(\mathbf{w}_\lambda \mathbf{d}'_{I1})(\mathbf{w}_\lambda \mathbf{d}'_{I2})^2 \,. \tag{43}$$

Evolution of the relative displacement vector $\mathbf{w}_\lambda$ is realized in two possible dominant directions $\mathbf{d}'_{I1}$ or $\mathbf{d}'_{I2}$. Evolution along $\mathbf{d}'_{I1}$ generates strong energetic barrier for evolution in $\mathbf{d}'_{I2}$ direction and inversely. Micro nonhomogeneous shear is characterized by collective development of the whole group of vectors $\mathbf{w}_\lambda$, $\lambda \in \Lambda$ in the same direction. Therefore, we introduce constraints which allow to develop all $\mathbf{w}_\lambda$ in the same direction after the bifurcation.

The functions introduced above describe a process of collective evolution of relative displacement vectors in two possible directions. During evolution of $\mathbf{w}_\lambda$, $\lambda \in \Lambda$, different arrangements of these vectors appear. Above discussion does not provide appropriate justification for considering separate evolutions $\mathbf{w}_\lambda$ for different λ. However, special arrangements of these vectors lead to two-path martensitic transformation. This previously discussed phenomenon occurs, for instance, in CuAlNi alloy. During loading and unloading, vectors $\mathbf{w}_\lambda$ change in two different ways. Then, different stress-induced phases appear. They can be distinguished only by positions of the relative displacement vectors. Possibility of modelling such a phenomenon gives the following function

$$M_{WI\lambda} = \Psi(a_\lambda(e_{I12}) + w_\lambda) - f_\lambda(e_{I12})(a_\lambda(e_{I12}) + w_\lambda) \, , \tag{44}$$

where $w_\lambda = |\mathbf{w}_\lambda|$. Form of this function allows to model the evolution of $\mathbf{w}_\lambda$ by dependence on e_{I12} and by control positions of minima of the introduced functions with the help of a_λ and f_λ.

The part of free energy which describes shuffles is finally suggested in the form

$$F_{W(J)} = \sum_\lambda M_{I\lambda} + \sum_\lambda M_{WI\lambda} \, , \tag{45}$$

where $J = (I, \alpha)$. The function (45) allows to model large variety of particular phenomena related to shuffles.

We have introduced $\mathbf{e}$ and $\mathbf{w}_\lambda$ as components of measure of deformation. Twelve kinds of structures can be created by six kinds of $\mathbf{e}$ related to shear systems and two kinds of $\mathbf{w}_\lambda$ obtained by possible bifurcations.

The free energy depends also on internal rotation of created hitherto structures. There are two habit planes for each of them. Thus, bifurcation process is related also to internal rotation. Dependence of free energy on $\mathbf{R}^I$ is introduced by means of additional variables introduced by (4) and based on material directors. The material directors $\mathbf{p}_{K\mu}$, $\mu = 1, 2$, determine positions of habit planes.

Internal rotations are accompanied by transformation of austenite to a martensite variant. Furthermore, an internal rotation of structure is accompanied by transition between different martensite variants. We admit that all pairs of martensite variants can be transformed one into another. However, we have observed that martensite occurs in self-accommodating groups. Under applying stress interfaces of twin type or habit type between these variants move. It means that the dominant phenomenon rests on transformation through mentioned interfaces.

Let us consider first austenite to martensite transformation. To this end the variables $\mathbf{a}_{K\mu}$ are introduced in the following form

$$\mathbf{a}_{K\mu} = \mathbf{R}^{-1}(\mathbf{F}^{ea})(\mathbf{F}^s\mathbf{F}^{ea} - \mathbf{R}^{-1}(\mathbf{F}^{ea}))\mathbf{p}_{K\mu} \, . \tag{46}$$

where $\mathbf{F}^{ea}$ is the gradient of deformation responsible for attaining deformation related to ∂S_A in a shear system $I \subset K$. Consequently, let us notice that $\mathbf{F}^s$ is the only independent variable. Let V_s be space of admissible $\mathbf{F}^s$.

