

Thermodynamics of solids which undergo displacive phase transformations and micro-nonhomogeneous deformations

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IN THE PAPER an approach to the thermodynamical description of materials undergoing displacive phase transitions and micro-nonhomogeneous deformations is proposed. First, one considers the thermodynamics of materials which undergo the micro-nonhomogeneous deformation only. Next, a model of the free energy for materials with DO_3 structure and undergoing displacive phase transformations is introduced into the thermodynamics previously proposed. A model of material damping, the source of which are micro-nonhomogeneous deformation and displacive phase transitions is considered.

1. Introduction

DISPLACIVE phase transformations are characterized by cooperative movement of atoms in the transition area. They are diffusionless and have moving interfaces. Such transformations can be induced by stresses or temperature. We can distinguish several situations depending on temperature. They can be illustrated qualitatively by means of a one-dimensional model of the Helmholtz free energy (Fig.1) as a function of the shear deformation γ . The free energy related to temperature T_1 is connected with existence of the martensite only. In the case of the one-dimensional model there are two martensite variants. Each of them is connected with a different minimum of the free energy. At temperature T_2 the austenite and the martensite can co-exist. At temperature T_3 the pseudoelasticity appears. Finally, at temperature T_4 the austenite phase exists only. Displacive phase transformations are connected with shape memory.

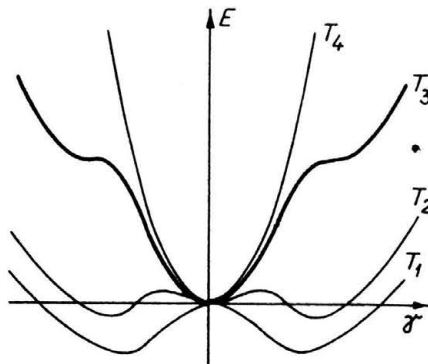


FIG. 1. The Helmholtz free energy for a one-dimensional model undergoing the martensitic transformation.

The mentioned phenomena have been considered in the literature. One-dimensional models and their generalizations connected with some symmetry groups can be found in papers by MÜLLER, WILMAŃSKI [1], FALK [2,3], JAMES [4,5], BARSCH, KRUMHANSL [6]. Many experimental investigations have been carried out for alloys based on copper. Among others, one can mention CuAl and CuAlNi alloys which are connected with DO₃ structure. They undergo a micro-nonhomogeneous deformation during the phase transformation. The micro-nonhomogeneous deformation consists in deviation of atoms from the positions indicated by the homogeneous deformation. The importance of such a deformation has been shown in the paper by KACZMAREK [7]. There, a one-dimensional mechanical model of two-path displacive phase transformations has been proposed. The two-path phase transition appears in CuAlNi alloy. During the loading process the alloy undergoes subsequent phase transition: from the γ' -phase to the β'' -phase and then to the α -phase. During unloading, however, it returns to the γ' -phase through the β' -phase, which is different from the β'' -phase [8]. Thus, we can see that the sequence of phases which appear during the loading process is different from that which appears during unloading. It is just the two-path process. The relative displacement vector which describes the micro-nonhomogeneous deformation is the main feature of the model proposed in [7]. Only with the aid of this variable, different paths of the phase transformation can be distinguished. Furthermore, the micro-nonhomogeneous deformation is necessary in order to distinguish different phases in CuAl alloy. There, two different structural phases in equilibrium are described by means of the same deformation given by the Green strain tensor but they have different micro-nonhomogeneous deformations.

The present author has not come across any approach in the literature which takes into consideration displacive phase transformations and micro-nonhomogeneous deformations occurring together. On the other hand, the majority of models considered are one-dimensional. The author would like to fill partly this gap and to propose a thermodynamical, three-dimensional description of materials which undergo displacive phase transformations and the micro-nonhomogeneous deformation. The material considered has the DO₃ structure. First, one proposes a thermodynamics of materials which undergo the micro-nonhomogeneous deformation only. Next, a model of free energy for materials with DO₃ structure and undergoing displacive phase transformations is introduced into this thermodynamics. The model of the free energy has been proposed in the paper [9]. Here, some aspects of this model and the character of its variables will be described only. Furthermore, a model of dumping for the material considered is proposed in the paper.

2. Thermodynamics of materials which undergo micro-nonhomogeneous deformations

2.1. Description of the micro-nonhomogeneous deformation

The micro-nonhomogeneous deformation appears during the deformation of crystals with the complex crystal lattice. In particular, such a deformation is accompanied by displacive phase transformations (for instance in CuAl, CuAlNi alloys which have the complex crystal lattice). The micro-nonhomogeneous deformation consists in deviation of crystal sublattices from the positions indicated by a homogeneous deformation. It is

illustrated at Fig. 2. At Fig. 2a an undeformed crystal lattice is shown. A homogeneous deformation of this crystal lattice is shown at Fig. 2b. At Fig. 2c the micro-nonhomogeneous deformation is illustrated. There, the vector ξ indicates translation of the crystal sublattice from the position indicated by the homogeneous deformation. The vector ξ can be seen as a measure of the micro-nonhomogeneous deformation.

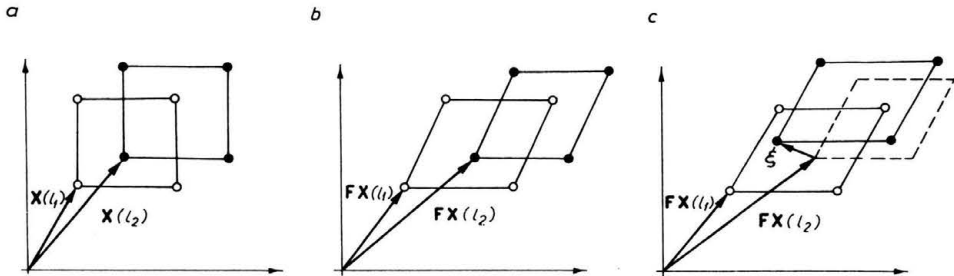


FIG. 2. Illustration of the micro-nonhomogeneous deformation.

At that moment, an order concerning deformations considered in the paper should be introduced. Thus, we will consider a macroscopic deformation. It relates to an area larger than the material point and is described by means of the Green tensor field. This deformation can be homogeneous or not. Next, we will consider a micro-nonhomogeneous deformation. It is a homogeneous deformation of the material point and is described by the Green tensor in this point. Finally, we will consider the micro-homogeneous deformation. It is a nonhomogeneous deformation of the material point (Fig. 2).

The micro-nonhomogeneous deformation has been investigated, among others, in papers [10, 11]. There, elastic constants connected with relative displacement vectors describing such a deformation and thermodynamics of perfect crystals are studied. In these papers dynamical problems and higher gradients of deformation are not considered. Theories connected with higher gradients of deformation without any relative displacement vectors have been the subject of many papers. We quote here the papers [12, 13, 14]. In the present paper the description of the displacive phase transformations needs higher gradients of the deformation as well as relative displacement vectors. Therefore, these gradients will be introduced into thermodynamics connected with the micro-nonhomogeneous deformation.

At present, we introduce a mathematical description of the micro-nonhomogeneous deformation. We assume that a crystal consists of N simple crystal sublattices (the crystal shown at Fig. 2 has two simple sublattices). Such crystal can be seen as a multicomponent body (eg. [20, 21, 22]). The aim of this paper is to give a thermomechanical description of materials which undergo displacive phase transformations and micro-nonhomogeneous deformations. In the description of the displacive phase transformations [9] relative displacement vectors are a measure of the micro-nonhomogeneous deformation. These variables are also important in order to distinguish different phases. However, the whole body is seen as a one-component body. Therefore the description should be suitable for one-component body with relative displacement vectors connected with the micro-nonhomogeneous deformation. On the other hand, derivations of motion equations are more correct and convenient if we assume that we are dealing with a multicomponent

body. Thus, we will start with the assumption that the deformation is given by N_λ fields. Further, these fields will be reduced to one field of deformation and $N_\lambda - 1$ fields of relative displacement vectors.

