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FIFTY YEARS OF THE ARCHIVES OF MECHANICS

A thermodynamical description of the martensitic transformation
A model with small volume of averaging

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IN THE PAPER a thermomechanical model of the martensitic transformation in a single crystal is introduced. The model is related to a small volume of averaging. It means that detailed phenomena such as motion of single interfaces, internal rotations towards habit planes, separate mechanisms of dissipation or nucleation of different martensite variants can be discussed in the framework of the model. Such a description is attained mainly by means of the introduced free energy. Therefore, the construction of this function is a central part of this paper. The free energy depends on the Lagrangean strain tensor which describes the dominant part of deformation, relative displacement vectors for modelling shuffles and variables which are introduced with the aid of material directors. With the help of the last variables, an internal rotation is discussed. Furthermore, higher gradients of deformation are also taken into account. A general thermodynamical formulation for this small scale model is considered.

1. Introduction

THE MARTENSITIC TRANSFORMATION appears in many alloys, organic materials and even in living organisms. This transformation is diffusionless and is characterized by dominant shear strain. In case of moving interfaces between martensite variants or between martensite and austenite, such a transformation leads to shape memory phenomenon [1].

In general, the martensitic transformation creates complicated microstructure. In the case of moving interfaces, the microstructure has its own complex dynamics. This dynamics becomes still much more complicated when thermal processes are taken into account. They cause the stabilization martensite phenomenon. The stabilization can considerably influence temperatures of the transformation.

The martensitic transformation is a subject of intensive investigations in metallurgy. Such a transformation is the main mechanism of the shape memory phenomenon [1]. Increasing interest in this phenomenon appears in mechanics for the last twenty years. This is possible owing to results which were attained in metallurgy. Very helpful in mechanical description are, for instance, crystallographic structures of CuAl [2] or CuAlNi [3] alloys, positions of their habit planes or forms in which their martensitic structures appear in the material.

Miscellaneous points of view are presented in mechanical description of the martensitic transformation. One-dimensional models are discussed in order to give a qualitative mechanical description for some special behaviour of a material (see for instance [4, 5]). There are some models related to a single crystal [6, 7, 8]. A statistical approach is presented in [9, 10]. On the other hand, very averaged descriptions over the composition of martensite variants and austenite are discussed in the literature, see for instance [11 – 16]. They are simpler and are more applicable.

Complicated behaviour of materials which undergo the discussed transformation suggests a multiscale approach. Such point of view is presented by the author of this paper. Consequently, two models should be introduced. The first one is a model with small scale of averaging. It means that many detailed phenomena are taken into account in this description. There are single martensite variants, moving interfaces, shuffles which are usually neglected in description of the martensitic transformation, internal rotations towards habit planes or separated mechanisms of dissipation. However, such a model is rather complicated and difficult in applications. Some elements of such a description are discussed in [17, 18].

The model with small scale of averaging is viewed to be a theoretical and numerical basis for a more averaged model. The last one would have a reduced number of variables and more simple constitutive equations which would be derived from the small scale model. A concept of multiscale approach of this kind has been discussed in [20]. The program discussed here is too large for one paper. On the other hand, the model of small volume of averaging is complicated itself. Therefore, the purposes should be more limited at the moment.

Consequently, the aim of this paper is to introduce a thermomechanical model of the martensitic transformation related to a small volume of averaging which takes into account the detailed phenomena accompanied by this transformation.

2. Crystallographic considerations related to the martensitic transformation

The model of small volume of averaging will be constructed mainly by introduction of appropriate form of the free energy. Properties of the free energy are responsible for the detailed behaviour of the material in the frame of the model. However, in order to determine this function, variables which are appropriate for description of kinematics of the martensitic transformation and some internal state variables should be introduced. Selection of these variables depends on understanding the crystallographic properties of the material undergoing the considered phase transformation.

The crystallographic structure of the martensitic transformation will be discussed with the help of the CuAl alloy. Properties of this alloy are representative for a large class of shape memory alloys based on copper.

Let us discuss a process of nucleation of martensite variant from austenitic structure in a single crystal.

The austenite single crystal has a cubic body-centered structure bcc which is shown in Fig. 1. This structure is also called the β phase [2]. A face-centered structure which is not cubic can be distinguished in the frame of the bcc one. This is marked by a bold line. Furthermore, four planes are displayed by means of thin lines. They are called basal planes and are connected with the $0Y$ axis. We can distinguish in a similar manner next four basal planes assigned to $0X$ and next to $0Z$ axes, respectively. Thus, we have twelve basal planes. Some of them coincide in the undeformed state of austenite. Thus, in this undeformed state we have six different basal planes.

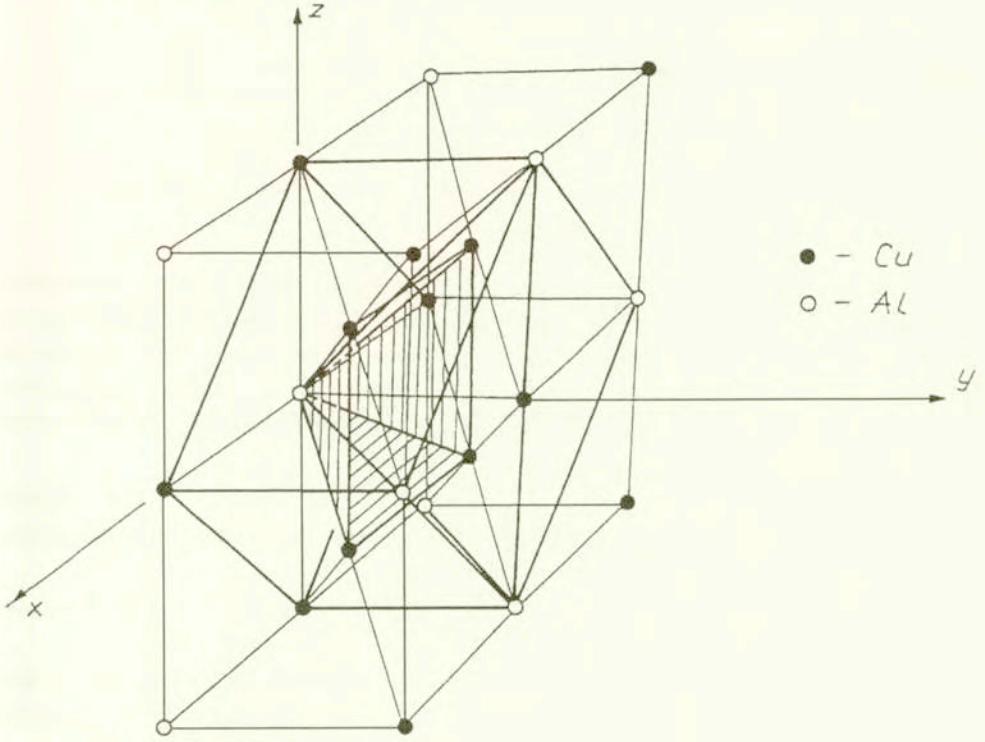

FIG. 1. Structure of austenite for CuAl alloy.

We can distinguish three stages of the martensitic transformation. The first stage consist in realization of the Bain strain. Let us select, for instance, $0Y$ axis. If we apply an extension along $0Y$ then, the previously discussed face-centered structure can be transformed into a cubic fcc one. The strain of this kind is called just the Bain strain.

The second stage of the martensitic transformation is a micrononhomogeneous shear. This deformation appears on one of four possible basal planes related to the $0Y$ axis. Micrononhomogeneous deformation of this kind is shown at Fig. 2 and

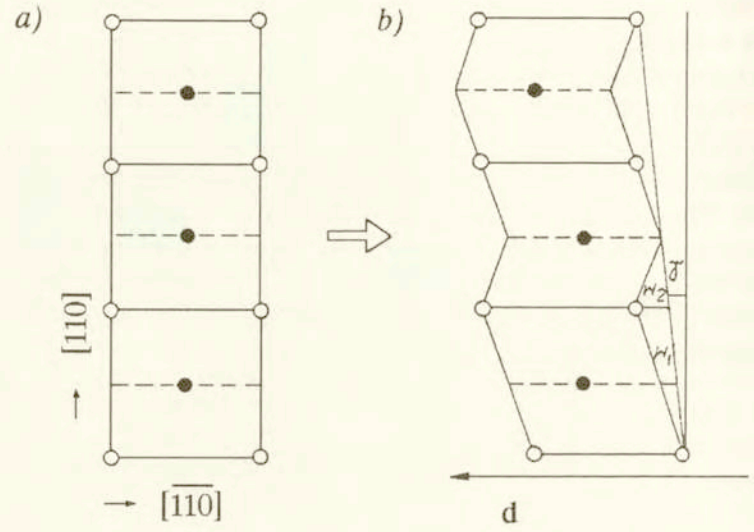

FIG. 2. Micrononhomogeneous shear on the basal plane of CuAl alloy.

is connected with shuffles. The micrononhomogeneous shear occurs in direction **d** which lies on the basal plane. We have four such directions accompanied by the $0Y$ axis. They are fixed to point 0 and lie on each of the basal planes and on the ZY and XY plane, respectively. The shuffles marked by w_1 and w_2 in Fig. 2 are a measure of deviation of atoms from the position indicated by a homogeneous deformation.

The third stage of transformation considered is a rotation of the hitherto obtained structure towards a habit plane. We have two possible habit planes related to each structure obtained in the discussed manner.

In real evolution of the crystal structure these three stages are not separated so clearly.

Thus, we can obtain twenty four martensite variants. Indeed, we have four micrononhomogeneous shears accompanied by the $0Y$ axis and next two possible rotations. This gives eight martensite variants related to the $0Y$ axis. Similarly, martensite variants can be obtained for the remaining axes.

Orientations of basal planes and habit planes are shown at Fig. 3 where notations from [21] are used. Capital letters denote Bain axes. Small letters are connected with directions of nonhomogeneous shear. Variants which are different by rotation are marked by primes at the capital letter.

Possible twenty four martensite variants appear in the material in six self-accommodating groups. Consequently, each group has four marensite variants separated by habit-type or twin-type planes. Four martensite variants organized in one self-accommodating group are shown at Fig. 4.