Let us define two one-dimensional paths $G_{J\beta}(e_{I12})$, $\beta = 1, 2$, parameterized by $e_{I12} \in N_{IS}$. They have the following properties: $G_{J1}(e_{I12}) = G_{J2}(e_{I12})$ for $e^*_{I12} < e_{I12} < e^b_{I12}$, where e^b_{I12} is value of the parameter at the bifurcation point. Thus, $G_{J1}(e^b_{I12}) = G_{J1}(e^b_{I12}) = B \in V_s$. Then, G_{J1} and G_{J2} do not coincide for $e_{I12} > e^b_{I12}$. Introduced paths reflect assumption that internal rotation appears after exceeding e^*_{I12} and next can bifurcate towards one from two possible habit planes. Furthermore, we assume that $\mathbf{a}_{J1} = 0$, $\mathbf{a}_{J2} \neq 0$ for $G_{J1}(e^{**}_{I12})$, and $\mathbf{a}_{J1} \neq 0$, $\mathbf{a}_{J2} = 0$ for $G_{J2}(e^{**}_{I12})$. The last assumption means that austenite and martensite are fitted together at the end of each curve discussed on separate habit planes. Accordingly, the paths G_{J1}, G_{J2} are elements of geometrical skeleton for constructing this part of free energy.

Let us introduce a function $g : G_{J\beta} \to R$ which has the following properties:

1. $g(G_{J1}(e_{I12})) = g(G_{J2}(e_{I12}))$ for $e_{I12} \in N_{IS}$,
2. $g(G_{J1}(e^*_{I12})) = 0$, $\frac{\partial g}{\partial e_{I12}}(e^*_{I12}) = 0$, $\frac{\partial^2 g}{\partial e^2_{I12}}(e^*_{I12}) = 0$,
3. g monotonically decreases on N_{IS} ,
4. $\frac{\partial g}{\partial e_{I12}}(e^{**}_{I12}) = 0$, $\frac{\partial^2 g}{\partial e^2_{I12}}(e^{**}_{I12}) > 0.$

These properties prove the symmetry of evolution for two possible internal rotations and attaining minimum for e^{**}_{I12}.

Construction of the part of free energy which depends on $\mathbf{R}^I$ is carried out with the help of idea of expression its graph as a fiber bundle. To this end we assume that the domains can be expressed as generalized products

$$D_{RJ\beta} = G_{J\beta}(e_{I12}) \times D_{J\beta}(e'_{J\beta}) \subset V_s \tag{47}$$

and $D_{RJ1} \cap D_{RJ2} \neq \emptyset$, $e'_{J\beta} \in (e^*_{I12},\ e^{**}_{I12})$ is a given value of the parameter. Thus, $G_{J\beta}$ is considered to be the basis and $D_{J\beta}$ a chosen fiber assigned to $e'_{J\beta}$. Basis of the fiber bundle related to graph of free energy is determined by

$$b_{J\beta}(e_{I12}) = \{\{\mathbf{F}^s,\ g(\mathbf{F}^s)\},\ \mathbf{F}^s \in G_{J\beta}(e_{I12})\}\ . \tag{48}$$

With the help of two introduced domains we define fibers related to the graph for each part of the domain as

$$f_{J\beta}(e_{I12}) = \{\{\mathbf{F}^s,\ g_f(\mathbf{F}^s)(e_{I12})\},\ \mathbf{F}^s \in D_{J\beta}(e_{I12})\}\ , \tag{49}$$

where g_f is a function with the property $\inf_F g_f(\mathbf{F}^s)(e_{I12}) = g(G_{J\beta}(e_{I12}))$. In other words infimum of value of function defining the fiber is attained on intersection with basis manifold.

Discussed part of free energy graph is introduced as

$$F_{R(K)}(\mathbf{F}^s) = \begin{cases} b_{J1}(e_{I12}) \times f_{J1}(e'_{I12}), & \mathbf{F}^s \in D_{RJ1} \\ b_{J2}(e_{I12}) \times f_{J2}(e'_{I12}), & \mathbf{F}^s \in D_{RJ2} \end{cases} \tag{50}$$

It is assumed that for $\mathbf{F}^s \in D_{RJ1} \cap D_{RJ2}$ these functions coincide.