Let us assume that the deformation of the crystal with N_λ sublattices is described by the traditional deformation function

$$(2.1) \quad \mathbf{x} = \chi(\mathbf{X}, t)$$

given for a distinguished sublattice and $N_\lambda - 1$ deformation functions

$$(2.2) \quad \mathbf{y}_\lambda = \mathbf{x} + \mathbf{R}\mathbf{w}_\lambda$$

for the remaining sublattices, where $\lambda = 1, \dots, N_\lambda - 1$, \mathbf{R} stands for a rotation tensor in the polar decomposition of the gradient deformation tensor $\mathbf{F} = \mathbf{V}\mathbf{R}$. The relative displacement vectors \mathbf{w}_λ indicates the deviation of the sublattice from the position determined by a micro-homogeneous deformation.

At this stage we should consider in more detail the variable \mathbf{w}_λ . A good illustration of the \mathbf{w}_λ is given in Fig. 4. This variable develops together with increasing of the micro-homogeneous deformation given there by γ . The way of change of \mathbf{w}_λ is determined by the free energy. Vector \mathbf{w}_λ is defined on undeformed configuration as $w_{\lambda M} = w_{\lambda M}(\mathbf{X}, t)$, $M = 1, 2, 3$. The vector $\mathbf{u}_\lambda = \mathbf{R}\mathbf{w}_\lambda$ is a displacement from the position given by \mathbf{x} . With the help of the formula (2.2) it gives the position of the λ -component particle. Let us investigate the transformation properties of the vector $\mathbf{w}_\lambda = \mathbf{R}^{-1}(\mathbf{y}_\lambda - \mathbf{x})$. Let us introduce the transformation $\mathbf{x}^* = \mathbf{Q}\mathbf{x} + \mathbf{c}$, $\mathbf{y}_\lambda^* = \mathbf{Q}\mathbf{y}_\lambda + \mathbf{c}$ and $\mathbf{R}^* = \mathbf{Q}\mathbf{R}$, where $\mathbf{Q} = \mathbf{Q}(t)$ is an orthogonal tensor. Vector \mathbf{w}_λ^* is defined as $\mathbf{w}_\lambda^* = \mathbf{R}^{*-1}(\mathbf{y}_\lambda^* - \mathbf{x}^*) = \mathbf{R}^{-1}\mathbf{Q}^{-1}\mathbf{Q}(\mathbf{y}_\lambda - \mathbf{x}) = \mathbf{w}_\lambda$ and does not undergo any change during this transformation. It means that \mathbf{w}_λ is the objective Langrangean vector according to the definition given in the paper [23].

A position of a body particle described by Eq. (2.1) is connected with the density ρ_h of the distinguished crystal lattice. The other described by Eq. (2.2) are connected with densities ρ_λ . Furthermore, we have $\rho_h + \sum \rho_\lambda = \rho$, where ρ is the total mass density of the crystal.

In the paper the summation convention does not apply to the index λ .

2.2. The balance of energy

The balance of energy will be a starting point to the derivation of thermomechanical equations for a body which undergoes the micro-nonhomogeneous deformation. It has been mentioned previously that the higher gradients of deformation as well as the relative displacement vectors should be introduced into the theory.

We start from the balance equation suggested in [21] for the multicomponent body. Let us consider a body \mathcal{P} and its deformed configurations $\chi_\lambda(\mathcal{P})$, $\chi_h(\mathcal{P})$ determined with the help of Eqs. (2.1) and (2.2). The energy of a body \mathcal{P} is the sum of the following components given in deformed configurations

$$(2.3) \quad \Psi_\lambda = \int_{\chi_\lambda(\mathcal{P})} \left(\rho_\lambda e + \frac{1}{2} \rho_\lambda \dot{y}_{\lambda i} \dot{y}_{\lambda i} \right) dv_\lambda, \quad \Psi_h = \int_{\chi_h(\mathcal{P})} \left(\rho_h e + \frac{1}{2} \rho_h \dot{x}_i \dot{x}_i \right) dv_h,$$

where $e = E/\rho$, E is the total internal energy of the body.

The measure Φ of efflux of Ψ_λ, Ψ_h through the boundary of the body \mathcal{P} , the production P of Ψ_λ, Ψ_h in \mathcal{P} and the supply S of Ψ_λ, Ψ_h in \mathcal{P} we assume as

$$(2.4) \quad \Phi(\Psi_\lambda, \Psi_h) = \sum_\lambda \int_{\partial\chi_\lambda(\mathcal{P})} \left(q_\lambda - \sum_{\phi=1}^L t_{\lambda M_1 \dots M_{\phi-1} i} \dot{x}_{i, M_1 \dots M_{\phi-1}} - \sum_{\phi=1}^M f_{\lambda N_1 \dots N_{\phi-1} N} \dot{w}_{\lambda N, N_1 \dots N_{\phi-1}} \right) da_\lambda + \int_{\partial\chi_h(\mathcal{P})} \left(q_h - \sum_{\phi=1}^L t_{h M_1 \dots M_{\phi-1} i} \dot{x}_{i, M_1 \dots M_{\phi-1}} \right) da_h,$$

$$(2.5) \quad P(\Psi_\lambda, \Psi_h) = \sum_\lambda \int_{\chi_\lambda(\mathcal{P})} p_{\lambda e} dv_\lambda + \int_{\chi_h(\mathcal{P})} p_{he} dv_h,$$

$$(2.6) \quad S(\Psi_\lambda, \Psi_h) = \sum_\lambda \int_{\chi_\lambda(\mathcal{P})} \rho_\lambda (r_{\lambda e} + b_{\lambda i} \dot{y}_{\lambda i}) dv_\lambda + \int_{\chi_h(\mathcal{P})} \rho_h (r_{he} + b_{hi} \dot{x}_i) dv_h,$$

where q_λ, q_h are heat fluxes for components marked by λ and h , $t_{\lambda M_1 \dots M_{\phi-1} i}$, $f_{\lambda N_1 \dots N_{\phi-1} N}$, $t_{h M_1 \dots M_{\phi-1} i}$ are multipolar tensors [12]. Furthermore, for $\phi = 1$ indices M_i and N_j vanish and the derivative of the zero order appears for \dot{x}_i and $\dot{w}_{\lambda N}$. $b_{\lambda i}, b_{hi}$ are densities of volume forces, $p_{\lambda e}, p_{he}$ are productions of energy density and $r_{\lambda e}, r_{he}$ are sources of heat.