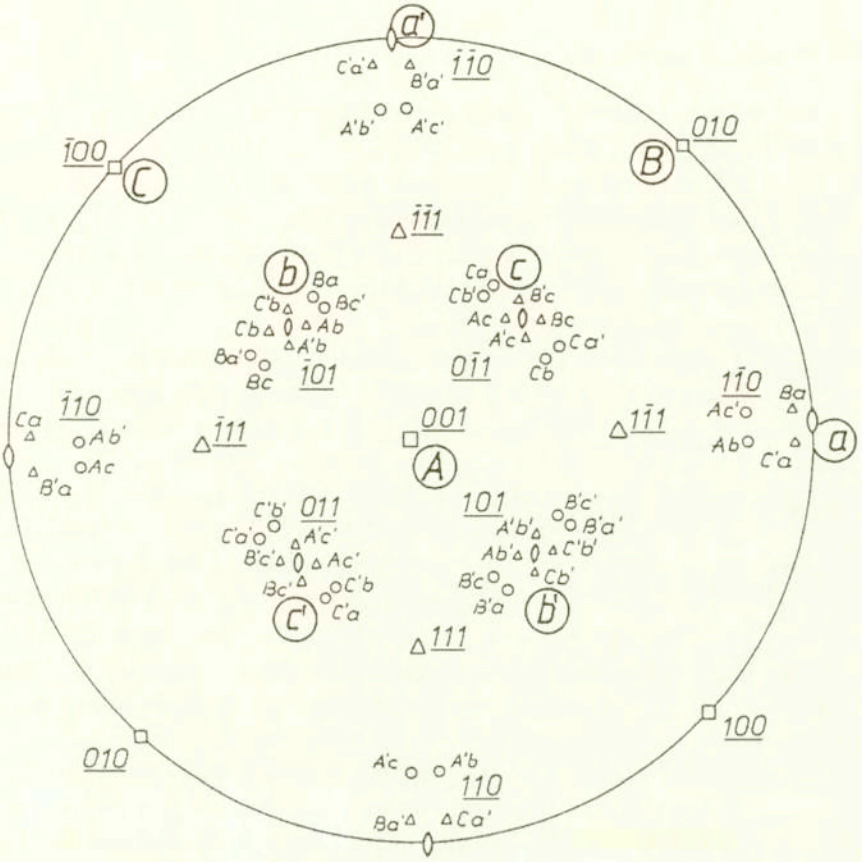

FIG. 3. Distribution of basal planes and habit planes for CuAl alloy.

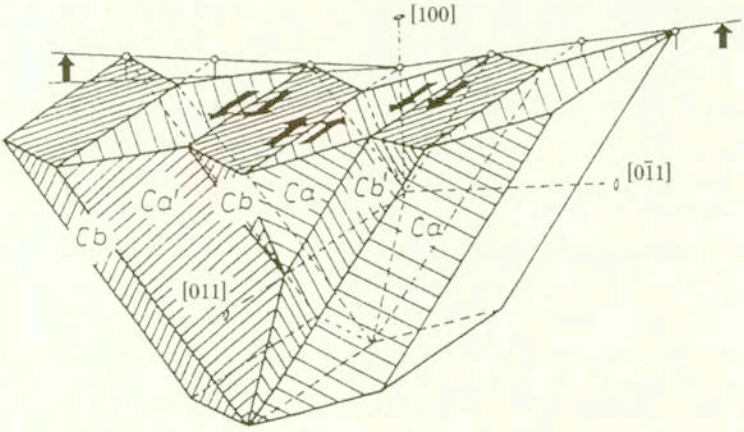

FIG. 4. A selfaccommodating group of four martensite variants in CuAl alloy.

3. Kinematical considerations

Crystallography of the martensitic transformation discussed in the last section suggests the measures of deformation which should be assumed. They should give a possibility of classification of martensite variants.

Let us introduce a system of orthonormal base vectors $\mathbf{b} = \{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3\}$. Directions of these vectors coincide with axes $0X$, $0Y$, $0Z$ as in Fig. 1, respectively.

We introduce also the sets of vectors which define the shear systems connected with the micrononhomogeneous shears.

Let us consider a vector $\mathbf{b}_i$. We assign to this vector two planes which contain the vector $\mathbf{b}_i$ and vectors $\mathbf{b}_j$, $j \neq i$, respectively. Thus, a double index is assigned to each plane of this kind as $I = \{i, j\}$, $j \neq i$. The first index is related to the Bain axis and the second one determines the plane introduced.

With the help of these planes we define vectors $\mathbf{d}_{I\alpha}$, $\alpha = 1, 2$. They are unit vectors with their initial points in 0 and lie on the lines which appear as intersections of plane I with a pair of basal planes related to axis i. Their positions are illustrated in Fig. 6. Pair of vectors $\{\mathbf{d}_{I1}, \mathbf{d}_{I2}\}$ determine a shear system. Furthermore, we create new basis $\mathbf{d}_I = \{\mathbf{d}_{I1}, \mathbf{d}_{I2}, \mathbf{d}_{I1} \times \mathbf{d}_{I2}\}$.

Let $\mathbf{e}$ be the Lagrangean strain tensor. Then $e_{I12} = \mathbf{d}_{I1}\mathbf{e}\mathbf{d}_{I2}$ is a measure of shear strain in this shear system. Vectors $\mathbf{d}_{I1}$ and $\mathbf{d}_{I2}$ indicate possible directions of shuffles.

Let us notice that structures given on Fig. 5 c and Fig. 5 d have the same strain given by e_{I12}. They differ only by shuffles. Thus, the shuffles which are small and usually neglected in description of the martensitic transformation are important for distinguishing different martensite variants. Moreover, we can say that during deformation given by $\mathbf{e}$, a bifurcation between two direction of shuffles appears.

However, qualitative meaning of shuffles is still greater. Namely, the possible habit planes towards which the structures rotate, depend just on the kind of shuffles which have previously appeared. Accordingly, the shuffles influence the kind of internal rotation.

Let us notice that micrononhomogeneous deformation appears as a consequence of complex crystal lattice accompanied by a multicomponent alloy. Therefore, a natural way of introducing the shuffles follows from multicomponent considerations.

Consequently, let us introduce a set of displacement functions

$$\mathbf{z}_\mu(\mathbf{X}, t) = \{\mathbf{x}(\mathbf{X}, t), \mathbf{y}_\lambda(\mathbf{X}, t)\}, \tag{3.1}$$

where $\lambda \in \Lambda = \{1, ..., N_\lambda\}$. It is assumed that the function $\mathbf{x}$ is accompanied by the microhomogeneous deformation assigned to the body, and functions $\mathbf{y}_\lambda$ indicate the positions which differ from the homogeneous one. Thus, the relation between $\mathbf{x}$ and $\mathbf{y}_\lambda$ has the form

$$\mathbf{y}_\lambda = \mathbf{x} + \boldsymbol{\xi}_\lambda. \tag{3.2}$$

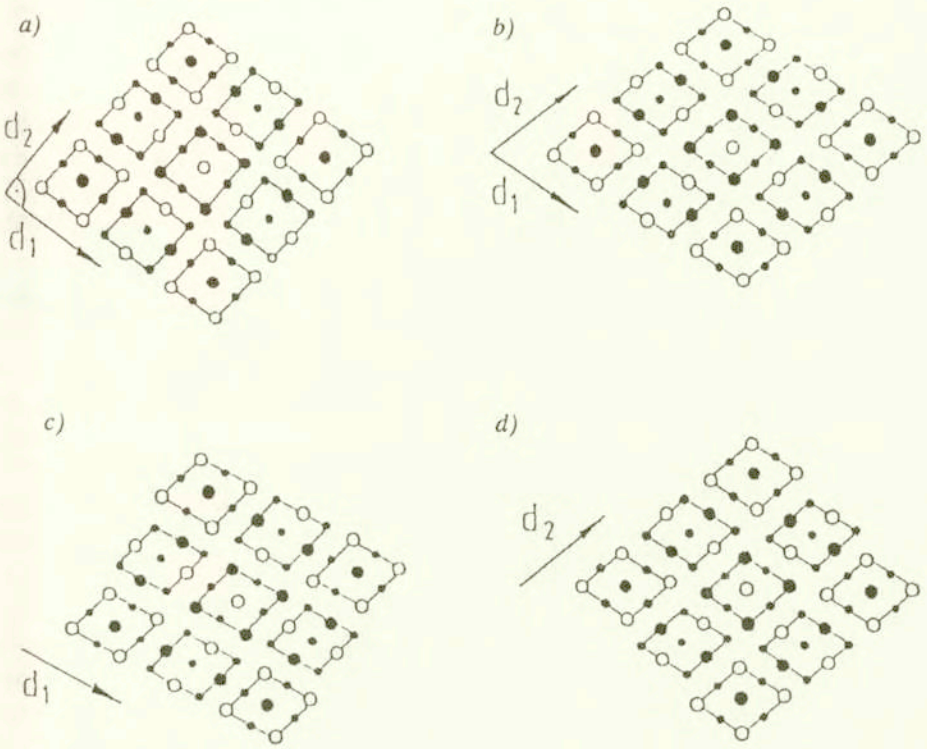

FIG. 5. Evolution of crystal structure during shear strain in the shear system $(\mathbf{d}_1, \mathbf{d}_2)$.

ξ_λ is an independent variable. However, we have observed that shuffles appear in $\mathbf{d}_{I1}$ or $\mathbf{d}_{I2}$ direction in the I-th shear system. Let us note that the base vectors $\mathbf{d}_{I1}$, $\mathbf{d}_{I2}$ can be also viewed as material directors which are deformed as $\mathbf{d}'_{I\alpha} = \mathbf{F}\mathbf{d}_{I\alpha}$ for $\alpha = 1, 2$, where $\mathbf{F}$ is the deformation gradient related to $\mathbf{x}$.

Taking into account the above remark we can assume that $\xi_\lambda = w_\lambda \mathbf{d}'_{I1}$ or $\xi_\lambda = w_\lambda \mathbf{d}'_{I2}$. Then, for instance for $\alpha = 1$, we obtain $\xi_\lambda = w_\lambda \mathbf{F}\mathbf{d}_{I1}$. Putting $\mathbf{w}_\lambda = w_\lambda \mathbf{d}_{I1}$ we have $\xi_\lambda = \mathbf{F}\mathbf{w}_\lambda$.

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 polar decomposition $\mathbf{F} = \mathbf{V}\mathbf{R}$ [28]. Taking into considerations (3.2) we can also write that $\mathbf{y}_\lambda = \mathbf{x} + \mathbf{F}\mathbf{w}_\lambda \approx \mathbf{x} + \mathbf{R}\mathbf{w}_\lambda$. Such an approximation will be useful in further derivations.

Let us notice that the approximation $\mathbf{F}\mathbf{w}_\lambda \approx \mathbf{R}\mathbf{w}_\lambda$ suggests some constraints related to the gradient of deformation. However, this approximation appears in displacement function $\mathbf{y}_\lambda$ only. Then, the gradient of deformation $\mathbf{F}$ related to $\mathbf{x}$ defines $\mathbf{y}_\lambda$. As a result of this, constraints are related to $\mathbf{y}_\lambda$ and finally to $\mathbf{w}_\lambda$ but not to $\mathbf{F}$.