Let us consider the transformation of K-th to K'-th martensite variant. Then, we have discussed two cases related to transformation through habit type interface and twin type interface. The same kind of variables $\mathbf{a}_{K\mu}$ is applied in both cases. However, critical conditions are accompanied by gradient of deformation $\mathbf{F}^{em}$ attaining ∂S_K in martensite. Therefore, $\mathbf{a}_{K\mu}$ is assumed as

$$\mathbf{a}_{K\mu} = \mathbf{R}^{-1}(\mathbf{F}^{em})(\mathbf{F}^s\mathbf{F}^{em} - \mathbf{R}^{-1}(\mathbf{F}^{em}))\mathbf{p}_{K\mu}\,, \tag{51}$$

where $\mathbf{p}_{K1}$, $\mathbf{p}_{K2}$ represent common habit plane on which considered martensite variants are matched.

Let us consider path $G_H = S \cap G(K, K')$ associated with transition through habit type plane and parameterized by parameter s. Then, we introduce function $g(G_H(s))$ for $s \in [s^*,\ s^{**}]$ defined by conditions similar to 2-4. The first condition is omitted since one path is considered in this case.

The domain of $\mathbf{F}^s \in V_{Hs}$ is expressed as

$$D_{RH} = G_H(s) \times D_H(s') \subset V_{Hs}\,, \tag{52}$$

where D_H is a chosen fiber and $s' \in [s^*, s^{**}]$ takes a given value. Basis of the fiber bundle connected with graph of free energy is constructed as

$$b_H(s) = \{\{\mathbf{F}^s, g(\mathbf{F}^s)\}, \mathbf{F}^s \in G_H(s)\}\,. \tag{53}$$

The fiber related to the graph is determined by

$$f_H(s) = \{\{\mathbf{F}^s, g_f(\mathbf{F})(s)\},\ \mathbf{F}^s \in D_H(s)\} \tag{54}$$

by analogy to $f_{J\beta}$.

Consequently, considered part of free energy is determined as a generalized product in the following form

$$F_{R(H)}(\mathbf{F}^s) = b_H(s) \times f_H(s') \tag{55}$$

for a given value of $s' \in [s^*,\ s^{**}]$.

Generalization of these considerations into $K \to K'$ transformation through twin plane is immediate. Then, material directors $\mathbf{p}_{K\mu}$ are replaced by $\mathbf{t}_{T\mu}$ which determine the twin plane. Then,

$$F_{R(T)}(\mathbf{F}^s) = b_T(s) \times f_T(s') \tag{56}$$

is defined by analogy to (55) by replacement of H by T in all definitions applied. Then, $\mathbf{F}^s \in V_{Ts}$.

Considerations related to small scale are inherently connected with possible nonlocal effects. Then, interfaces are considered with a "thickness" generated by higher gradients of deformation terms. On the other hand, introducing of slips on discontinuity slip surfaces is accompanied by generating dislocations and defects. Such phenomena easily destroy fine structure of well organized material. Consequently, we have to model fine structure with the help of higher gradients and simultaneously have to introduce model of destroying this structure by slip generated inhomogeneities.

Let us consider a concept of introducing higher gradients of deformations by means of hierarchy of distinguished directions in the crystal structure.

Let ϕ be a field defined in the three-dimensional space. Let furthermore, three linearly independent directions $\{\mathbf{r},\ \mathbf{s},\ \mathbf{t}\}$ be distinguished in this space. The directions have hierarchy determined by their sequence. The first two determine a plane and distinguished directions on it. Let us consider an example of free energy in the following form

$$F_\phi = C_r(D_\mathbf{r}\phi)^2 + C_s(D^k_\mathbf{r}\phi)(D_\mathbf{s}\phi)^2 + C_t(D^k_\mathbf{r}\phi,\ D^l_\mathbf{s}\phi)(D_\mathbf{t}\phi)^2\,. \tag{57}$$

Properties of functions $C_s(D^k_\mathbf{r}\phi)$ and $C_t(D^k_\mathbf{r}\phi,\ D^l_\mathbf{s}\phi)$ determine behaviour of field ϕ. We assume that the function C_s is symmetric, positive, has maximum in 0 and tends strongly to zero if argument increases. The function C_t is defined on the plane as positive with maximum in (0, 0) and tending strongly to zero with increasing distance of point of its domain from (0, 0).

If $D^k_\mathbf{r}\phi$ is big sufficiently then C_s and C_t vanish and propagation of ϕ in $\mathbf{r}$ direction takes place. This happens since gradient dependence in $\mathbf{r}$ direction accelerates equalizing field in this direction. Then, $D_\mathbf{r}\phi$ becomes gradually smaller. As a result activity on $\mathbf{s}$ direction increases until $D_\mathbf{s}\phi$ becomes sufficiently small. Then, motion of the whole surface becomes more active.