A general balance statement for a multicomponent body based on [21] takes the form

$$(2.7) \quad \sum_\lambda \frac{d\Psi_\lambda}{dt} + \frac{d\Psi_h}{dt} = -\Phi(\Psi_\lambda, \Psi_h) + P(\Psi_\lambda, \Psi_h) + S(\Psi_\lambda, \Psi_h).$$

After substitution of Eqs. (2.3)–(2.6) to Eq. (2.7), transforming the time derivative of the integrals on the left-hand side of Eq. (2.7) and grouping the suitable terms we obtain

$$(2.8) \quad \sum_\lambda \int_{\chi_\lambda(\mathcal{P})} \left\{ \left[\frac{\partial \rho_\lambda}{\partial t} + (\rho_\lambda \dot{y}_{\lambda j})_{,j} \right] \left(e + \frac{1}{2} \dot{y}_{\lambda i} \dot{y}_{\lambda i} \right) + \rho_\lambda \left(\frac{\partial e}{\partial t} + \dot{y}_{\lambda j} e_{,j} \right) + \rho_\lambda \dot{y}_{\lambda j} \dot{y}_{\lambda j} \right\} dv_\lambda + \int_{\chi_h(\mathcal{P})} \left\{ \left[\frac{\partial \rho_h}{\partial t} + (\rho_h \dot{x}_j)_{,j} \right] \left(e + \frac{1}{2} \dot{x}_i \dot{x}_i \right) + \rho_h \left(\frac{\partial e}{\partial t} + \dot{x}_j e_{,j} \right) + \rho_h \dot{x}_i \dot{x}_i \right\} dv_h + \sum_\lambda \int_{\chi_\lambda(\mathcal{P})} [q_{\lambda j, j} - \rho_\lambda (r_{\lambda e} + b_{\lambda i} \dot{y}_{\lambda i}) - p_{\lambda e}] dv_\lambda + \int_{\chi_h(\mathcal{P})} [q_{h j, j} - \rho_h (r_{hi} + b_{hi} \dot{x}_i) - p_{he}] dv_h = \sum_\lambda \int_{\partial\chi_\lambda(\mathcal{P})} \left(\sum_{\phi=1}^L t_{\lambda M_1 \dots M_{\phi-1} i} \dot{x}_{i, M_1 \dots M_{\phi-1}} + \sum_{\phi=1}^M f_{\lambda N_1 \dots N_{\phi-1} N} \dot{w}_{\lambda N, N_1 \dots N_{\phi-1}} \right) da_\lambda + \int_{\partial\chi_h(\mathcal{P})} \left(\sum_{\phi=1}^L t_{h M_1 \dots M_{\phi-1} i} \dot{x}_{i, M_1 \dots M_{\phi-1}} \right) da_h.$$

At this stage we transform the multicomponent body into a one-component body. It

will happen by assumption that $R_{iN}w_{\lambda N}$ tends to zero. Then, $\chi_{\lambda}(\mathcal{P})$ tends to $\chi_h(\mathcal{P})$ and the differentiation with respect to configuration y_{λ_i} changes into the differentiation with respect to configuration x_i . $\chi_h(\mathcal{P})$ will be further denoted by $\chi(\mathcal{P})$. Taking into account the mass conservation laws for individual components and the suggested limit transformation, we obtain the balance equation

$$(2.9) \quad \int_{\chi(\mathcal{P})} \left[\dot{E} + \rho_h \dot{x}_i \dot{x}_i + \sum_{\lambda} \rho_{\lambda} \dot{y}_{\lambda_j} \dot{y}_{\lambda_j} + q_{j,j} - p_e - \rho b_i \dot{x}_i \right] dv \\ - \int_{\partial \chi(\mathcal{P})} \sum_{\phi=1}^L t_{M_1 \dots M_{\phi-1} i} \dot{x}_i,_{M_1 \dots M_{\phi-1}} + \sum_{\lambda} \sum_{\phi=1}^M f_{\lambda N_1 \dots N_{\phi-1} N} \dot{w}_{\lambda N, N_1 \dots N_{\phi-1}} da = 0.$$

During the limit transformation new quantities have appeared $q_j = \sum_{\lambda} q_{\lambda_j} + q_{h_j}$, $t_{M_1 \dots M_{\phi-1} i} = \sum_{\lambda} t_{\lambda M_1 \dots M_{\phi-1} i} + t_{h M_1 \dots M_{\phi-1} i}$, $r_e = \sum_{\lambda} r_{\lambda e} + r_{he}$, $b_i = \sum_{\lambda} b_{\lambda i} + b_{hi}$. We can notice that the limit transformation has not been carried out consistently. In fact, we have retained the expression $\sum_{\lambda} \rho_{\lambda} \dot{y}_{\lambda_j} \dot{y}_{\lambda_j}$ and the last summand in Eq. (2.9). These expressions will be helpful in description of motion of relative displacement vectors. At this stage we have to consider some components which appear in Eq. (2.9) in details. First we will investigate the expression $\rho_h \dot{x}_i \dot{x}_i + \sum_{\lambda} \rho_{\lambda} \dot{y}_{\lambda_i} \dot{y}_{\lambda_i}$

$$(2.10) \quad \rho_h \dot{x}_i \dot{x}_i + \sum_{\lambda} \rho_{\lambda} \dot{y}_{\lambda_i} \dot{y}_{\lambda_i} = \rho_h \dot{x}_i \dot{x}_i + \sum_{\lambda} \rho_{\lambda} (\dot{y}_{\lambda_i} - \dot{x}_i + \dot{x}_i) (\dot{x}_i + \dot{u}_{\lambda_i}) \\ = \rho \dot{x}_i \dot{x}_i + \sum_{\lambda} \rho_{\lambda} (\dot{y}_{\lambda_i} - \dot{x}_i) \dot{x}_i + \sum_{\lambda} \rho_{\lambda} (\dot{y}_{\lambda_i} - \dot{x}_i) \dot{u}_{\lambda_i} + \sum_{\lambda} \rho_{\lambda} \dot{x}_i \dot{u}_{\lambda_i} \approx \rho \dot{x}_i \dot{x}_i \\ + \sum_{\lambda} \rho_{\lambda} (\dot{y}_{\lambda_i} - \dot{x}_i) R_{iN} \dot{w}_{\lambda N}.$$

Influences of inertia of the mass connected with relative displacement vectors on the motion of the body and acceleration of the body on the motion of the relative displacement vectors are neglected in the last step. Furthermore, it is assumed that $(R_{iN}w_{\lambda N}) \cdot = \dot{R}_{iN}w_{\lambda N} + R_{iN}\dot{w}_{\lambda N} \approx R_{iN}\dot{w}_{\lambda N}$. It means neglecting the rotational velocity effects on the motion of relative displacement vectors. If we also neglect the rotational acceleration, then the last expression in Eq. (2.10) takes the form $\sum_{\lambda} \rho_{\lambda} (\dot{y}_{\lambda_i} - \dot{x}_i) R_{iN} \dot{w}_{\lambda N} \approx \sum_{\lambda} \rho_{\lambda} R_{iM} \ddot{w}_{\lambda M} R_{iN} \dot{w}_{\lambda N} = \sum_{\lambda} \rho_{\lambda} \ddot{w}_{\lambda N} \dot{w}_{\lambda N}$.