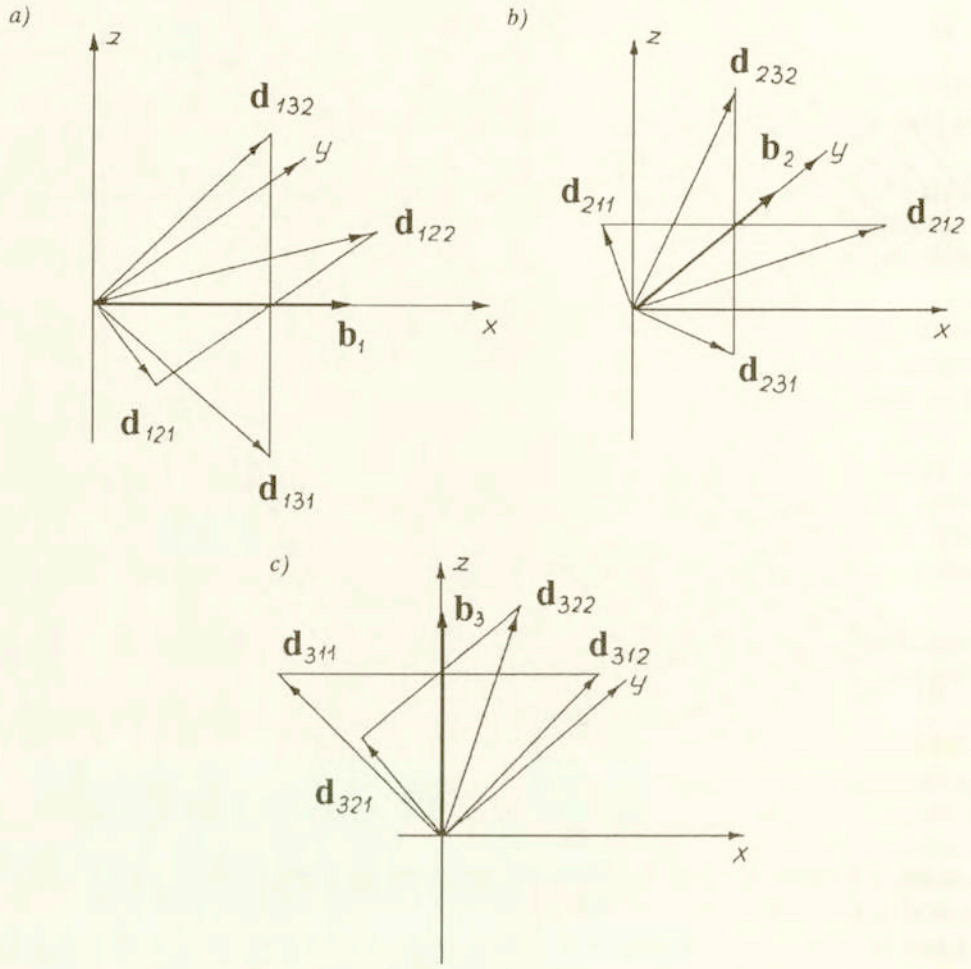

FIG. 6. Distributions of vectors $\mathbf{d}_{I\alpha}$ in the austenite structure.

The vector $\mathbf{w}_\lambda$ is a variable which characterizes relative translation of sublattices. Thus, in the above approximation, it is assumed that the rotation is the most valid part of the gradient of deformation for kinematics. It characterizes the change of directions in rotating lattice. In general, relative displacement vectors should depend on the remaining components of the gradient of deformation. However, such a dependence should not follow from kinematics but from dependence of the free energy on $\mathbf{F}$ and $\mathbf{w}_\lambda$. This kind of dependence in the equilibrium case is discussed in what follows.

In general, the relative displacement vector $\mathbf{w}_\lambda$ has not to be considered as $\mathbf{w}_\lambda = w_\lambda \mathbf{d}_{I1}$ because the last relation is a constraint in fact. Consequently, the vector $\mathbf{w}_\lambda$ will be viewed as an independent variable which is convenient for modelling the shuffles in the free energy.

The approximations discussed above related to $\mathbf{w}_\lambda$ have an interpretational meaning and are applied further during the derivation of equations. It is assumed that they do not influence integrability of the finally obtained fields. The main interpretational aspect related to $\mathbf{w}_\lambda$ rests on elucidating the fact that $\mathbf{w}_\lambda$ appears as a result of multicomponent considerations and is not directly related to defects.

Next problem is connected with a 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 variants. The habit plane is a plane on which 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. Thus, a bifurcation process related to the internal rotation can take place.

The internal rotation will be introduced here with the help of variables which are defined by means of material directors. Let $\mathbf{p}_1$ and $\mathbf{p}_2$ be a pair of material directors which lie on a habit plane. In other words, the habit plane is spanned by these directors. They transform as $\mathbf{p}'_\beta = \mathbf{F}\mathbf{p}_\beta$, $\beta = 1, 2$.

The directors are transformed during the martensitic transformation. We try to describe the forces in the material. Therefore, the discussed variable should exclude an external rotation. Taking it into account, the following measure of deviation of directors is introduced:

$$\mathbf{a}_\beta = \mathbf{R}^{-1}(\mathbf{F} - \mathbf{R})\mathbf{p}_\beta = (\mathbf{R}^{-1}\mathbf{F} - 1)\mathbf{p}_\beta \,, \tag{3.3}$$

where $\mathbf{R}$ is an external rotation. At this moment, a problem of separation of internal and external rotations appears. An idea of this separation is introduced by assuming some additional auxiliary configurations.

It is assumed that the internal rotation develops only when the shear strain e_{I12} in the I-th shear system is between the given values e^*_{I12} and e^{**}_{I12}. This follows from the fact that the internal rotation appears only if an elastic region is exceeded. Indeed, in the usual elasticity problems related to such a rotation are not observed.

Let us distinguish some special configurations. The first one is the reference configuration which coincides with the natural state of austenite. The second configuration $x_\alpha = x_\alpha(X_N)$ is connected with the deformation for which the strain e^*_{I12} is attained in a given point of the body. The third configuration $x_\mu = x_\mu(x_\alpha)$ is connected with deformation for which the strain e^{**}_{I12} is attained and the fourth configuration is an actual configuration x_i.

Configurations x_α and x_μ are fixed and are different for different points $\mathbf{X}$. Thus, they are accompanied by retaining in memory the state of deformation in a given point attained in the past.

The deformation gradients are assigned to the mentioned configurations $\mathbf{F}^{ea} = [x_{\alpha,N}]$, $\mathbf{F}^s = [x_{\nu,\alpha}]$, $\mathbf{F}^{em} = [x_{i,\nu}]$ and the total gradient takes the form $\mathbf{F} = \mathbf{F}^{em}\mathbf{F}^s\mathbf{F}^{ea}$.

At the moment we are able to separate internal and external rotations. Let us assume that deformation occurs in region S, i.e. between the second and third fixed configurations. Then, an external rotation follows from polar decomposition $\mathbf{F}^{ea} = \mathbf{VR}$. Then, the definition of variable $\mathbf{a}_\beta$ is more precise. Let us assume $\mathbf{F}^s = \mathbf{R}^s\mathbf{U}^s$. In such a case, Eq. (3.3) can be rewritten as

$$\mathbf{a}_\beta = \mathbf{R}^{-1}(\mathbf{R}^s\mathbf{U}^s\mathbf{VR} - \mathbf{R})\mathbf{p}_\beta \,. \tag{3.4}$$

It is assumed that the internal rotation is identified with $\mathbf{R}^s$. It means that in the S domain only this rotation appears. Thereby, the evolution of the internal rotation is viewed as relatively faster than the external rotation in the considered domain.

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 the number of variables is reduced.

Let $\mathbf{U}^c = \mathbf{U}^s\mathbf{V}$ and $\mathbf{Rp}_\beta = \overline{\mathbf{p}}_\beta$. With the help of this, a variable $\overline{\mathbf{a}}_\beta = \mathbf{Ra}_\beta$ is introduced. This variable can also be expressed as $\overline{\mathbf{a}}_\beta = (\mathbf{R}^s\mathbf{U}^c - 1)\overline{\mathbf{p}}_\beta$. With the help of the last formula we can discuss a problem of existence of the internal rotation.

The plane spanned on $\overline{\mathbf{p}}_1$, $\overline{\mathbf{p}}_2$ is undeformed if

$$\begin{aligned} \mathbf{U}^c\overline{\mathbf{p}}_1\mathbf{U}^c\overline{\mathbf{p}}_1 &= \overline{\mathbf{p}}_1\overline{\mathbf{p}}_1 \,, \\ \mathbf{U}^c\overline{\mathbf{p}}_1\mathbf{U}^c\overline{\mathbf{p}}_2 &= \overline{\mathbf{p}}_1\overline{\mathbf{p}}_2 \,, \\ \mathbf{U}^c\overline{\mathbf{p}}_2\mathbf{U}^c\overline{\mathbf{p}}_2 &= \overline{\mathbf{p}}_2\overline{\mathbf{p}}_2 \,. \end{aligned} \tag{3.5}$$

Furthermore, we assume that austenite and martensite are fitted together if $\overline{\mathbf{a}}_\beta = 0$. It means that

$$(\mathbf{R}^s\mathbf{U}^c - 1)\overline{\mathbf{p}}_1 = 0, \qquad (\mathbf{R}^s\mathbf{U}^c - 1)\overline{\mathbf{p}}_2 = 0. \tag{3.6}$$

It is known from crystallographic considerations that $\mathbf{U}_c$ can be interpreted to be responsible for the Bain strain and micrononhomogeneous shear. On the other hand, we have obtained in (3.5) and (3.6) nine equations and nine variables $\mathbf{U}^c$ and $\mathbf{R}^s$. It is known from crystallographic considerations that for equilibrium martensite $\mathbf{U}^c \neq 1$. Thus, if $\mathbf{R}^s = 1$ then Eqs. (3.6) are not satisfied. Consequently, there exist $\mathbf{R}^s \neq 1$.

4. Free energy

A model of the free energy plays a key role in the discussed small-scale approach. Detailed phenomena modelled by the free energy give evidence of what

kind of averaging is used. We have discussed the evolution of crystal structure during the martensitic transformation. As a result, components of the deformation measure are introduced in order to describe this process.

Consequently, we take into account the shear strain in separate shear systems, shuffles represented by relative displacement vectors, internal rotations towards habit planes which can be modelled with the help of directors. Furthermore, we observe in Fig. 4 that the interfaces are flat. Such a phenomenon should appear as a result of mechanical properties of interfaces. Therefore, this fact should also influence the free energy form.

Accordingly, the most important independent variables of the free energy were discussed in the previous section. Furthermore, we assume that the free energy depends on temperature and some internal state variables which will be discussed later.

The free energy will be introduced with the help of the following program:

1. The skeleton of the free energy is based on geometrical objects distinguished in crystal structure of austenite. They are:
   - Bain axes,
   - six different basal planes in undeformed state of austenite,
   - twenty four habit planes,
   - directions of micrononhomogeneous shear.
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. In this region the phase transformation is initiated.
4. The first stage of construction of the free energy consists in defining its part which depends mainly on the strain tensor.
5. The second stage consists in introducing relative displacement vectors in order to describe the evolution of shuffles.
6. The third stage consists in taking into account internal rotations towards possible habit planes.
7. The last stage consists in introducing higher gradients of deformation.

First, the part of the free energy which depends mainly on the Lagrangean strain tensor $\mathbf{e}$ is introduced. As follows from crystallographic considerations, this part of the free energy should have six minima for martensite and one for austenite. Furthermore, the elastic properties of austenite and martensite near their equilibrium position are assumed to be modelled by a quadratic form with respect to the strain tensor $\mathbf{e}$.