This idea is introduced in order to underline fact that crystal structure is felt by the model. The habit and twin interfaces are observed to be flat. Thus, curvature induced by stress has to be leveled with perception of directions. In some cases fracture of interfaces is observed [26]. Evidently, evolution of such process has connections with distinguished directions.

Let us introduce a function $p(\mathbf{X}) = \{\mathbf{k}_K,\ \mathbf{l}_K,\ \mathbf{v}_K\}$ which assigns a triplet of vectors to point $\mathbf{X}$ by recognition of state of deformation measure in a neighbourhood of this point. Vectors $\mathbf{k}_K$, $\mathbf{l}_K$ represent distinguished directions on the habit plane HP_K. Let, furthermore, $\mathbf{M} = \{M_q\} = \{F_{iM},\ w_{\lambda N}\}$ be a set of variables and $\boldsymbol{\rho} = \{\rho_1, ..., \rho_k\}$ are internal state variables describing inhomogeneities generated by defects and dislocations.

Taking into account concept expressed by formula (57) we introduce the following form of free energy dependent on higher gradients of deformation

$$F_{G(K)} = \sum_q [C_{kq}(\boldsymbol{\rho})(D_\mathbf{k}M_q)^2 + C_{lq}(D_\mathbf{k}M_q,\ \boldsymbol{\rho})(D_\mathbf{l}M_q)^2 + \\ + C_{vq}(D_\mathbf{k}M_q,\ D_\mathbf{l}M_q,\ \boldsymbol{\rho})(D_\mathbf{v}M_q)^2]\,. \tag{58}$$

The activity of this part of the free energy depends on recognition, with the help of function $p(\mathbf{X})$, of the kind of habit plane and next introduce distinguished directions. Then, the functions C_{kq}, C_{lq}, C_{vq} take properties by analogy to those defined in (57).

Introduced in this paper complicated system of indexes I, J, K, H, T reflects complicated microstructure of martensite variants and their interfaces. In order to gain more clarity in this description, the domain of the free energy should be more precisely elucidated.

If a stress is applied to the natural state of austenite the deformation develops in order to attain ∂S_A. If ∂S_A is attained on ∂S_α then the deformation measured by $e_{\alpha mn}$ does not increase. Further, a slip is continued. If ∂S_A is attained on ∂S_I then transition to region S is realized. Furthermore, the index I is remembered. Then, the remaining elements of deformation measure are activated. First, vectors $\mathbf{w}_{J\lambda}$ develop and bifurcate. Next, the index J is remembered and then internal rotation $\mathbf{F}^s$ is developed and represent a rotation towards a habit plane indexed by $K = (I,\ \alpha,\ \beta) = (J,\ \beta)$.

We assume that values of introduced components of deformation measure are not quite arbitrary. They are admissible in the neighbourhood of equilibrium paths. The equilibrium paths for the relative displacement vector $\mathbf{w}_\lambda$ are given by $\mathbf{w}_{\lambda\alpha} = w_\lambda \mathbf{d}'_{I\alpha}$. We assume that these vectors develop only in some neighbourhood $U(\mathbf{w}_{\lambda\alpha})$ of these paths. It means that the domain of admissible $\mathbf{w}_\lambda$ is

$$W_J = W_{I\alpha} = \{\mathbf{w}_\lambda :\ \mathbf{w}_\lambda \in U(\mathbf{w}_{\lambda\alpha}),\ \lambda \in \Lambda\}\,. \tag{59}$$

The part of domain related to internal rotation is connected with $\mathbf{F}^s$ development in a neighbourhood of $G_{J\beta} = G_K$. We assume it in the form

$$V_K = V_{J\beta} = \{\mathbf{F}^s :\ \mathbf{F}^s \in U(G_{J\beta})\}\,. \tag{60}$$

Higher gradients of deformation are concentrated around a zero value. If they are connected with the habit plane then the domain H_K is defined as

$$H_K = \Big\{\{\frac{\partial}{\partial X_i} M_q\} : \{\frac{\partial}{\partial X_i} M_q\} \in U(0),\quad i = 1, 2, 3\Big\}\,. \tag{61}$$