Now, we will investigate more exactly the first summand in Eq. (2.9). Let us assume that $E = F + \rho sT$ and $\dot{E} = \dot{F} + \rho s\dot{T} + \rho \dot{s}T$, where F is the free energy. Let us introduce the latter formula into the balance equation (2.9) and study an expression which is an integral of \dot{F} . We assume furthermore that the function F depends on the following variables: $F = F(x_{i, M_1}, \dots, x_{i, M_1 \dots M_L}, w_{\lambda N}, w_{\lambda N, N_1}, \dots, w_{\lambda N, N_1 \dots N_M}, T)$. Taking it into account we obtain

$$(2.11) \quad \int_{\chi(\mathcal{P})} \dot{F} dv = \int_{\chi(\mathcal{P})} \left[\frac{\partial F}{\partial T} \dot{T} + \sum_{\delta=1}^L (-1)^{\delta} \left[\frac{\partial F}{\partial x_{i, M_1 \dots M_{\delta}}} \right]_{, M_{\delta} \dots M_1} \dot{x}_i \right. \\ \left. + \sum_{\nu=0}^M \sum_{\lambda} (-1)^{\nu} \left[\frac{\partial F}{\partial w_{\lambda N, N_1 \dots N_{\nu}}} \right]_{, N_{\nu} \dots N_1} \dot{w}_{\lambda N} \right] dv$$

$$\begin{aligned}
(2.11) \quad & + \int_{\partial\chi(\mathcal{P})} \left[\sum_{\phi=1}^L \sum_{\delta=\phi}^L (-1)^{\delta+1} \left[\frac{\partial F}{\partial x_{i,M_1\dots M_\delta}} \right]_{,M_\delta\dots M_{\phi-1}} (x_{k,M_\phi} n_k) \dot{x}_{i,M_1\dots M_{\phi-1}} \right. \\
& \left. + \sum_{\phi=1}^M \sum_{\nu=\delta}^M \sum_{\lambda} (-1)^{\nu+1} \left[\frac{\partial F}{\partial w_{\lambda N,N_1\dots N_\nu}} \right]_{,N_\nu\dots N_{\phi+1}} x_{k,N_\phi} n_k \dot{w}_{\lambda N,N_1\dots N_{\phi-1}} \right] da \\
& = \int_{\chi(\mathcal{P})} \left[\frac{\partial F}{\partial T} \dot{T} + A_i \dot{x}_i + \sum_{\lambda} B_{\lambda N} \dot{w}_{\lambda N} \right] dv + \int_{\partial\chi(\mathcal{P})} \left[\sum_{\phi=1}^L A_{\phi i} \dot{x}_{i,M_1\dots M_{\phi-1}} \right. \\
& \qquad \qquad \qquad \left. + \sum_{\phi=1}^M \sum_{\lambda} B_{\phi\lambda N} \dot{w}_{\lambda N,N_1\dots N_{\phi-1}} \right] da.
\end{aligned}$$

New quantities A_i , $A_{\phi i}$, $B_{\lambda N}$, $B_{\phi\lambda N}$ have been defined during the transformation of this identity. For $\nu = 0$ the derivation rank is equal to zero in the third summand on the right-hand side of the first equality sign in Eq. (2.11). Derivatives of rank equal to zero for \dot{x}_i and $\dot{w}_{\lambda N}$ appear there for $\phi = 1$. If $\delta = \phi$ and $\nu = \phi$, then the derivatives connected with indices M_δ and N_ν vanish in the fourth and the fifth summands on the right-hand side in Eq. (2.11). $A_{\phi i}$ and $B_{\phi\lambda N}$ are equal to zero for $\delta < \phi$ and $\nu < \phi$.

The components $\rho T \dot{s}$ and $\rho \dot{T} s$ have appeared as a consequence of the introduction of the free energy into Eq. (2.9). On the other hand, the expression $\frac{\partial F}{\partial T} \dot{T}$ has appeared during differentiation of F . We can transform the latter two expressions $\rho \dot{T} s + \frac{\partial F}{\partial T} \dot{T}$ into $\rho \dot{T} \left(s + \frac{1}{\rho} \frac{\partial F}{\partial T} \right)$. Let us assume that the latter formula is equal to zero. It provides

$$(2.12) \quad s = -\frac{1}{\rho} \frac{\partial F}{\partial T}$$

in agreement with classical thermodynamics of continuum [20]. The remaining term $\rho T \dot{s}$ will be represented in two different forms. In the first form we obtain the following formula:

$$\begin{aligned}
(2.13) \quad \rho T \dot{s} = & - \sum_{\phi=1}^L T \frac{\partial}{\partial T} \left[\frac{\partial F}{\partial x_{i,M_1\dots M_\phi}} \right] \dot{x}_{i,M_1\dots M_\phi} \\
& - \sum_{\nu=0}^M \sum_{\lambda} T \frac{\partial^2 F}{\partial T \partial w_{\lambda N,N_1\dots N_\nu}} \dot{w}_{\lambda N,N_1\dots N_\nu} - T \frac{\partial^2 F}{\partial T^2} \dot{T}.
\end{aligned}$$

In the second form we consider an integral of $\rho T \dot{s}$ and then we obtain

$$\begin{aligned}
(2.14) \quad \int_{\chi(\mathcal{P})} \rho T \dot{s} dv = & \int_{\chi(\mathcal{P})} -T \frac{\partial \dot{F}}{\partial T} dv = - \int_{\chi(\mathcal{P})} \left[T \frac{\partial^2 F}{\partial T^2} \dot{T} + A_i^T \dot{x}_i + \sum_{\lambda} B_{\lambda N}^T \dot{w}_{\lambda N} \right] dv \\
& - \int_{\partial\chi(\mathcal{P})} \left[\sum_{\phi=1}^L A_{\phi i}^T \dot{x}_{i,M_1\dots M_{\phi-1}} + \sum_{\phi=1}^M \sum_{\lambda} B_{\phi\lambda N}^T \dot{w}_{\lambda N,N_1\dots N_{\phi-1}} \right] da,
\end{aligned}$$

where the quantities A_i^T , $B_{\lambda N}^T$, $A_{\phi i}^T$, $B_{\phi\lambda N}^T$ are defined with the aid of the following

expressions

$$(2.15) \quad A_i^T = \sum_{\delta=1}^L (-1)^\delta \left(T \frac{\partial}{\partial T} \left(\frac{\partial F}{\partial x_{i,M_1 \dots M_\delta}} \right) \right)_{,M_\delta \dots M_1},$$

$$(2.16) \quad B_{\lambda N}^T = \sum_{\nu=0}^M (-1)^\nu \left(T \frac{\partial^2 F}{\partial T \partial w_{\lambda N, N_1 \dots N_\nu}} \right)_{,N_\nu \dots N_1},$$

$$(2.17) \quad A_{\phi_i}^T = \sum_{\delta=\phi}^L (-1)^{\delta+1} \left(T \frac{\partial}{\partial T} \partial \left(\frac{\partial F}{\partial x_{i,M_1 \dots M_\delta}} \right) \right)_{,M_\delta \dots M_{\phi+1}} (x_{k,M_\phi} n_k),$$

$$(2.18) \quad B_{\phi \lambda N}^T = \sum_{\nu=\phi}^M (-1)^{\nu+1} \left(T \frac{\partial^2 F}{\partial T \partial w_{\lambda N, N_1 \dots N_\nu}} \right)_{,N_\nu \dots N_{\phi+1}} (x_{k,N_\phi} n_k).$$

2.3. The motion equations and the heat conduction equation

Taking into account Eqs. (2.10), (2.11), (2.12), (2.14) we can transform the balance equation (2.9) into the form

$$(2.19) \quad \int_{\chi(\mathcal{P})} \left((A_i - A_i^T - \rho b_i + \rho \ddot{x}_i) \dot{x}_i + \sum_{\lambda} [B_{\lambda N} - B_{\lambda N}^T + \rho_{\lambda} (\ddot{y}_{\lambda i} - \ddot{x}_i) R_{iN}] \dot{w}_{\lambda N} \right. \\ \left. - \frac{\partial^2 F}{\partial T^2} \dot{T} + q_{j,j} - p_e - \rho r_e \right) dv \\ + \int_{\partial \chi(\mathcal{P})} \left(\sum_{\phi=1}^L [A_{\phi i} - A_{\phi i}^T - t_{M_1 \dots M_{\phi-1} i}] \dot{x}_{i,M_1 \dots M_{\phi-1}} \right. \\ \left. + \sum_{\phi=1}^M \sum_{\lambda} [B_{\phi \lambda N} - B_{\phi \lambda N}^T - f_{\lambda N_1 \dots N_{\phi-1} N}] \dot{w}_{\lambda N, N_1 \dots N_{\phi-1}} \right) da.$$

Equation (2.19) provides the following motion equation

$$(2.20) \quad A_i - A_i^T - \rho b_i + \rho \ddot{x}_i = 0$$

and the equation for relative displacement vectors

$$(2.21) \quad B_{\lambda N} - B_{\lambda N}^T + \rho_{\lambda} (\ddot{y}_{\lambda i} - \ddot{x}_i) R_{iN} = 0$$

together with suitable boundary conditions following from the second part of the formula (2.19).