Let E be a set of all strain tensors $\mathbf{e}$ expressed in the basis $\mathbf{b}$. Let us assume that E can be decomposed into the sum $E = A \cup S \cup \bigcup_I M_I$ of sets which represents elastic range for austenite, a spinodal region and elastic range for the

I-th variant of martensite, respectively. These sets are defined as

$$A = \{\mathbf{e} : F_{ijkl}(\mathbf{e}) > 0,\ l(\mathbf{0},\ \mathbf{e}) \subset A\}, \tag{4.1}$$

$$M_I = \{\mathbf{e} : F_{ijkl}(\mathbf{e}) > 0,\ l(\mathbf{e}_{MI},\ \mathbf{e}) \subset M_I\}, \tag{4.2}$$

where

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

$l(\mathbf{e}',\ \mathbf{e}'')$ means a segment with ends $\mathbf{e}'$, $\mathbf{e}''$, $\mathbf{e}_{MI}$ is a strain assigned to I-th martensite variant in equilibrium. The set S is a domain where $F_{ijkl}(\mathbf{e})$ is not positive definite. Let us remark that $\partial S_A = \partial A$ and $\partial S_{MI} = \partial M_I$.

Let $\overline{F}_A = c_{ijkl}e_{ij}e_{kl}$ be a positive definite form which describes elastic properties of austenite near the equilibrium point $\mathbf{e} = \mathbf{0}$. Such elastic properties are real only in some neighbourhood U_A of this point. On the ∂S_A the free energy is not positive definite. Thus, the function $\overline{F}_A$ should be appropriately modified in domain $A - U_A$. Similarly, a positive definite quadratic form $\overline{F}_{MI} = c_{MIijkl}(e_{ij} - e_{MIij})(e_{kl} - e_{MIkl}) + d$ which represents elastic properties of I-th martensite is introduced. Furthermore, we assume that a critical stress as well as the corresponding strain for which martensitic transformation is initiated is known. It means that forms of hipersurfaces ∂S_A and ∂S_{MI} are postulated in E where the free energy should be semipositive only.

It is convenient to discuss the form of the free energy or, more exactly, the graph of the free energy as a fiber bundle. The fiber bundle is understood here as a generalization of Cartesian product of basis manifold and a fiber manifold [30].

Let $A_I : E \to E_I$ be a mapping which transforms the strain tensors expressed in basis $\mathbf{b}$ into the strain tensors expressed in basis $\mathbf{d}_I$. Let $e_{I12} = \mathbf{d}_{I1}\mathbf{e}\mathbf{d}_{I2}$ be a component of strain tensor $\mathbf{e}_I \in E_I$. It is known from previous considerations that the most characteristic feature of the martensitic transformation is the shear strain. In the discussed case it is the shear strain in shear system $\{\mathbf{d}_{I1},\ \mathbf{d}_{I2}\}$. Accordingly, e_{I12} is just the main feature of martensite variants created in this shear system.

Let us introduce sets $N_{IA} = \{e_{I12} : 0 \leq e_{I12} \leq e^*_{I12}\}$, $N_{IS} = \{e_{I12} : e^*_{I12} \leq e_{I12} \leq e^{**}_{I12}\}$, $N_{IM} = \{e_{I12} : e^{**}_{I12} \leq e_{I12} \leq e_{MI12}\}$ and $N_I = N_{IA} \cup N_{IS} \cup N_{IM}$, where e^*_{I12} and e^{**}_{I12} are components of strains such that $e^*_I \in \partial S_A$ and $e^{**}_I \in \partial S_{MI}$. Functions $\overline{F}_A$ and $\overline{F}_{MI}$ are expressed in the basis $\mathbf{d}_I$ as $\overline{F}_{AI}(\mathbf{e}_I) = \overline{F}_A \circ A_I^{-1}(\mathbf{e}_I)$ and $\overline{F}_{MII}(\mathbf{e}_I) = \overline{F}_{MI} \circ A_I^{-1}(\mathbf{e}_I)$.

Let $h_{AI}(e_{I12}) : \partial S_A \to f(e_{I12})$, $e_{I12} \in N_{IA} - \{0\} = N_0$ be a family of homeomorphisms. Then, N_0 can be seen as a basis of a fiber bundle and $f(e_{I12})$ as a family of fibers. As a result, we consider the elastic domain $A = \bigcup_{e_{I12} \in N_0}\{e_{I12},\ f(e_{I12})\} = N_0 \times \partial S_A$ as a fiber bundle or, in other words, as a generalized Cartesian product of N_0 and ∂S_A. The projection in this bundle acts as $\pi(f(e_{I12})) = e_{I12}$. We discuss one coordinate representation. Then, the structural group consists of one element only.

Let us introduce the following sets in $E_I \times R$ space:

$$\overline{B}_{IA} = \{b_{IA12} = \{e_{I12}, \overline{F}_{AI}(e_{I12})\} : e_{I12} \in N_{IA}\}$$

and

$$\overline{B}_{IM} = \{b_{IM12} = \{e_{I12}, \overline{F}_{MI}(e_{I12})\} : e_{I12} \in N_{IM}\}.$$

Let us consider also the sets $\overline{F}_{\partial S} = \{\{e_I, \overline{F}_{AI}|_{\partial S_A}\} : e_I \in \partial S_A = f(e^*_{I12})\}$ and $F_{f(e_{I12})} = \{\{e_I, \overline{F}_{AI}|_{f(e_{I12})}\} : e_I \in f(e_{I12})\}$. With the help of these sets we can determine the graph of $\overline{F}_{AI}$ as a fiber manifold

$$\overline{F}_{AI} = \bigcup_{e_{I12} \in N_0} \left\{b_{IA12}, F_{f(e_{I12})}\right\} = \overline{B}_{IA} \times \overline{F}_{\partial S} \tag{4.3}$$

with projection π in the bundle as $\pi(F_{f(e_{I12})}) = b_{IA12}$.

As it was mentioned previously, $\overline{F}_A$ has not an appropriate form because it is not positive definite on ∂S_A. Therefore, $\overline{F}_A$ should be modified on $A - U_A$.

It is assumed that $\mathbf{0} \in U_A$, $U_A \subset \operatorname{int} A$ and there exists e_{I12} which gives $\partial U_A = f(e_{I12})$. The idea of modification (4.3) consists in introduction of a modifying function C such that we obtain from $\overline{F}_{AI}$ a new function F_{AI} in the form

$$F_{AI} = \begin{cases} \overline{F}_{AI}|_{U_A}, & \mathbf{e}_I \in U_A, \\ \overline{F}_{AI} + C, & \mathbf{e}_I \in A - U_A. \end{cases} \tag{4.4}$$

The graph of the map C is assumed as

$$C = \begin{cases} \{\mathbf{e}_I, 0\}, & \mathbf{e}_I \in U_A, \quad e_{I12} \leq \bar{e}_{I12} = N_{IA} \cap \partial U_A, \\ \{\mathbf{e}_I, C_{e_{I12}}(\mathbf{e}_I)\}, & \mathbf{e}_I \in f(e_{I12}), \quad \bar{e}_{I12} < e_{I12} < e^*_{I12}, \end{cases} \tag{4.5}$$

where the condition

$$\frac{\partial^2(\overline{F}_{AI} + C)}{\partial e^2_{I12}}(e^*_{I12}) = 0$$

is fulfilled and F_{AI} is semipositive definite on the whole ∂S_A.

Let furthermore $B_{IA} = \{\{e_{I12}, F_{AI}(e_{I12})\} : e_{I12} \in N_{IA}\}$ and $F_{\partial S_A} = \{\{e_I, (\overline{F}_{AI} + C)\}|_{\partial S}\} : e_I \in \partial S_A\}$. Then, we have defined the free energy F_{AI} in the domain A and the graph of this function can be identified with the generalized product $B_{IA} \times F_{\partial S_A}$.

The function F_{AI} can be expressed in basis $\mathbf{b}$ as $F_A = F_{AI} \circ A_I(\mathbf{e})$. There are six shear systems I. Such a construction can be carried out in six ways. We assume that they lead to the same results since we have only one variant of austenite.

Similar construction will be carried out for martensite variants. Let $h_{MI}(e_{I12})$: $\partial S_{MI} \to f(e_{MI})$, $e_{I12} \in N_{IM} - \{e_{MI12}\} = N_{IMo}$ be a family of homeomorphisms. Then, the elastic domain for the I-th martensite variant can be expressed as $M_I = \bigcup_{e_{I12} \in N_{IMo}} \{e_{I12}, f_{MI}(e_{I12})\} = N_{IMo} \times \partial S_{MI}$.

Let us consider the sets $\overline{F}_{\partial S_{MI}} = \{\{e_I,\ \overline{F}_{MII}|_{\partial S_{MI}}\} :\ e_I \in \partial S_{MI} = f(e^{**}_{I12})\}$ and $F_{MIf}(e_{I12}) = \{\{e_I,\ \overline{F}_{MII}|_{f_{MI}(e_{I12})}\} :\ e_I \in f_{MI}(e_{I12})\}$. Then, the function $\overline{F}_{MII}$ takes the form

$$\overline{F}_{MII} = \bigcup_{e_{I12} \in N_{IMo}} \{b_{IM_{12}},\ F_{MIf}(e_{I12})\} = \overline{B}_{IM} \times \overline{F}_{\partial S_{MI}}\,. \tag{4.6}$$

Let us assume that the elastic properties of the I-th martensite are given in elliptic form only in a set $U_{MI} \subset intM_I$, and that there exists $\check{e}_{I12} \in N_{IMo}$ which gives $\partial U_{MI} = f_{MI}(\check{e}_{I12})$. Then, a correction function C_{MI} induces a new form $\overline{F}_{MII}$ as

$$F_{MII} = \begin{cases} \overline{F}_{MII}\,, & \mathbf{e}_I \in U_{MI}\,, \\ \overline{F}_{MII} + C_{MI}\,, & \mathbf{e}_I \in M_I - U_{MI}\,. \end{cases} \tag{4.7}$$

The map C_{MI} is assumed in the following form:

$$C_{MI} = \begin{cases} \{\mathbf{e}_I,\ 0\}, & \mathbf{e}_I \in U_{MI}\,, \\ \{\mathbf{e}_I,\ C_{MI}(e_{I12})\}, & \mathbf{e}_I \in f(e_{I12}),\quad e^{**}_{12} \le e_{I12} \le \check{e}_{I12} \end{cases} \tag{4.8}$$

with the following condition

$$\frac{\partial^2(\overline{F}_{MII} + C_{MI})}{\partial e^2_{I12}}(e^{**}_{I12}) = 0,$$

and F_{MII} is semipositive definite on the whole ∂S_{IM}.

Let furthermore $B_{IM} = \{\{e_{I12}, F_{MII}(e_{I12})\} :\ e_{I12} \in N_{IM}\}$ and $F_{\partial S_{MI}} = \{\{e_I, (\overline{F}_{IMI} + C_{MI})\}|_{\partial S_{MI}}\} :\ e_I \in \partial S_{MI}\}$. Then, we have defined the free energy F_{MII} in the domain M_I and the graph of this function can be identified with generalized product $B_{IM} \times F_{\partial S_{MI}}$.

