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Internal variables in description of martensitic transformation in a single crystal

The problem of kinds of internal state variables which should be used in modelling dissipation for materials undergoing martensitic transformation is discussed. This problem is considered on two levels of description. The first one (L1) is connected with a small volume of averaging. In this instance detailed phenomena involved in the martensitic transformation are taken into account. A group of internal variables is suggested for this level of description. The second one (L2) is related to a larger volume of averaging. However, it is assumed that the L1-description should be used as a theoretical framework for L2-models. As a result one defines an internal variable for which the evolution equation could base on L1-model.

1. Introduction

The martensitic transformation exhibits a complicated form of microstructure. On the other hand this phenomenon can appear as a very well organized transformation with a high degree of reversibility. This is observed, for instance, in shape memory alloys [1], [6].

In order to give a detailed mechanical description of this phenomenon it should be first considered in a single crystal. Then, the description can be related to a small volume of averaging (L1-models) or to a larger volume of averaging (L2-models). In the first instance we distinguish separate phenomena such as martensite variants, interfaces between them, internal rotations and so on. A mechanical model of this kind has been considered in [2], [3]. The models suggested in papers [4], [5] could also be seen as those with the small volume of averaging. The L2-models carry out averaging through the composition of martensite variants. Then, for instance, previously mentioned interfaces are not studied. The L1-models could be deemed a theoretical basis for L2-models.

The aim of the present paper is to discuss kinds of internal variables whereby the dissipation process could be modelled on both L1 and L2 levels.

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An internal variable pertaining to martensitic transformation is considered in the literature [7÷10],[19÷20] for L2- description. In these papers the internal state variable stands for volume fraction of components connected with martensite variants.

A new variable for description of dissipation on L2-level related to the martensitic transformation is suggested in the paper. The construction of this variable is adjusted to using L1-model as a theoretical framework.

2. The L1-model and internal variables related to it

During averaging through a small enough volume we can take into account detailed phenomena involved in martensitic transformation. We can distinguish different martensite variants, interfaces between them and between martensite and austenite, the motion of interfaces, internal rotations which appear during creating martensitic structure matches with austenite or other martensite variants, shuffles which play a role in differentiation of variants.

The small volume of averaging is introduced with the help of the free energy. This fact is expressed by the number of fields which are considered and details which are taken into account in a suggested form of the free energy.

The free energy [2] depends on Green strain tensor $\underline{\mathbf{e}}$, relative displacement vectors $\underline{\mathbf{w}}_\lambda$, $\lambda = 1, \dots, N-1$, where N stands for the number of relative displacement vectors considered and variable $\underline{\mathbf{a}}$ related to internal rotation of martensite toward a habit plane. The Green strain tensor describes the dominant part of deformation connected with martensitic transformation. The shuffles are described by the relative displacement vectors. These vectors are important in description of creating martensite variants.

In our considerations we assume that deformation-temperature configuration takes the form

$$\underline{\mathbf{h}} = (\underline{\mathbf{e}}, \underline{\mathbf{w}}_\lambda, \underline{\mathbf{a}}, T, \underline{\mathbf{g}}), \quad (1)$$

where T is absolute temperature and $\underline{\mathbf{g}}$ stands for $\text{grad } T$. For simplicity, higher gradients of deformation are neglected in comparison with [2].

In the paper [3] the constitutive relations are involved with the following functions: free energy Ψ , the stress tensor $\underline{\mathbf{t}}$, forces related to shuffles $\underline{\mathbf{f}}_\lambda$, entropy S and heat flux $\underline{\mathbf{q}}$. The martensitic transformation is characterized by significant dissipation which appears during creation of martensite and motion of interface [11].

Creation of martensite is involved in shuffles [2]. Shuffles described with the help of relative displacement vectors means relative motion of atoms lying in different simple sublattices of the crystal. This motion is generated by micro-homogeneous deformation described by the Green strain tensor. This relative motion of atoms evidently generates heat. Thus, a group of internal variables $\underline{\mathbf{a}}$ should be distinguished in order to describe this kind of dissipation.

The second source of dissipation is associated with a jump through a potential barrier during the transformation. Then considerable accelerations act on the crystal lattice and as a result heat is generated. We assume that the group of internal variables α is connected with this form of dissipation.

The evolution equations for the above suggested variables are assumed in a general form of

$$\dot{\alpha} = A(\underline{h}, \alpha, \xi), \quad (2)$$

$$\dot{\beta} = B(\underline{h}, \beta, \xi), \quad (3)$$

where $\underline{h}$ stands for deformation-temperature configuration (1) and ξ stands for all remaining used internal variables.

Identification of a detailed form of evolution equations (2), (3) with the help of experiments seems to be rather difficult. Perhaps calculations based on methods of phonon mechanics or molecular dynamics will be helpful in this instance.

Material can undergo different forms of heat treatment. In the case of shape memory the heat treatment can cause stabilization of martensite [12÷14]. The stabilization of martensite influences temperatures of transformation M_s , M_f , A_s , A_f , [14]. Internal friction accompanied with the martensitic transformation strongly depends just on these temperatures [14]

In Fig. 1 the dependence of internal friction on temperature during the first

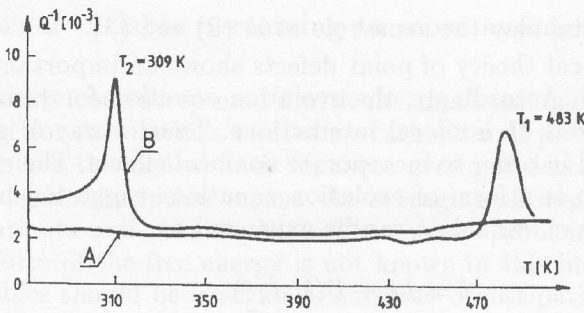


Fig. 1. Dependence of internal friction Q^{-1} on temperature for CuZnAl for first cycle of heating-cooling

cycle of heat treatment is shown. Considerable difference between the positions of internal friction maxima related to the process of heating and that of cooling is observed. During the second cycle of heating and cooling this difference decays (Fig. 2).