In order to derive the equation of thermal conductivity we use the first form of $\rho T \dot{s}$ (2.13). Next, using the balance equation (2.9) we obtain the following equation:

$$(2.22) \quad - \sum_{\phi=1}^L T \frac{\partial}{\partial T} \left(\frac{\partial F}{\partial x_{i,M_1 \dots M_\phi}} \right) \dot{x}_{i,M_1 \dots M_\phi} \\ - \sum_{\phi=0}^M \sum_{\lambda} T \frac{\partial^2 F}{\partial T \partial w_{\lambda N, N_1 \dots N_\phi}} \dot{w}_{\lambda N, N_1 \dots N_\phi} - T \frac{\partial^2 F}{\partial T^2} \dot{T} + q_{j,j} = \rho r_e.$$

In this equation we have obtained the same components which appear in the paper by GREEN-RIVLIN [12] and, additionally, the component with variables $w_{\lambda N}$ and their gradients.

3. The free energy for materials which undergo displacive phase transformations

Previously, the thermodynamics of materials undergoing micro-nonhomogeneous deformation has been considered. The aim of the paper is to suggest a thermodynamical theory for materials undergoing both the micro-nonhomogeneous deformation and the displacive phase transformations. An idea of taking into consideration the displacive phase transformations consists in determination of a form of the free energy and, next, in introducing it into the previously proposed thermodynamics of materials with the micro-nonhomogeneous deformation. The free energy has been proposed in the paper [9]. In this paper we confine ourselves to a rather general discussion connected with its formulation.

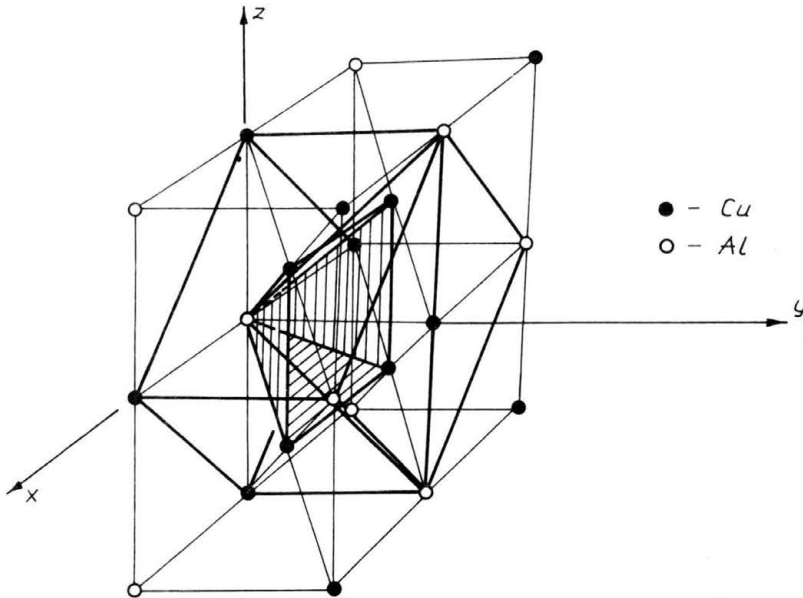


FIG. 3. Structure of β_1 -phase (CuAl alloy).

The free energy is related to the DO_3 structure. In order to understand the motivations as well as the character of variables which appear in the free energy, first we recognize geometrical properties of this structure. An example of such a structure is the CuAl alloy. It is a cubic body-centered structure (b.c.c) and is called also β -phase. It is shown at Fig. 3. There a face-centered structure is shown by means of a bold line in the frame of b.c.c.. However, this face-centered structure is not cubic in the undeformed state. With the aid of thin lines, a system of four planes oriented with respect to the OY axis is marked. These planes will be called basal planes. One can create similar systems of planes with respect to the axes OX and OZ . Then, we take into account twelve planes. However,

some of them coincide and finally the DO_3 structure has six different basal planes in undeformed state.

Let us select an axis, for instance OY , according to Fig. 3. If we apply a suitable extension along the OY axis and contraction along OX and OZ axes, then the face-centered structure marked by the bold line can transform to a cubic force-centered structure (f.c.c.). The strain which leads from b.c.c. to f.c.c. structure will be called the Bain strain along the Bain axis OY . The Bain strain can be considered as a stage of the martensitic transformation.

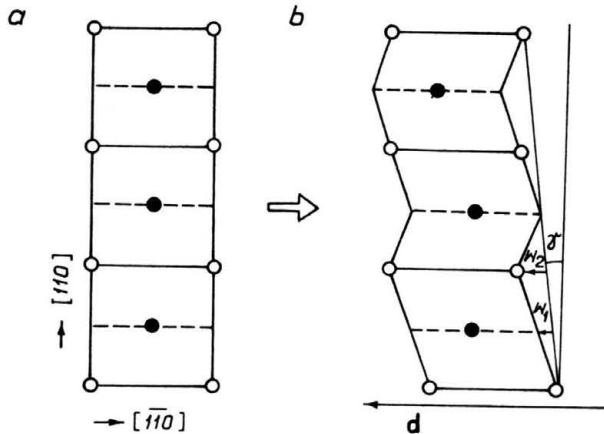


FIG. 4. The micro-nonhomogeneous deformation pertaining to the transformation of β_1 -phase to β_1' -phase (CuAl alloy).

The second stage of the martensitic transformation is a micro-nonhomogeneous shear connected with the falling of crystal lattice. As a result of this micro-nonhomogeneous shear, the micro-nonhomogeneous deformation appears. It is illustrated in Fig. 4. The micro-nonhomogeneous shear takes place in d direction on the basal plane. Further a shear system will be connected with plane of Fig. 4 (perpendicular to two opposite basal planes). For a given Bain axis we have four basal planes. Thus, four kinds of micro-nonhomogeneous deformations can appear in connection with this axis. Each of them is related to a different basal plane. At this stage we can get twelve martensite variants. For each of Bain axes we obtain four micro-nonhomogeneous deformations.

The next stage of the austenite-martensite transformation is a rotation of each of martensite variants obtained towards the habit planes. There are two different habit planes for a given martensite variant. Habit planes appear as a result of highly coherent motion of atoms during phase transformation. As a result, the parent phase (austenite) and the martensite are adapted on habit planes. The habit plane is undeformed and unrotated (as far as parent phase is unrotated). The determination of the habit plane can follow as a result of geometrical considerations taking into account the Bain strain and the shear on the basal plane [16]. Habit planes can also be determined with the aid of matrix calculus [17].