The function F_{MII} can be expressed as $F_{MI} = F_{MII} \circ A_I(\mathbf{e})$ in basis $\mathbf{b}$. Let us note that an internal rotation can appear. Then, the martensite becomes rotated with respect to the austenite. As a result of this, elastic constants undergo a transformation being dependent on the possible rotation. In order to stress this fact we write $F_{MI} = F_{MII}(\mathbf{R}) \circ A_I(\mathbf{e})$. It is assumed that $\mathbf{R}$ is not variable at this place but is fully determined.

The form of the free energy function in the S domain 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:

$$\begin{aligned} &F_S|_{N_{IS}} = B_{IS}\,, \qquad F_S|_{\partial S_A} = F_A|_{\partial S_A}\,, \qquad F_S|_{\partial S_{MI}} = F_{MI}|_{\partial S_{MI}}\,, \\ &\frac{\partial F_S}{\partial \mathbf{e}}\Big|_{\partial S_A} = \frac{\partial F_A}{\partial \mathbf{e}}\Big|_{\partial S_A}\,, \qquad \frac{\partial F_S}{\partial \mathbf{e}}\Big|_{\partial S_{MI}} = \frac{\partial F_{MI}}{\partial \mathbf{e}}\Big|_{\partial S_{MI}}\,, \\ &\frac{\partial^2 F_S}{\partial \mathbf{e}\partial \mathbf{e}}\Big|_{\partial S_A} = \frac{\partial^2 F_A}{\partial \mathbf{e}\partial \mathbf{e}}\Big|_{\partial S_A}\,, \qquad \frac{\partial^2 F_S}{\partial \mathbf{e}\partial \mathbf{e}}\Big|_{\partial S_{MI}} = \frac{\partial^2 F_{MI}}{\partial \mathbf{e}\partial \mathbf{e}}\Big|_{\partial S_{MI}}\,, \end{aligned} \tag{4.9}$$

where B_{IS} should be postulated.

General features of temperature dependence are presented by means of plotting components of the free energy $c_{ijkl}(T)$, $\partial S_A(T)$, $C(T)$, $c_{MIijkl}(T)$, $\partial S_{MI}(T)$, $C_{MI}(T)$ with temperature. Increasing temperature we can pass from stable martensite to a pseudoelastic case. It is displayed by conditions $\frac{\partial F}{\partial \mathbf{e}}(\mathbf{e}_{MI}) = 0$ in the first case, and by $\frac{\partial F}{\partial \mathbf{e}}(\mathbf{e}_{MI}) \neq 0$ in the second case.

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

$$F_E = \begin{cases} F_A\,, & \mathbf{e} \in A\,, \\ F_{MII}(\mathbf{R}) \circ A_I\,, & \mathbf{e} \in M_I\,, \\ F_S\,, & \mathbf{e} \in S\,. \end{cases} \tag{4.10}$$

Another part of the free energy is related to micrononhomogeneous deformation. We have discussed previously that the shuffles appear in two possible directions $\mathbf{d}_{I1}$ or $\mathbf{d}_{I2}$ in a given I-th shear system. Thus, 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.

With the help of C_α, a bifurcation for evolution of $\mathbf{w}_\lambda$ can be modelled. To this end let us introduce a function of variable $\mathbf{w}_\lambda$ given by

$$M_{I\lambda} = C_1(\mathbf{w}_\lambda \mathbf{d}'_{I2})(\mathbf{w}_\lambda \mathbf{d}'_{I1})^2 + C_2(\mathbf{w}_\lambda \mathbf{d}'_{I1})(\mathbf{w}_\lambda \mathbf{d}'_{I2})^2\,. \tag{4.11}$$

Properties of functions C_α produce evolution of the relative displacement vector $\mathbf{w}_\lambda$ in two possible dominant directions $\mathbf{d}'_{I1}$ or $\mathbf{d}'_{I2}$. Evolution along $\mathbf{d}'_{I1}$ eliminates evolution in $\mathbf{d}'_{I2}$ and inversely. However, we have a group of vectors $\mathbf{w}_\lambda$ since $\lambda \in \Lambda$. Kinematical considerations indicate that all vectors of this group should develop in the same directions after a bifurcation (Fig. 2). Thus, we have a collective bifurcation. Therefore, an energetic barrier should make impossible a bifurcation of $\mathbf{w}_\lambda$ and $\mathbf{w}_{\lambda'}$, $\lambda \neq \lambda'$ in two different directions.

Let us introduce some additional notations. By $d_{\alpha\lambda\lambda'} = d(\mathbf{w}_\lambda \mathbf{d}'_{I\alpha},\ \mathbf{w}_{\lambda'} \mathbf{d}'_{I\alpha})$ we denote a distance between $w_{\lambda\alpha} = \mathbf{w}_\lambda \mathbf{d}'_{I\alpha}$ and $w_{\lambda'\alpha}$. We use functions C_α again. Let us consider next the function of variables $\mathbf{w}_\lambda$ and $\mathbf{w}_\lambda$ in the form

$$M_{I\lambda\lambda'} = C_1(d_{2\lambda\lambda'})d^2_{1\lambda\lambda'} + C_2(d_{1\lambda\lambda'})d^2_{2\lambda\lambda'}\,. \tag{4.12}$$

This function has a similar structure as function (4.11). Therefore, if $\mathbf{w}_\lambda$ develops in one direction then an energetic barrier appears and blocks evolution of $\mathbf{w}_{\lambda'}$ in the other direction.

The functions introduced above describe the 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. Previous 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 phenomenon happens, for instance, in CuAlNi alloy. In this case, during loading and unloading, vectors $\mathbf{w}_\lambda$ change in two different ways. Then, new stress-induced phases appear. They can be distinguished only by positions of the relative displacement vectors. In order to obtain a possibility of modelling such a phenomenon, the following function is postulated:

$$M_{WI\lambda} = \Psi(a_\lambda(e_{I12}) + w_\lambda) - f_\lambda(e_{I12})(a_\lambda(e_{I12}) + w_\lambda), \tag{4.13}$$

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. By means of similar functions, the two-path martensitic transformation has been discussed in [19].

Finally, the part of the free energy which describes shuffles is suggested in the form

$$F_{W(J)} = \sum_\lambda M_{I\lambda} + \sum_{\lambda \neq \lambda',\ \lambda > \lambda'} M_{I\lambda\lambda'} + \sum_\lambda M_{WI\lambda}\,, \tag{4.14}$$

where $J = (I,\ \alpha)$.

Next component of the free energy describes the evolution of internal rotation towards a habit plane. We have twenty four possible habit planes. They can be marked by multi-index $K = (I,\ \alpha,\ \beta) = (J,\ \beta)$, $\alpha, \beta = 1,\ 2$. The habit plane can be represented by a pair of linearly independent vectors $\mathbf{p}_{K\mu}$, $\mu = 1,\ 2$ which are determined in the crystal structure of austenite. In Sec. 3 we have discussed variables which are appropriate for description of the internal rotation. Let us introduce these variables in a convenient form

$$a_{K\mu} = \mathbf{R}^{-1}(\mathbf{F}^{ea})(\mathbf{F}^s\mathbf{F}^{ea} - \mathbf{R}^{-1}(\mathbf{F}^{ea}))\mathbf{p}_{K\mu}\,. \tag{4.15}$$

The deformation gradient $\mathbf{F}^{ea}$ is assigned to the configuration known and fixed at the moment. Thus, all variables $\mathbf{a}_{K\mu}$ depend in fact only on $\mathbf{F}^s$ as independent variable.

Let V_s be a space of all admissible $\mathbf{F}_s \in V_s(x_\alpha(\mathbf{X}_P))$. V_s depends on a fixed configuration $x_\alpha(\mathbf{X}_P)$ for the considered point $\mathbf{X}_P$.

In the space V_s we define curves $K_{J\beta}(e_{I12})$ which are parameterized by $e_{I12} \in N_{IS}$. They have the following properties: $K_{J1}(e_{I12}) = K_{J2}(e_{I12})$ for $e^*_{I12} < e_{I12} < \bar{e}_{I12}$, where $\bar{e}_{I12}$ only slightly exceeds e^*_{I12}. $K_{J1}(\bar{e}_{I12}) \cap K_{J2}(\bar{e}_{I12}) = B \in V_s$, where B is a bifurcation point for these curves which do not coincide for points $e_{I12} > \bar{e}_{I12}$. Thus, the two curves coincide up to the bifurcation point B accompanied by $\bar{e}_{I12}$. By this we introduce the assumption that internal rotation appears

directly after exceeding e^*_{I12}, and then also the bifurcation process starts. We assume that for $K_{J1}(e^{**}_{I12})$ and $K_{J2}(e^{**}_{I12})$, the following conditions are satisfied: $\mathbf{a}_{J1} = 0$, $\mathbf{a}_{J2} \neq 0$ and $\mathbf{a}_{J2} = 0$, $\mathbf{a}_{J1} \neq 0$, respectively. It means that austenite and martensite are fitted together at the end of these curves. Thus, the $K_{J\beta}$ are viewed as certain paths of deformation and create a skeleton for this part of the free energy.

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

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

These properties prove the symmetry of evolution for two possible internal rotations.

Construction of the part of the free energy which depends on rotation is introduced also with the help of the basis and fibers which together create a graph manifold as a fiber bundle. Let us consider a basis

$$b_{J\beta}(e_{I12}) = \{K_{J\beta}(e_{I12}),\ g(K_{J\beta}(e_{I12}))\}.$$

It is assumed also that parts of the domain can be represented as a generalized product in the form $D_{RJ\beta} = K_{J\beta}(e_{I12}) \times D_{J\beta}(e_{I12}) \subset V_s$ and $D_{RJ1} \cap D_{RJ2} \neq \emptyset$, $D_{RJ1} \cup D_{RJ2} = V_s$. Then, we are able to define

$$f_{J\beta}(e_{I12}) = \{\{D_{J\beta}(e_{I12}),\ g_f(\mathbf{F})(e_{I12})\} :\ \mathbf{F} \in D_{J\beta}(e_{I12})\}$$

with the property that $\inf_{\mathbf{F}} g_f(\mathbf{F}) = g(K_{J\beta}(e_{I12}))$. The infimum is attained for $\mathbf{F} \in K_{J\beta}(e_{I12}) \cap D_{J\beta}(e_{I12})$. $f_{J\beta}$ is viewed as a fiber for defining the graph of the considered part of the free energy. Function g_f attains minimum at intersection of $D_{J\beta}$ and $K_{J\beta}$ or, in other words, at the intersection with the basis $b_{J\beta}$.