The deformation can start also from K-th martensite variant. If $\partial S_{K\beta}$ is attained then $e_{K\beta mn}$ cannot further increase and slip in β-th slip system in martensite is activated on the slip surface. The deformation can attain ∂S_{KA}. Then, the deformation path is directed towards austenite and active domain is placed in the framework of hitherto discussed sets for austenite-martensite transformation. The last case rests on attaining $\partial S_{KK'}$ by the deformation what leads to changing martensite variants. Then, we have assumed one path G_H or G_T for transformation by habit plane or by twin plane. In this case we introduce the following sets

$$W_H = \{\mathbf{w}_\lambda :\ \mathbf{w}_\lambda \in U_H\}\,,\ W_T = \{\mathbf{w}_\lambda :\ \mathbf{w}_\lambda \in U_T\}\,, \tag{62}$$

$$V_H = \{\mathbf{F}^s : \mathbf{F}^s \in U(G_H)\}\,, \; V_T = \{\mathbf{F}^s : \mathbf{F}^s \in U(G_T)\}\,. \tag{63}$$

Introduced multiindex $K = \{I, \alpha, \beta\}$ determines a sequence of activity of distinguished parts of domain expressed by $D_K = E \times W_J \times V_K \times H_K$. If index I is remembered then J must have the form $\{I,\ \alpha\}$ and next $K = \{J,\ \beta\}$. Let $I_P = \{H,\ T\}$. Finally, the total domain is expressed as

$$D = \bigcup_{K \in I_K} (E \times W_J \times V_K \times H_K) \cup \bigcup_{P \in I_P} (E \times W_P \times V_P \times H_P) = \bigcup_K D_K \cup \bigcup_P D_P\,. \tag{64}$$

The total form of free energy is given by

$$F = F_K(g) = F_E + F_{W(J)} + F_{R(K)} + F_{G(K)}, \; g \in D_K\,, \; K \in I_K$$

$$F = F_P(g) = F_E + F_{W(P)} + F_{R(P)} + F_{G(P)}, \; g \in D_P\,, \; P \in I_P. \tag{65}$$

In the case of the function F_P we have not defined all components in detail. $F_{W(P)}$ determines evolution of shuffles between martensite variants. In order to determine such a term precisely many additional information on crystal structure behaviour are necessary. $F_{G(P)}$ is defined by analogy to $F_{G(K)}$.

4. Model of plasticity with distinguished slip surfaces

Model of plasticity with distinguished slip surfaces is characterized by slips realized on discontinuity surfaces of the deformation function χ. As a result, the bulk of material is described by usual model of material without slips. In this paper we consider the model of the martensitic transformation. Then, conditions on slip surface determine a kind of boundary conditions for part of material lying between the slip surfaces.

Balance equations for small scale model of the martensitic transformation have been discussed in [19]. Consequently, we concentrate our considerations around surface conditions related to discontinuity generated by slips.

Let us consider a slip surface $\mathcal{S}$ at an initial instant when $\mathbf{u}_S = \mathbf{0}$. Then, $\mathcal{S} = \mathcal{S}^+ = \mathcal{S}^-$, where $\mathcal{S}^+$ and $\mathcal{S}^-$ are material surfaces related to parts of the body which are in contact on $\mathcal{S}$. We assume also that $\mathcal{S}$ intersects the whole body. Then, $\mathcal{S}^+ = \chi^+(\mathcal{S},\ t)$ and $\mathcal{S}^- = \chi^-(\mathcal{S},\ t)$. We can distinguish parts of surfaces defined as $\partial\mathcal{B}_{S^+} = \mathcal{S}^+ - \mathcal{S}^-$, $\partial\mathcal{B}_{S^-} = \mathcal{S}^- - \mathcal{S}^+$ and $\mathcal{S}_S = \mathcal{S}^+ \cap \mathcal{S}^-$.