Ending this discussion on the geometry let us pay attention to an important aspect of the martensitic transformation related to the micro-nonhomogeneous deformation. At

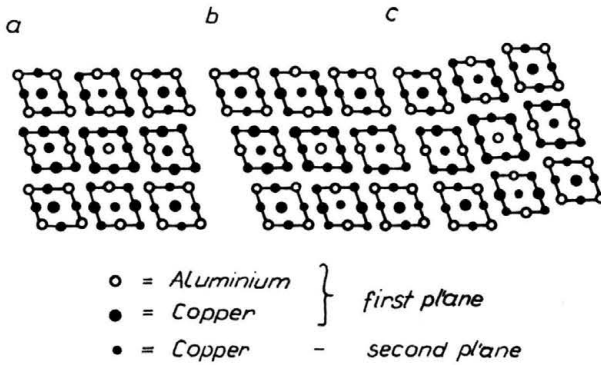


FIG. 5. Two different micro-nonhomogeneous deformations applied to the f.c.c. structure.

the Fig. 5b the f.c.c. structure as a Bain strain of the b.c.c. structure is shown. At Fig. 5a and Fig. 5c two different micro-nonhomogeneous deformations accompanied by the shear on opposite basal planes are illustrated. The shear deformation described by means of the Green tensor \mathbf{e} will coincide in both cases. However, micro-deformations are different in each of them. This example shows the validity of using relative displacement vectors in description of the displacive phase transformations. These variables are necessary in order to distinguish such different phases.

For further convenience we introduce the following sets: $T = 1, 2, 3$, $T_i = \{j : j \in T, j \neq i\}$, $\Delta = \{1, 2\}$ and multi-indices $I = (i, j)$, $J = (i, j, \delta) = (I, \delta)$, $K = (i, j, \delta, h) = (J, h)$, $i \in T$, $j \in T_i$, $\delta \in \Delta$, $h \in \Delta$. The multi-indices I , J , K are dependent because they have common first indices.

Taking into considerations the geometrical properties of the DO_3 structure we will introduce suitable mathematical objects. The body will be considered in an unchanging orthonormal basis $\mathbf{a} = \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$. In connection with the Bain axes, an orthonormal basis $\mathbf{b} = \{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3\}$ consisting of vectors which lie on these axes is introduced. To each of the Bain axes with index $i \in T$ we can assign a plane in which a micro-nonhomogeneous shear can occur. There are two planes of such kind. They contain the axes with indices i and $j \in T_i$. Thus, the index I can be assigned to such a plane. The plane with index I is perpendicular to two opposite basal planes (Fig. 3). Therefore, two different micro-nonhomogeneous shears can take place in this plane. The first one in the direction determined by the intersection of the plane considered with the first basal plane, and the second one with the second basal plane. We mark the directions determined in this way by \mathbf{d}_{I1} and \mathbf{d}_{I2} (Fig. 6). One can assume that index I determines a shear system with two possible micro-nonhomogeneous shears. For this shear system we can introduce another orthonormal basis $\mathbf{d}_I = (\mathbf{d}_{I1}, \mathbf{d}_{I2}, \mathbf{d}_{I3})$, where $\mathbf{d}_{I3} = \mathbf{d}_{I1} \times \mathbf{d}_{I2}$ (Fig. 6).

Let us consider a shear system \mathbf{d}_I . In the plane of this system two micro-nonhomogeneous shears can appear (Fig. 5). One of them has direction \mathbf{d}_{ij} and the second \mathbf{d}_{ik} , $j, k \in T_i$. A scheme of such a micro-nonhomogeneous shear is shown at Fig. 4. There, γ is a measure of the micro-homogeneous deformation. The micro-nonhomogeneous deformation presented there can be described by means of vectors \mathbf{w}_1 and \mathbf{w}_2 which means deviation of distinguished atom layers from positions indicated by homogeneous deformation. In practice, the number of atom layers which are necessary to give the full characteristics of the micro-nonhomogeneous deformation can be various. In the case of

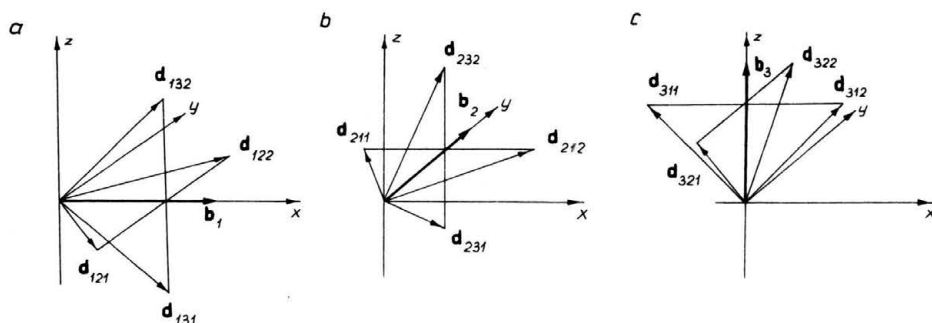


FIG. 6. Locations of vectors \mathbf{d}_{ijk} and \mathbf{b}_i .

CuAlNi alloy this number is equal to eighteen [8]. The above considerations suggest a way of indexing for relative displacement vectors connected with the micro-nonhomogeneous deformation. Namely, these variables can take the form $\mathbf{w}_{ij\alpha m}$. The first index $i \in T$ is connected with the Bain axis, the second index $j \in T_i$ chooses the shear system $I = (i, j)$, the third index means the shear direction \mathbf{d}_{I1} or \mathbf{d}_{I2} . The index $m \in P = \{1, 2, \dots, p\}$ is connected with the number of atom layers considered in a given shear direction. A short notation for $\mathbf{w}_{ij\alpha m} = \mathbf{w}_{I\alpha m} = \mathbf{w}_{Jm}$ by means of multi-indices introduced is reached. The domain for the relative displacement vectors as $K = \{\mathbf{w}_{Jm} : \mathbf{w}_{Jm} = w_{Jm} \mathbf{d}_J(F)\}$ can be determined. In general, we can admit that vector \mathbf{d}_J depends on the gradient deformation F . However, here it is assumed that the vector \mathbf{d}_J depends on internal rotation only.

Two kinds of rotations will be considered in the paper. The internal rotation \mathbf{R}^i is related to a rotation of the martensite relatively to the parent phase (austenite) towards a habit plane and the external rotation \mathbf{R}^e is understood as a rotation of the Bain axes with respect to the basis \mathbf{a} .

Summing up the above considerations we assume the following assumptions pertaining to the symmetry:

1. There exist six basal planes in underformed DO_3 structure (distributed according to Fig. 3).
2. The free energy function is a positive definite quadratic form in a neighbourhood of the deformation equal to zero and has the symmetry properties suitable for the austenitic structure considered.
3. The free energy function has the symmetry properties suitable for a given martensite variant structure in a neighbourhood of equilibrium state of this variant.
4. There exist twenty four habit planes strictly determined in the crystal structure considered.

Furthermore we introduce the following kinematical assumptions:

1. Relative displacement vectors \mathbf{w}_{Jm} act in direction \mathbf{d}_J . They are the measure of deviation of atomic layers from position indicated by homogeneous deformation. The micro-nonhomogeneous deformation can start only after exceeding a critical shear stress τ in a given shear system.

2. The basis $\mathbf{d}_I = \{\mathbf{d}_{I1}, \mathbf{d}_{I2}, \mathbf{d}_{I3}\}$ can undergo an internal rotation \mathbf{R}^i . The process of internal rotation can start only after exceeding a critical shear stress τ in a given shear system.

The free energy has been constructed in [9] with the following program:

1. Assuming as a starting point a free energy $F = F(e_{ij}, T)$ as a positive definite quadratic form. The free energy has suitable symmetry conditions in a neighbourhood of the deformation equal to zero for a given crystal structure.