Now the mentioned part of graph of the free energy can be defined as

$$F_{R(K)}(\mathbf{F}^s) = \begin{cases} b_{J1}(e_{I12}) \times f_{J1}(e_{I12}), & \mathbf{F}^s \in D_{RJ1}, \\ b_{J2}(e_{I12}) \times f_{J2}(e_{I12}), & \mathbf{F}^s \in D_{RJ2}. \end{cases} \tag{4.16}$$

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

The model considered is related to a small volume of averaging. Then, nonlocal effects become more important. These effects can be approximated by higher gradients of deformation.

During the martensitic transformation we observe, in a small scale, the thickness of the interface. On the other hand, the interfaces are flat during the transformation. Furthermore, we can consider breaking of interfaces during the appropriate loading process [27]. Thus, interfaces have many fine features which

should be modelled in a small scale. These phenomena suggest the necessity of taking into consideration higher gradients of deformation as an approximation of nonlocal effects.

Some models which take into account this kind of description of the martensitic transformation are considered in literature. See for instance [22, 23, 4].

In the paper, a concept of application of higher gradients in description of fine features of the interfaces is discussed. First, let us introduce this concept with the aid of a two-dimensional example on a plane. Let ϕ be a field on the plane and $\mathbf{m}$ and $\mathbf{n}$ be two linearly independent vectors. Let us consider a free energy as an example, in the following form:

$$F_\phi = C_m(D_{\mathbf{m}}\phi)^2 + C_n(D^s_{\mathbf{m}}\phi)(D_{\mathbf{n}}\phi)^2. \tag{4.17}$$

It is assumed that the function C_n has properties shown at Fig. 7. It means that it is a symmetric positive function of its argument, it has maximum at point 0 and strongly decreases to zero if the argument increases. If the derivative of rank s in direction $\mathbf{m}$ is large enough, then the dependence of F_ϕ on $D_{\mathbf{n}}\phi$ vanishes. Consequently, propagation of ϕ will be continued first in the $\mathbf{m}$ direction. It happens since the gradient dependence on $D_{\mathbf{m}}\phi$ accelerates the equalization of field ϕ in the $\mathbf{m}$ direction. As a consequence, $D^s_{\mathbf{m}}\phi$ gradually vanishes and propagation in direction $\mathbf{n}$ becomes more active. This concept will be next generalized to a three-dimensional model.

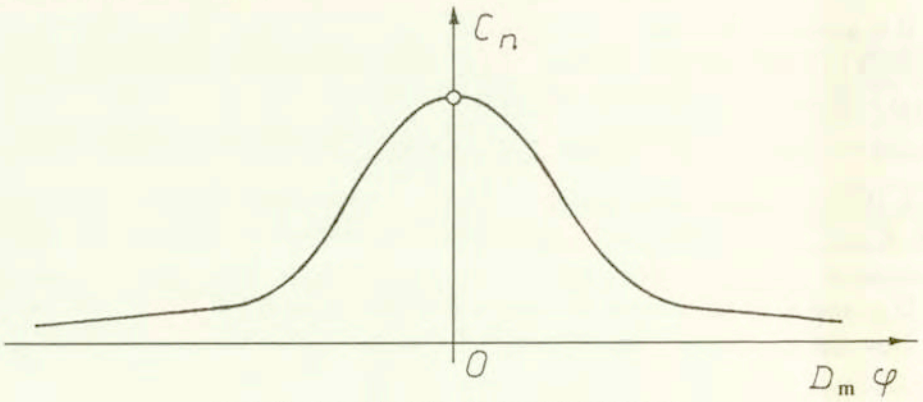

FIG. 7. A qualitative form of function C_n.

A crystal structure, in general, has some distinguished directions. They are connected with arrangement of the atoms. If the interface appears, then some directions can be distinguished on this interface for the same reason.

Let $B_K = \{\mathbf{b}_1, .., \mathbf{b}_N\}$ be a set of distinguished directions on the habit plane HP_K and $\mathbf{v}_K$ be a vector which is perpendicular to this plane. Vectors $\mathbf{b}_1, .., \mathbf{b}_N$ are in general linearly dependent.

Let us consider a point $\mathbf{X}$ which lies on the interface. This fact can be recognized by the state of deformation. Furthermore, we can investigate a deformation

in the neighbourhood of this point and determine what is a preferred direction lying on this habit plane HP_K for this point. More exactly, if the point lies on a flat interface, no direction is preferred. However, if the interface is curved at this point then, it is assumed, a kind of edge on this plane appears. This "edge" reflects the arrangement of atoms and, as a consequence, a preferred direction of the crystal structure. It is assumed that the set B_K is just a set of these preferred directions and they can be recognized by the analysis of deformation near the point $\mathbf{X}$.

Let us introduce a function $p(\mathbf{X}) = \{\mathbf{k},\ \mathbf{l},\ \mathbf{v}_K\}$ which assigns a triplet of vectors to point $\mathbf{X}$. The vector $\mathbf{k} \in B_K$ indicates the preferred direction, $\mathbf{l} \in HP_K$ and $\mathbf{lk} = 0$. Let, furthermore, $\mathbf{M} = \{M_q\} = \{F_{iM},\ w_{\lambda N}\}$ be a set of variables.

After these preparations, the following form of the free energy dependent on higher gradients of deformation is assumed:

$$F_{\mathcal{B}(K)} = \sum_q \Big[C_{kq}(p(\mathbf{X}),\ \mathbf{k})(D_{\mathbf{k}}M_q)^2 + C_{lq}(p(\mathbf{X}),\ \mathbf{l},\ D_{\mathbf{k}}M_q)(D_{\mathbf{l}}M_q)^2 + C_{vq}(p(\mathbf{X}),\ \mathbf{v}_K,\ D_{\mathbf{k}}M_q,\ D_{\mathbf{l}}M_q)(D_{\mathbf{v}}M_q)^2\Big]. \tag{4.18}$$

The idea of dependence of C_{lq} and C_{vq} on $D_{\mathbf{k}}M_q$ and $D_{\mathbf{l}}M_q$ follows from (4.17). If $D_{\mathbf{k}}M_q$ is large enough then C_{lq} and C_{vq} vanishes and development in the $\mathbf{k}$ direction is preferred. Next degree of this hierarchy consists in the fact that the surface is straight in direction $\mathbf{k}$. As a result, we have $D_{\mathbf{k}}M_q = 0$ and then $\mathbf{l}$ is the second direction of development. Third degree of this hierarchy is evidently the $\mathbf{v}_K$ direction.

Let us note that formula (4.18) takes into considerations the symmetry of crystal structure of both the austenite and martensite. It consists in taking into account the distribution of directors $\mathbf{p}_{K\mu}$ which define the habit planes and vectors $\mathbf{v}_K$. Position of habit planes uniquely defines the kind of martensite variant which is fitted together with austenite on this plane. This is just connected with crystal symmetries of these two structures.

Summing up the above considerations, let us notice that we have constructed four summands of the free energy. However, they depend on multi-indices I, J, K. Therefore, the domain of the free energy is not determined clearly enough.

Let us observe that independent variables and their higher gradients do not take all possible values but only some admissible ones. Indeed, we do not expect that, for instance, $\mathbf{w}_\lambda$ takes a very large value. Rather, we define only some admissible domains in the set of all possible values of variables. These domains are defined here by means of multi-indices I, J, K.

Let $\partial S_{AI} = \{\mathbf{e} :\ \mathbf{d}_{I1}\mathbf{e}\mathbf{d}_{I2} = e^*_{I12},\ \mathbf{d}_{I'1}\mathbf{e}\mathbf{d}_{I'2} < e^*_{I'12},\ I \neq I'\}$. With the help of this we obtain $\partial S_A = \bigcup \partial S_{AI}$. The set ∂S_{AI} determines the validity of index I for a further stage of deformation. If the deformation attains this set then it means that the first e^*_{I12} is attained still before $e^*_{I'12}$. As a result, two paths for bifurcation for $\mathbf{w}_\lambda$ are determined and two other for the internal rotation given

in $\mathbf{F}^s$. 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 this paths. It means that the domain of admissible $\mathbf{w}_\lambda$ is

$$W_J = W_{I\alpha} = \{\mathbf{w}_\lambda : \mathbf{w}_\lambda \in U(\mathbf{w}_{\lambda\alpha}),\ \lambda \in \Lambda\} = \Pi_\lambda U(\mathbf{w}_{\lambda\alpha}) . \tag{4.19}$$

Similarly, we assume that $\mathbf{F}_s$ develops near its path $K_{J\beta} = K_K$ in some neighbourhood $U(K_{J\beta})$. Thus, we have

$$V_K = V_{J\beta} = \{\mathbf{F}^s : \mathbf{F}^s \in U(K_{J\beta})\}. \tag{4.20}$$

Dependence of the free energy on higher gradients is connected with the habit plane HP_K. Thus, the set of admissible higher gradients of deformation takes the form

$$H_K = \left\{ \left\{ \frac{\partial}{\partial X_i} M_q \right\} : \quad i = 1, 2, 3 \right\} . \tag{4.21}$$

Finally, we define subdomains of the free energy with the help of multi-indices $K = (I,\ \alpha,\ \beta) = (J,\ \beta)$ as $D_K = E \times W_J \times V_K \times H_K$. Thus, the total domain is assumed as

$$D = \bigcup_K (E \times W_J \times V_K \times H_K). \tag{4.22}$$

The total form of the free energy is then described by means of the expression

$$F_K(g) = F_E + F_{W(J)} + F_{R(K)} + F_{G(K)}, \qquad g \in D_K . \tag{4.23}$$

The free energy can be also expressed with the aid of graph manifold in the following form,

$$\{g,\ F(g)\} = \bigcup_K \bigcup_{g \in D_K} \{g,\ F_K(g)\}. \tag{4.24}$$

It is assumed that in regions where $D_K \cap D_{K'} \neq \emptyset$, the free energy is determined equivalently.

Let us note that such a form of the free energy is relatively simple in comparison with those given in the Landau theory [29]. The expression given by (4.23) reflects many properties which are introduced by the geometrical skeleton of this construction. This skeleton is based on ∂S_A, $\mathbf{d}_I$, symmetries near $\mathbf{e} = \mathbf{0}$, $\mathbf{e} = \mathbf{e}_{MI}$ and directors $\mathbf{p}_{K\mu}$. Accordingly, we are able to introduce terms of the free energy which are responsible for separate phenomena.

Let us observe that second or third-order terms of the free energy in three-dimensional case in the Landau theory [29] are very long polynomials. They are difficult for physical interpretations. In order to express the free energy which is discussed in the paper, the degrees of polynomials have to be much more higher.

The expression (4.23) has a good physical interpretation. It takes place owing to the mentioned geometrical skeleton which is connected just with interpretation of the physical processes.

Summing up this comment we may say that the form of the free energy is relatively simple in comparison with those known from the Landau theory. On the other hand, this form is relatively complicated in comparison with those from the more averaged level of description.

5. Thermodynamical description of the martensitic transformation

The model with small volume of averaging describes the detailed behaviour of microstructure. Therefore, the free energy introduced in the previous section is relatively complicated. This function is a basis for the model discussed in the paper. As a next step, balance equations and a more general form of constitutive equations will be discussed.