We assume that during the slip a surface force $\mathbf{f}_S$ is generated on $\mathcal{S}_S$ as a reaction of the material. Following the well known form of balance equations on the surface [27], we obtain the conditions

$$\mathbf{t}^-(\mathbf{x}^-)\mathbf{n} - \mathbf{t}^+(\mathbf{x}^+ = \mathbf{x}^-)\mathbf{n} = \mathbf{f}_S(\mathbf{x}^-)\,, \; \mathbf{x}^- \in \mathcal{S}_S\,,$$

$$\mathbf{t}^-(\mathbf{x}^-)\mathbf{n} = 0\,, \ \mathbf{x}^- \in \partial\mathcal{B}_{S^-}\,,$$
$$\mathbf{t}^+(\mathbf{x}^+)\mathbf{n} = 0\,, \ \mathbf{x}^+ \in \partial\mathcal{B}_{S^+} \tag{66}$$

and

$$-(\mathbf{q}^- - \mathbf{t}^-\mathbf{v}^-)(\mathbf{x}^-)\mathbf{n} + (\mathbf{q}^+ - \mathbf{t}^+\mathbf{v}^+)(\mathbf{x}^+ = \mathbf{x}^-)\mathbf{n} - (\mathbf{f}_S\dot{\mathbf{u}}_S)(\mathbf{x}^-) = 0\,, \ \mathbf{x}^- \in \mathcal{S}_S\,. \tag{67}$$

We have furthermore conditions related to new parts of boundary which appear during slip on the surface intersecting whole body considered

$$\mathbf{q}^-(\mathbf{x}^-)\mathbf{n} = \bar{q}^-\,, \ \mathbf{x}^- \in \partial\mathcal{B}_{S^-}\,,$$
$$\mathbf{q}^+(\mathbf{x}^+)\mathbf{n} = \bar{q}^+\,, \ \mathbf{x}^+ \in \partial\mathcal{B}_{S^+}\,. \tag{68}$$

In order to describe evolution of slip, an evolution equation for $\mathbf{u}_S$ defined by (11) has to be introduced. We assume that evolution of $\mathbf{u}_S$ is determined by the formula

$$\dot{\mathbf{u}}_S = \Phi(\mathbf{t}^+, \mathbf{t}^-, \mathbf{f}_S)\,. \tag{69}$$

The equation (69) is not entirely determined since we do not know form of $\mathbf{f}_S$. Therefore, a kind of constitutive equation has to be added. This equation is assumed in the following form

$$\mathbf{f}_S = \mathbf{f}_S(\dot{\mathbf{u}}_S, T, \boldsymbol{\rho}^+, \boldsymbol{\rho}^-)\,. \tag{70}$$

Equations (69) and (70) define in turn the equation expressed as $\dot{\mathbf{u}}_S = \Phi \circ \mathbf{f}_S(\dot{\mathbf{u}}_S)$ for given values of the remaining variables. Let us notice that given forms of Φ and $\mathbf{f}_S$ allow to solve the equation and determine $\dot{\mathbf{u}}_S$ uniquely for given values of the remaining variables. As a result $\mathbf{f}_S(\dot{\mathbf{u}}_S)$ also takes a determined value.

In reality $\mathbf{f}_S$ depends also on $\boldsymbol{\rho}^+$, $\boldsymbol{\rho}^-$, T which induce dependence of $\dot{\mathbf{u}}_S$ on these variables. Determination of $\boldsymbol{\rho}^+$, $\boldsymbol{\rho}^-$ depends on the kind of particular modelling of inhomogeneities. In general, evolution equations have to be introduced in the bulk of crystal for the variable $\boldsymbol{\rho}$. Furthermore, conditions on the slip surface which determine dependence between $\boldsymbol{\rho}^+$ and $\boldsymbol{\rho}^-$ have to be postulated.

Evolution of $\boldsymbol{\rho}$ can be useful in description of creep since this variable influences hardening expressed by the form of free energy. However, then described effects have to be transformed into a larger scale where constant external stress can be considered.

5. Final remarks

The aim of introduced in this paper nanoscale model of the transformation-induced plasticity is the description of interactions of martensitic transformation with slips in detail. Model of this kind is related to scale of averaging between 10^{-9} m and 10^{-8} m. This induces complicated model and considerable number of constants necessary for identification. It is not sure that these constants can be determined with the help of experiments since it is difficult to investigate experimentally separate phenomena for such a small scale. However, this scale creates convenient conditions for supporting the model by discrete calculations. This is the case since a relatively small number of atoms is contained in a representative volume related to the nanoscale model. In particular, molecular dynamics, which is widely applied in material science [28, 29], could be useful in determination of considerable number of constants necessary for identification of this model.

It is expected that presented model will be helpful in creating foundations for the development of the transformation-induced plasticity in a single crystal related to scale 10^{-6} m when the gradient of deformation can be applied for description of plastic slips or evolution of the martensitic structure.

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