2. Determination of a validity domain for the free energy assumed in point 1 with the aid of the assumption about critical shear stress. Exceeding this stress causes the phase transformation.

3. For each of the shear system I separately, cutting-off the domain of the free energy F by means of the critical shear condition. Next, modelling $F = F_I$ again in cutting domain, taking into account properties of the phase transformation.

4. Constructing a new form of the free energy from six functions F_I obtained in former point.

5. Introduction of relative displacement vectors for the description of the micro-nonhomogeneous deformation.

6. Introduction of higher deformation gradients in order to describe the phenomena: the rotation towards a habit plane, flat propagating interfaces.

The free energy derived in the paper [9] takes the form

$$(3.1) \quad F = F_t + M + A + G_H.$$

The previously mentioned critical shear condition determines an area in the space of stresses as well as in the space of strains. In this area the material does not undergo phase transformations yet. Only after exceeding a critical shear the phase transformation can start. Then the micro-nonhomogeneous deformation and internal rotations can also appear. Taking into account internal rotations and dependence on relative displacement vectors, the component of the free energy F_t takes the form [9]

$$(3.2) \quad F_t(\mathbf{e}) = \inf_I \{ F_I \circ A_I(\mathbf{R}^i)(\mathbf{e}, \mathbf{w}_{I\delta m}) \},$$

where F_I is a free energy defined in the basis \mathbf{d}_I , A_I is a map transforming strain components from the basis \mathbf{d}_I to the basis \mathbf{b} .

The component of the free energy connected with the micro-nonhomogeneous deformation takes the form [9]

$$(3.3) \quad M = \sum_I \left(\sum_{\delta \in \Delta} \sum_{m \in P} [\Psi_{\delta m}(w_{I\delta m}) - f_m(\gamma)w_{I\delta m}] + \sum_{\alpha \in \Delta} \sum_{\delta \in \Delta_\alpha} \sum_{m \in P} c_\delta(w_{I\alpha m})(w_{I\delta m})^2 \right),$$

where $\Delta_\alpha = \{ \delta : \delta \neq \alpha, \delta \in \Delta \}$, γ is a measure of shear deformation. In the above equation the sum runs through all multi-indices I . However, if the micro-nonhomogeneous deformation starts in a given shear system, then all the relative displacement vectors pertaining to other systems vanish. The first summand in Eq. (3.3) models the micro-nonhomogeneous deformation. Function $\Psi_{\delta m}$ models the shape of the free energy connected with individual atom layer m . The essence of the micro-nonhomogeneous deformation consists in deviation of different atom layers from positions indicated by micro-homogeneous deformation measured by γ in the shear system. The function $\Psi_{\delta m}$ can take the form $\Psi_{\delta m} = C_{i\delta m} w_{I\delta m}^2$ with minimum equal to zero. With the aid of the

function $f_m(\gamma)w_{I\delta m}$ which is linear with respect to variable $w_{I\delta m}$ we can control the position of minimum of the function $\Psi_{\delta m} - f_m(\gamma)w_{I\delta m}$ and in this way we can introduce the micro-nonhomogeneous deformation. The positions of minima depend on γ and on the number of atom layer m . The second summand in Eq. (3.3) causes the bifurcation between variables w_{I1m} and w_{I2m} owing to the suitable shape of the function C_δ . The bifurcation between these variables is connected with two micro-nonhomogeneous shears on opposite habit planes.

The component A is related to internal rotations of martensitic structures towards habit planes. Directional derivatives \mathbf{a}_K of vectors connected with the crystal structure are assumed as variables. These vectors can be seen as material directors introduced in the paper [18]. These vectors are connected with habit planes. If the phase transformation occurs, then, due to the component of free energy A , the directions of the directors will be adapted on a habit plane. There are two habit planes for the forming variant of martensite. Thus, A has to cause a bifurcation between internal rotations.

The component of the free energy G_H is connected with higher gradients of the deformation as well as relative displacement vectors. A mechanics of flat propagating interfaces has been proposed by means of G_H .

The free energy F given by Eq. (3.1) depends on the deformation gradient because it contains the Green strain tensor. F depends also on higher gradients of deformation. It is because the variables \mathbf{a}_K can be expressed by higher gradients. Furthermore, higher gradients of deformation appear in G_H . F depends also on variables $\mathbf{w}_{I\alpha m}$ and their gradients which appear in G_H . Our aim is to construct the free energy function F in order to introduce it into the thermodynamics previously suggested. Therefore, connections between indices of variables $\mathbf{w}_{I\alpha m}$ and $w_{\lambda N}$ should be elucidated. Atom positions in the shear system I and in m -th atomic layer are determined by the vector $\mathbf{w}_{Im} = \mathbf{w}_{I1m} + \mathbf{w}_{I2m}$. \mathbf{w}_{Im} is the sum of their components in the basis d_I . Thus, the index α is related to the index N connected with components of the variable $\mathbf{w}_{\lambda N}$. The index m is connected evidently with λ . The index I plots the deformation with suitable internal state variables and can be neglected in these considerations.

Summing up, we can assert that the free energy F can be introduced into the thermodynamical model considered in the previous section.

4. The material damping

Materials which undergo displacive phase transformations have good damping properties [19]. Sources of the damping are related to both the micro-nonhomogeneous deformation and the phase transformations. The micro-nonhomogeneous deformation induced by micro-homogeneous deformation causes relative motion of atoms. Motion of this kind is evidently a source of heat. Therefore, we can postulate that the amount of heat emitted during the deformation is proportional to relative velocities of crystal sublattices. Bearing in mind the fulfilling of Clausius–Duhem inequality we assume as a starting point the positive definite quadratic form

$$(4.1) \quad L = \sum_{\lambda} C_{\lambda MN} \dot{w}_{\lambda M} \dot{w}_{\lambda N} + \sum_{(\lambda, \nu) \in I} C_{\lambda \nu MN} (\dot{w}_{\lambda M} - \dot{w}_{\nu M})(\dot{w}_{\lambda N} - \dot{w}_{\nu N}) \geq 0,$$

where $I = \{(\lambda, \nu) : \lambda < \nu, \lambda, \nu = 1 \dots N_\lambda - 1\}$. The L will determine the amount of heat emitted per unit time in a material point during the body motion. We can

transform Eq. (4.1) to the form

$$(4.2) \quad L = \sum_{\lambda=1}^{N_\lambda-1} D_{\lambda N} \dot{w}_{\lambda N} = \sum_{\lambda=1}^{N_\lambda-1} \left(C_{\lambda M N} \dot{w}_{\lambda M} + \sum_{\nu=\lambda+1}^{N_\lambda-1} C_{\lambda \nu M N} (\dot{w}_{\lambda M} - \dot{w}_{\nu M}) - \sum_{\alpha=1}^{\lambda-1} C_{\alpha \lambda M N} (\dot{w}_{\alpha M} - \dot{w}_{\lambda M}) \right) \dot{w}_{\lambda N},$$

where for $\lambda = N_\lambda - 1$ the second summand on the right-hand side vanishes and for $\lambda = 1$ the third summand vanishes. The formula (4.2) defines the dissipative force $D_{\lambda N}$.