Let us note that during kinematical considerations, a few displacement functions have been introduced. It follows from the micrononhomogeneous deformation which appears during the martensitic transformation. Such a deformation is connected with complex crystal lattice. It suggests a multicomponent description. However, in general, we would like to avoid such a description since it is too complicated. On the other hand, relative displacement of atoms are not a large deviation from homogeneity. Consequently, the one-component description is most appropriate. In such a case the presence of relative displacement vectors can be viewed as a result of a multicomponent approach.

In the first stage of our considerations, energy balance equations for multicomponent body are introduced. Next, we approximate them by a balance equation connected with one-component description, with some effects which are a result of the initial approach.

Let us introduce a set of displacement functions discussed in Sec. 3

$$\mathbf{z}_\mu(\mathbf{X},\ t) = \{\mathbf{x}(\mathbf{X},\ t),\ \mathbf{y}_\lambda(\mathbf{X},\ t) = \mathbf{x} + \mathbf{R}\mathbf{w}_\lambda\}, \tag{5.1}$$

where $\lambda \in \Lambda$, $\mu \in \{0\} \cup \Lambda$. The approximation assumed for function $\mathbf{y}_\lambda$ was discussed in the previous section.

Let us introduce the expressions for energy related to various components of the body

$$\Psi_0 = \int\limits_{\chi(\mathcal{B})} \left(\varrho_0 e + \frac{1}{2}\varrho_0 \dot{x}_i \dot{x}_i\right) dv\,, \qquad \Psi_\lambda = \int\limits_{\chi_\lambda(\mathcal{B})} \left(\varrho_\lambda e + \frac{1}{2}\varrho_\lambda \dot{y}_{\lambda i} \dot{y}_{\lambda i}\right) dv, \tag{5.2}$$

where e is the internal energy density, ϱ_0, ϱ_λ are densities related to individual components and $(\varrho_0 + \sum_\lambda \varrho_\lambda) = \varrho$. In this notation we have also $\Psi_\mu = \{\Psi_0,\ \Psi_\lambda\}$.

The following general form of the balance equation is assumed for considerations [26] as an initial stage

$$\sum_\mu \frac{d}{dt}\Psi_\mu = \sum_\mu \left(-\Phi_\mu(\Psi_\mu) + P_\mu(\Psi_\mu) + S_\mu(\Psi_\mu)\right), \tag{5.3}$$

where Φ_μ is outflow of the conserved quantity Ψ_μ through the boundary of the body, P_μ is the production and S_μ is the source of this quantity.

Taking into account higher gradients of deformation discussed in the model of the free energy, we assume the following form of the outflow Φ_μ:

$$\Phi_\mu(\Psi_\mu) = \int\limits_{\partial\chi_\mu(\mathcal{B})} \left(q_\mu - \sum_{\phi=0}^{G-1} t_{\mu M_1 \ldots M_\phi i} \dot{x}_{i,M_1 \ldots M_\phi} - \sum_{\phi=0}^{H-1} f_{\mu N N_1 \ldots N_\phi} \dot{w}_{\mu N, N_1 \ldots N_\phi} \right) da_\mu , \tag{5.4}$$

where the last term exists only for $\mu = \lambda > 0$.

The remaining parts of equation (5.3) are postulated as

$$P_\mu(\Psi_\mu) = \int\limits_{\chi_\mu(\mathcal{B})} p_{e\mu} dv_\mu \tag{5.5}$$

and

$$S_\mu(\Psi_\mu) = \int\limits_{\chi_\mu(\mathcal{B})} \varrho_\mu (r_\mu + b_{\mu i} \dot{z}_{\mu i}) dv_\mu . \tag{5.6}$$

Let us substitute (5.2), (5.4) – (5.6) into (5.3). Next we perform the limit approximation. Assuming that $\mathbf{w}_\lambda \to 0$ we obtain a one-component body. Then, we assume that

$$\chi_\mu(\mathcal{B}) \to \chi(\mathcal{B}), \qquad \sum_\mu q_\mu \to q, \qquad \sum_\mu t_{\mu M_1 \ldots M_\phi i} \dot{x}_{i,M_1 \ldots M_\phi} \to t_{M_1 \ldots M_\phi i} \dot{x}_{i,M_1 \ldots M_\phi} ,$$

$$\sum_\mu p_{e\mu} \to p_e , \qquad \sum_\mu \varrho_\mu r_{e\mu} \to r_e , \qquad \sum_\mu \varrho_\mu b_{\mu i} \dot{z}_{\mu i} \to b_i \dot{x}_i .$$

However, we do not carry out this transformation consistently. The last term of the sum (5.4) and the kinetic energy in (5.2) related to relative displacement vectors remain. After applying the well-known steps in deriving the balance equations and assuming that $q = \mathbf{qn}$, we obtain the following form of the energy balance equation:

$$\int\limits_{\chi(\mathcal{B})} \left[\varrho \dot{e} + \varrho_0 \ddot{x}_i \dot{x}_i + \sum_\lambda \varrho_\lambda \ddot{y}_{\lambda j} \dot{y}_{\lambda j} + q_{j,j} - p_e - r_e - b_i \dot{x}_i \right] dv$$

$$- \int\limits_{\partial\chi(\mathcal{B})} \left(\sum_{\phi=0}^{G-1} t_{M_1 \ldots M_\phi i} \dot{x}_{i,M_1 \ldots M_\phi} + \sum_\lambda \sum_{\phi=0}^{H-1} f_{\lambda N N_1 \ldots N_\phi} \dot{w}_{\lambda N, N_1 \ldots N_\phi} \right) da = 0. \tag{5.7}$$

Let us consider the kinetic energy part more carefully. Using definition of $\mathbf{y}_\lambda$ we have

$$(5.8)\qquad \sum_\mu \varrho_\mu \ddot{z}_{\mu i}\,\dot{z}_{\mu i} = \varrho_0\,\ddot{x}_i\,\dot{x}_i + \sum_\lambda \varrho_\lambda\,\ddot{y}_{\lambda i}\,\dot{y}_{\lambda i} = \left(\varrho_0 + \sum_\lambda \varrho_\lambda\right)\ddot{x}_i\,\dot{x}_i + \sum_\lambda \varrho_\lambda\,(\ddot{y}_{\lambda i} - \ddot{x}_i)\,\dot{x}_i + \sum_\lambda \varrho_\lambda\,(\ddot{y}_{\lambda i} - \ddot{x}_i)\,\dot{\xi}_i + \sum_\lambda \varrho_\lambda\,\ddot{x}_i\,\dot{\xi}_i \approx \varrho\,\ddot{x}_i\,\dot{x}_i + \sum_\lambda \varrho_\lambda\,\ddot{w}_{\lambda N}\,\dot{w}_{\lambda N}\,.$$

In the last step, interactions between the macroscopic inertia effects represented by time derivatives of x_i and the microscopic inertia effects represented by relative displacement vectors are neglected. It means that the influence of macroscopic motion on relative displacement vectors is due to the internal forces in the material represented by the free energy.

Next problem is related to the internal rotation. The free energy depends not only on the strain tensor but also on the internal rotation in the spinodal region. This suggests the necessity to investigate more carefully the balance of angular momentum. It will be done later. The internal rotation mentioned is connected also with certain inertia effects.

The moment of inertia tensor for the part $\mathcal{P}$ of the body $\mathcal{B}$ is defined by formula $I_{mn} = \int_{\mu(\mathcal{P})} \varrho\varepsilon_{mri}\varepsilon_{ink}r_r r_k dv$, where $\mathbf{r} = \mathbf{x} - \mathbf{x}_c$ is position of the point with respect to the center of mass of $\mathcal{P}$. The moment of inertia density can be defined as

$$i_{mn} = \frac{\partial I_{mn}}{\partial \mu(\mathcal{P})} = \varrho\varepsilon_{mri}\varepsilon_{ink}r_r r_k\,.$$

However, if $\mu(\mathcal{P}) \to 0$ then $\mathbf{r} \to 0$ and finally $i_{mn} = 0$.

The martensitic structure created during the phase transformation tends to fit together with austenite. It happens with the help of material forces which are created by locally nonhomogeneous deformation. It means that atoms are shifted from the averaged positions which are determined by the deformation function. As a result, a local distribution of density with respect to the assumed averaged density is changed. Consequently, we admit for qualitative considerations, that there is a translation $\delta\mathbf{r}$ of the averaged density from the material point in nonequilibrium state with respect to the internal rotation. This shift of density is not connected with the introduced relative displacement vectors since they characterize durable shift of atoms and are constant in martensitic phase. Accordingly, we assume that

$$i_{mn} = \frac{\partial I_{mn}}{\partial \mu(\mathcal{P})} = \varrho\varepsilon_{mri}\varepsilon_{ink}(r_r + \delta r_r)(r_k + \delta r_k) = \varrho\varepsilon_{mri}\varepsilon_{ink}\delta r_r \delta r_k\,.$$

We assume here that during $\mu(\mathcal{P}) \to 0$, an averaging shift of density $\delta\mathbf{r} \neq 0$ can be considered.

In order to take into account the inertia effects related to internal rotations, the kinetic energy term

$$I_k = \frac{1}{2}\int i_{mn}\omega_m\omega_n dv,$$

where $\omega_n = \frac{1}{2}\varepsilon_{nij}(\dot{x}_i)_{,j}$. The term I_k should be added to the formula for the total energy of the body. If we investigate the expression $\frac{d}{dt}I_k$ then we obtain a formula with two main parts. The first one is connected with conservation of i_{mn} and the second one has the form $\int i_{mn}\dot{\omega}_m\omega_n dv$. In the considered case we assume for simplicity, that the term related to conservation of i_{mn} is equal to zero. The author introduces this simplification in order to avoid complicated considerations accompanied by relatively simple effects of a rotational inertia. However, total neglecting of these inertial effects leads to qualitative complications in the balance of angular momentum. Therefore, in what follows, only the last term will be introduced into the balance of energy equation.