The material damping connected with displacive phase transformations has different mechanism from that for the micro-nonhomogeneous deformation. Heat emitted in this transformation will be mainly related to the acceleration connected with breaking after passing through the energetic barrier. Thus, we can assume that the dissipative stress is proportional to the acceleration of deformation

$$(4.3) \quad t_{iM}^D = C_{iMPQ} \ddot{e}_{PQ}.$$

Dissipative forces $D_{\lambda N}$ and stresses t_{iM}^D can be incorporated into the balance equation (2.19). Let us modify the balance equation by adding and subtracting suitable components suggested below

$$(4.4) \quad t_{iM}^D \dot{x}_{i,M} + \sum_{\lambda} D_{\lambda N} \dot{w}_{\lambda N} - t_{iM}^D \dot{x}_{i,M} - \sum_{\lambda} D_{\lambda N} \dot{w}_{\lambda N} = (t_{iM}^D \dot{x}_i)_{,M} - t_{iM,M}^D \dot{x}_i + \sum_{\lambda} D_{\lambda N} \dot{w}_{\lambda N} - t_{iM}^D \dot{x}_{i,M} - \sum_{\lambda} D_{\lambda N} \dot{w}_{\lambda N}.$$

Components $-t_{iM,M}^D \dot{x}_i + \sum_{\lambda} D_{\lambda N} \dot{w}_{\lambda N}$ take part in forming the balance momentum equation. The component $(t_{iM}^D \dot{x}_i)_{,M}$ will be transformed into the boundary conditions and components $-t_{iM}^D \dot{x}_{i,M} - \sum_{\lambda} D_{\lambda N} \dot{w}_{\lambda N}$ take part in forming the heat conductivity equation. Taking into consideration the damping connected with the micro-nonhomogeneous deformation and displacive phase transformations, the motion equations and heat conductivity equation (2.20), (2.21) and (2.22) finally can be written

$$(4.5) \quad A_i - A_i^T + t_{iM,M}^D - \rho b_i + \rho \ddot{x}_i = 0,$$

$$(4.6) \quad B_{\lambda N} - B_{\lambda N}^T + D_{\lambda N} + \rho_{\lambda} (\ddot{y}_{\lambda i} - \ddot{x}_i) R_{iN} = 0,$$

$$(4.7) \quad - \sum_{\phi=1}^L T \frac{\partial}{\partial T} \left(\frac{\partial F}{\partial x_{i,M_1 \dots M_\phi}} \right) \dot{x}_{i,M_1 \dots M_\phi} - \sum_{\phi=1}^M \sum_{\lambda} T \frac{\partial^2 F}{\partial T \partial w_{\lambda N, N_1 \dots N_\phi}} \dot{w}_{\lambda N, N_1 \dots N_\phi} - T \frac{\partial^2 F}{\partial T^2} \dot{T} + q_{j,j} = \rho r_e + \sum_{\lambda=1}^{N_\lambda-1} D_{\lambda N} \dot{w}_{\lambda N} + t_{iM}^D \dot{x}_{i,M}.$$

The two last terms connected with dissipation arise in Eq. (4.7) as sources of heat.

5. Constitutive equations

Constitutive equations consist of relations imposed on the free energy F , the heat flux q_m , the stress tensor t_{iM} and the entropy s . The free energy has been considered in the previous section. Let us concentrate now on the constitutive equation for the heat flux. In general, the multiphase body is considered. Heat coefficients are different for the austenite phase and for the martensite phase. Furthermore, the martensite can undergo internal rotations. It influences the heat conductivity coefficients expressed in the basis \mathbf{b} . The development of relative displacement vectors during the phase transition leads to the formation of different martensite variants with different structures. Thus, they have also different heat coefficients. In order to take into consideration the above mentioned elements we assume the Fourier equation expressed in the basis \mathbf{d}_I as a starting point. Let \bar{q}_l be the heat flux, $\bar{\lambda}_{lk}$ be the heat conductivity coefficients and $T_{,k}$ be the gradient of temperature. These quantities are expressed in the basis \mathbf{d}_I . The Fourier equation takes the form $\bar{q}_l = \bar{\lambda}_{lk} T_{,k}$ in this basis. The heat conductivity coefficients $\bar{\lambda}_{lk}$ do not depend on internal rotation \mathbf{R}^i because the basis \mathbf{d}_I rotates in agreement with internal rotations. Thus, as a consequence of the structure transformation during deformation, $\bar{\lambda}_{lk}$ should depend on the shear deformation measure γ and variables \mathbf{w}_J only. Therefore, we assume $\bar{\lambda}_{lk} = \bar{\lambda}_{lk}(\gamma, \mathbf{w}_J)$. The relation between the gradient of temperature $T_{,k}$ given in basis \mathbf{d}_{Ik} and the gradient of temperature $T_{,n}$ expressed in the basis \mathbf{b}_n has the form $T_{,k} = \mathbf{d}_{Ik} \mathbf{b}_n T_{,n}$. Connections between heat flux q_m in the basis \mathbf{b}_m and \bar{q}_l given in the basis \mathbf{d}_{Il} can be written as $q_m = \mathbf{b}_m \mathbf{d}_{Il} \bar{q}_l$. Internal rotations will be taken into account by assuming $\mathbf{d}_{Ik} = \mathbf{d}_{Ik}(\mathbf{R}^i)$. Bearing in mind the above considerations we propose the constitutive equations for the heat flux in the basis \mathbf{b}_m in the form

$$(5.1) \quad q_m = \mathbf{b}_m \mathbf{d}_{Il}(\mathbf{R}^i) \bar{\lambda}_{lk}(\gamma, \mathbf{w}_J) \mathbf{d}_{Ik}(\mathbf{R}^i) \mathbf{b}_n T_{,n}.$$

The constitutive relation for stresses can be given with the help of Eqs. (2.11), (2.15) and (4.3).

$$(5.2) \quad t_{iM_1} = \sum_{\delta=1}^L (-1)^\delta \left(\frac{\partial F}{\partial x_{i,M_1 \dots M_\delta}} + T \frac{\partial}{\partial T} \left(\frac{\partial F}{\partial x_{i,M_1 \dots M_\delta}} \right) \right)_{,M_\delta \dots M_2} + C_{iM_1 P Q} \ddot{e}_{P Q}.$$

The constitutive equation for entropy has the traditional form (2.12). Finally, the constitutive equation for the free energy takes the form (3.1).

These constitutive equations should fulfil the Clausius–Duhem inequality. Let us investigate this problem for equations considered in the paper. The Clausius–Duhem inequality will be introduced in the form [20]

$$(5.3) \quad \rho \dot{s} + \left(\frac{q_j}{T} \right)_{,j} - \frac{\rho r_e}{T} \geq 0.$$

Using Eq. (4.7) we can determine ρr_e as

$$(5.4) \quad \rho r_e = \rho T \dot{s} + q_{j,j} - \sum_{\lambda=1}^{N_\lambda-1} D_{\lambda N} \dot{w}_{\lambda N} - t_{iM}^D \dot{x}_{i,M}.$$

Introducing Eq. (5.4) into inequality (5.3) we obtain the following condition

$$(5.5) \quad \frac{t_{iM}^D \dot{x}_{i,M}}{T} + \frac{\sum_{\lambda} D_{\lambda N} \dot{w}_{\lambda N}}{T} - \frac{q_j T_{,j}}{T} \geq 0,$$

which represents the constraints imposed on the constitutive relations.

6. Conclusions

The two-path displacive phase transformations mentioned in the introduction can be incorporated into the model of the suggested thermodynamics. Mechanical description of the two-path process is given in [9]. The two-path process can be seen as a pseudoelastic transformation of the γ' -phase [8]. The γ' -phase is connected with the DO₃ structure and appears from β_1 phase through the micro-nonhomogeneous deformation in the same way as it has been considered in the paper. The essence of introducing this kind of transformation into the model of the thermodynamics consists in shaping functions $\Psi_{\delta m}$ and f_m from (3.3) similarly as it has been proposed for functions Ψ and F in [7].

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