In order to predict the final form of energy balance equation and balance of linear momentum, it is assumed that dissipation is introduced by adding and then subtracting the same term in the balance of energy equation (5.7).

$$\begin{aligned}(5.9)\qquad & T^d_{iM}\dot{x}_{i,M} + \sum_\lambda f^d_{\lambda N}\dot{w}_{\lambda N} - T^d_{iM}\dot{x}_{i,M} - \sum_\lambda f^d_{\lambda N}\dot{w}_{\lambda N} \\ & = -T^d_{iM,M}\dot{x}_i + \sum_\lambda f^d_{\lambda N}\dot{w}_{\lambda N} + (T^d_{iM}\dot{x}_i)_{,M} - T^d_{iM}\dot{x}_{i,M} - \sum_\lambda f^d_{\lambda N}\dot{w}_{\lambda N}.\end{aligned}$$

Let $F = \varrho\psi$ and $e = \psi + sT$. We assume that ψ depends on higher gradients of deformation and, furthermore, on some internal state variables $\boldsymbol{\mu}$ which will be discussed in what follows. Then, taking into account the above discussion, the energy balance equation (5.7) is modified and assumes the form

$$\begin{aligned}(5.10)\qquad & \int_{\chi(\mathcal{B})}\Bigg[(-T_{iM,M} + \varrho\,\ddot{x}_i - b_i)\dot{x}_i + \sum_\lambda (f_{\lambda N} + \varrho_\lambda\,\ddot{w}_{\lambda N})\dot{w}_{\lambda N} + \varrho\left(\frac{\partial\psi}{\partial T} + s\right)\dot{T} \\ & \qquad + \varrho\dot{s}T - T^d_{iM}\dot{x}_{i,M} - \sum_\lambda f^d_{\lambda N}\dot{w}_{\lambda N} + q_{i,i} - r_e + \varrho\frac{\partial\psi}{\partial\mu_i}\dot{\mu}_i\Bigg]\,dv \\ & + \int_{\partial\chi(\mathcal{B})}\Bigg[\sum_{\phi=0}^{G-1}(\bar{t}_{iM_1\ldots M_\phi j}n_j - t_{iM_1\ldots M_\phi})\dot{x}_{i,M_1\ldots M_\phi} + (T^d_{iM}x_{j,M})n_j\dot{x}_i \\ & \qquad + \sum_\lambda\sum_{\phi=0}^{H-1}(\bar{f}_{\lambda NN_1\ldots N_\phi j}n_j - f_{\lambda NN_1\ldots N_\phi})\dot{w}_{\lambda N,N_1\ldots N_\phi}\Bigg]\,da = 0,\end{aligned}$$

where

$$T_{iM} = \tilde{T}_{iM} + B_{iM} + T^d_{iM}, \qquad f_{\lambda N} = \varrho\frac{\partial\psi}{\partial w_{\lambda N}} + F_{\lambda NN_1,N_1} + f^d_{\lambda N},$$

and furthermore

$$\tilde{T}_{iM_1} = \sum_{s=1}^{G}(-1)^{s+1}\left(\varrho\frac{\partial\psi}{\partial x_{i,M_1\ldots M_s}}\right)_{,M_s\ldots M_2},$$

$$B_{iM} = \frac{1}{2}i_{mn}\dot{\omega}_m\varepsilon_{nij}x_{M,j},$$

$$F_{\lambda NN_1} = \sum_{s=1}^{H}(-1)^{s}\left(\varrho_\lambda\frac{\partial\psi}{\partial w_{\lambda N,N_1\ldots N_s}}\right)_{,N_s\ldots N_2},$$

$$\bar{t}_{iM_1\ldots M_\phi j} = \sum_{s=\phi+1}^{G}(-1)^{s-\phi+1}\left(\varrho\frac{\partial\psi}{\partial x_{i,M_1\ldots M_s}}\right)_{,M_sM_{s-1}\ldots M_{\phi+2}}x_{j,M_{\phi+1}},$$

$$\bar{f}_{\lambda NN_1\ldots N_\phi j} = \sum_{s=\phi+1}^{H}(-1)^{s-\phi+1}\left(\varrho_\lambda\frac{\partial\psi}{\partial w_{\lambda N,N_1\ldots N_s}}\right)_{,N_sN_{s-1}\ldots N_{\phi+2}}x_{j,N_{\phi+1}}.$$

Assuming the processes in Eq. (5.10) to be time-independent, the balance of linear momentum is expressed by

$$-T_{iM,M} + \varrho\,\ddot{x}_i - b_i = 0 \tag{5.11}$$

in the body $\mathcal{B}$, and

$$\bar{t}_{iM_1\ldots M_\phi j}n_j = t_{iM_1\ldots M_\phi} \tag{5.12}$$

on $\partial\mathcal{B}$, where $\phi = 0, \ldots, G-1$. Furthermore, the term $\bar{t}_{iM_1}$ is modified by adding $T^d_{iM_1}$ to the above defined expression. The remaining equations are

$$f_{\lambda N} + \varrho_\lambda\,\ddot{w}_{\lambda N} = 0 \tag{5.13}$$

in $\mathcal{B}$, and

$$\bar{f}_{\lambda NN_1\ldots N_\phi j}n_j - f_{\lambda NN_1\ldots N_\phi} = 0 \tag{5.14}$$

on $\partial\mathcal{B}$, $\lambda \in \Lambda$.

If the above linear momentum equations are fulfilled then the local form of energy balance equation is given by

$$\varrho\dot{s}T - T^d_{iM}\dot{x}_{i,M} - \sum_\lambda f^d_{\lambda N}\dot{w}_{\lambda N} + q_{i,i} - r_e + \varrho\frac{\partial\psi}{\partial\mu_i}\dot{\mu}_i = 0. \tag{5.15}$$

Let us consider the balance of angular momentum which can be expressed in the well-known form

$$\int_{\chi_\mu(\mathcal{B})}\left[\varepsilon_{ijk}x_j(t_{mk,m} + b_k - \varrho\,\ddot{x}_k) + \varepsilon_{ijk}t_{jk}\right]dv = 0, \tag{5.16}$$

where $t_{jk} = J^{-1}x_{k,M}T_{jM}$. Assuming that the balance of linear momentum is fulfilled we obtain $\varepsilon_{ijk}t_{jk} \equiv \varepsilon_{ijk}J^{-1}x_{k,M}T_{jM} = 0$ what leads to

$$\varepsilon_{ijk}x_{k,M}\overline{T}_{jM} = -\varepsilon_{ijk}x_{k,M}B_{jM}\,, \tag{5.17}$$

where $\overline{T}_{jM} = \tilde{T}_{jM} + T^d_{jM}$. Consequently, introducing the corrective moment of inertia density field gives a possibility of taking into account the inertial reaction of the material on the internal forces acting there during the martensitic transformation.

Equation (5.13) obtained as a result of balance of linear momentum is close to phonon dynamics and it is difficult to expect that in dynamical case it will give correct results. Therefore, rather an approximation procedure is suggested in this place. Equation (5.13) can be discussed in case of slow deformational processes. In such a case we can assume that $\dot{\mathbf{w}}_\lambda \approx 0$. Then, the relation $f_{\lambda N} = 0$ is obtained. Let us consider the theory with $H = 1$. It means that only the first gradients of $\mathbf{w}_\lambda$ are considered. Then, the discussed equation takes the form

$$-\left(\varrho\frac{\partial\psi}{\partial w_{\lambda N,N_1}}\right)_{,N_1} + \varrho\frac{\partial\psi}{\partial w_{\lambda N}} = 0. \tag{5.18}$$

Gradients of $\mathbf{w}_\lambda$ generate a bifurcation of $\mathbf{w}_\lambda$ in some neighbourhood occurring in the same direction.

Equation (5.18) creates a relation $\mathbf{w}^*_\lambda = \mathbf{w}^*_\lambda(g')$, where g' is the part of the deformation measure which does not contain $\mathbf{w}_\lambda$. However, this relation is not a function since bifurcation processes are considered. Therefore, it is difficult to neglect equation (5.13). This equation in the approximate form (5.18) allows to eliminate $\mathbf{w}_\lambda$ but all complications related to modelling the bifurcations remain. Finally, the variable $\mathbf{w}_\lambda$ seems to be appropriate for modelling the free energy even in the simplified version by means of the relation $\mathbf{w}^*_\lambda = \mathbf{w}^*_\lambda(g')$.

On the other hand, micrononhomogeneous deformation increases the amount of dissipation. Then, it is assumed, it would be appropriate to plot an internal state variable with evolution of $\mathbf{w}^*_\lambda$.

Summing up these considerations we state that equation (5.13) could be replaced by Eq. (5.18) and dynamical effects related to phonon mechanics level could be described by an internal state variable and their evolution equation.

The problem of dissipation is accompanied also by the stabilization of martensite. During heat treatment of the material undergoing the martensitic transformation we obtain considerable differences in temperatures of transformations for different cycles of this process. Such a phenomenon is called the stabilization of martensite. Main reason for the changes of transformation temperatures is the evolution of vacancy density ϱ which can block the interfaces [24, 25]. This is an important phenomenon from the termomechanical point of view. In general, we admit thermal processes with miscellaneous time scales. Deformational processes

are also responsible for defects and dislocation densities. Therefore, in general, internal state variables ϱ which represent densities of dislocations and defects should have influence on temperatures of transformations by the free energy.

Let us introduce notations $\mathcal{R} = \{\psi,\ \mathbf{T},\ \mathbf{f}_\lambda,\ s,\ \mathbf{q}\}$, $\mathcal{H} = \{g,\ T_{,j}\}$, where $g \in D$ was introduced in the previous section. Let $\boldsymbol{\alpha}$ be a group of internal state variables responsible for dissipation induced by micrononhomogeneous deformation and phase transformation. Let ϱ be a set of variables for description of the stabilization of martensite phenomenon. Then, a general form of constitutive equations is assumed in the form

$$\mathcal{R} = \mathcal{R}(\mathcal{H},\ \boldsymbol{\alpha},\ \varrho), \tag{5.19}$$

$$\dot{\boldsymbol{\alpha}} = A(\mathcal{H},\ \boldsymbol{\alpha},\ \varrho), \tag{5.20}$$

$$\dot{\varrho} = B(\mathcal{H},\ \boldsymbol{\alpha},\ \varrho), \tag{5.21}$$

where some equations have been previously discussed in detail.

The introduced constitutive equations have to satisfy the Clausius–Duhem inequality which in the considered case has the form

$$T^d_{iM}\dot{x}_{i,M} + \sum_\lambda f^d_{\lambda N}\dot{w}_{\lambda N} - (q_i T_{,i})/T - \varrho\frac{\partial\psi}{\partial\alpha_i}\dot{\alpha}_i - \varrho\frac{\partial\psi}{\partial\varrho_i}\dot{\varrho}_i \geq 0. \tag{5.22}$$

The last inequality is derived with the help of the well-known Clausius–Duhem inequality [28] and local form of the balance energy equation (5.15).

Internal state variables are considered in continuum theory in order to take into account phenomena or effects of a smaller scale. The model is related to small volume of averaging. Then, the question is what scale is appropriate for justification or interpretation of internal state variables and their evolution equations (5.20), (5.21). Undoubtedly, it has to be a discrete level of description. Thus, variables $\boldsymbol{\alpha}$ are related to phonon behaviour during micrononhomogeneous deformation or jump over an energetic barrier which appears during the phase transformation. Similarly, micrononhomogeneous deformation given by ϱ is close to a discrete level.

It follows that the model of the martensitic transformation discussed in the paper should be supported by discrete calculations.

6. Final remarks

The model with small volume of averaging introduced in the paper can be used for the description of evolution of microstructure which appears during the martensitic transformation. In particular, it is referred to motion of separate interfaces and their behaviour during various forms of loading. Therefore the model of the free energy is relatively complicated and consists of many constants and functions. Unfortunately, they are not entirely identified. Some of them can

be determined by experiments. In general, it is assumed that this model will be supported by discrete calculations. Consequently, the introduced description of the martensitic transformation is viewed to be a bridge between more averaged models and descriptions on atomic level.

Furthermore, the introduced scale of averaging seems to be very convenient for modelling the interactions between various phenomena occurring in materials and the martensitic transformation.

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