This temperature dependence of the internal friction maxima is explained by the process of stabilization of martensite connected with vacancy density. The stabilization of martensite is a complicated phenomenon in general. However, the motion of vacancies is probably a predominant source of this phenomenon [12÷14].

We assume that during a mechanical process the material can undergo also

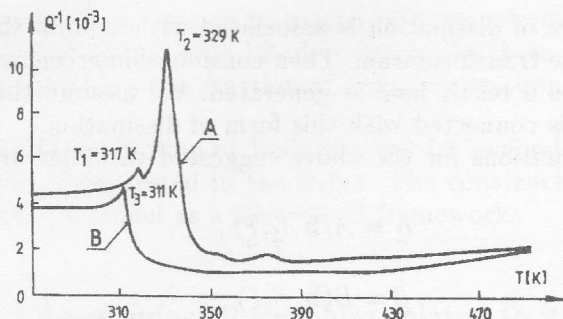


Fig. 2. Dependence of internal friction Q^{-1} on temperature for CuZnAl for second cycle of heating-cooling

large temperature changes and these temperature changes can initiate processes accompanied with evolution of vacancies density. Thus, as a consequence of stabilization of martensite, the vacancies density has a significant impact on transformation temperature and internal friction. Consequently, the vacancies density δ can be seen as an internal state variable. Evolution of point defect density is described in the literature with the help of first order differential equations [15]. Let us assume that the evolution equation for variable δ takes the form

$$\dot{\delta} = D(\underline{h}, \delta, \xi), \quad (4)$$

where variables $\underline{h}$ and ξ play the same role as in (2) and (3).

However, mechanical theory of point defects shows an important role of non-local interactions [16]. Accordingly, the evolution equation for variable δ should follow from assumptions on nonlocal interactions. Thus, a way of generalisation of (4) should be found in order to incorporate nonlocal effects. The expedient way for this generalisation is a form of evolution equations suggested by Perzyna in [17] which in the case of variable δ can be expressed as

$$\dot{\delta} = L\delta + D(\underline{h}, \delta, \xi), \quad (5)$$

where L is a linear operator connected with space variables. The internal variable should satisfy suitable boundary conditions in order to avoid control of δ by external interaction [17].

The operator L can describe nonlocal effects. If these effects are neglected the evolution equation takes a classical formulation (4) [18].

Constitutive equations for the martensitic transformation in a single crystal have been studied in [2÷3]. Here, we consider their general form only.

In the paper [3] the constitutive relations are involved with five functions previously mentioned. For the sake of simplicity we assume that $\mathcal{R}$ stands for these five functions $\mathcal{R} = (\Psi, \underline{t}, (\underline{f}_\lambda, S, \underline{q})$. Function $\mathcal{R}$ depends on deformation-temperature configuration given by (1). Furthermore the constitutive function $\mathcal{R}$ should be plotted with internal state variables introduced in the paper.

Let $\underline{\mu}$ stands for triple $(\underline{\alpha}, \underline{\beta}, \underline{\delta})$. Then, the general form of constitutive relations can be expressed as

$$\mathcal{R} = \mathcal{R}(\underline{\mathbf{h}}, \underline{\mu}), \quad (6)$$

The evolution equation for $\underline{\mu}$ can be assumed in the generalized form

$$\dot{\underline{\mu}} = \mathcal{L}\underline{\mu} + \mathcal{M}(\underline{\mathbf{h}}, \underline{\mu}), \quad (7)$$

where $\mathcal{L}$ is a linear operator related to space variables and contains operator L from (5). The form of $\mathcal{L}$ makes it possible to incorporate nonlocal effects in connection with all variables $\underline{\alpha}, \underline{\beta}, \underline{\delta}$. Neglecting nonlocal interactions we obtain function $\mathcal{M}$ only in (7). This function encompass functions A, B, D from (2) (3) and (4).

The constitutive relations discussed here undergo constraints imposed by the Clausius-Duhem inequality [18] in the following form

$$\frac{1}{\rho}(\underline{\mathbf{t}} - \rho \partial_{\underline{\mathbf{F}}} \Psi) \dot{\underline{\mathbf{F}}} + \frac{1}{\rho} \sum_{\lambda} (\underline{\mathbf{f}}_{\lambda} - \rho \partial_{\underline{\mathbf{w}}_{\lambda}} \Psi) \dot{\underline{\mathbf{w}}}_{\lambda} - (\partial_T \Psi + S) \dot{T} - \partial_{\underline{\mu}} \Psi \{ \mathcal{L}\underline{\mu} + \mathcal{M}(\underline{\mathbf{h}}, \underline{\mu}) \} - \frac{1}{\rho T} \underline{\mathbf{q}} \underline{\mathbf{g}} \geq 0. \quad (8)$$

Here it is assumed that the free energy Ψ does not depend on gradients of temperature.

3. An internal variable pertaining to more averaged description

The previously considered model with the small volume of averaging (L1) could be applied for calculations related to rather small pieces of monocrystal or could be used as a theoretical basis for more averaged description.

More averaged description means the averaging through the composition of martensite variants and parent phase. Then many problems appear. In general the detailed form of the free energy is not known in this instance. What kind of internal variables should be used for description of dissipation.

In the literature we can come across the internal variable x which means volume fraction of martensitic structure related to the total volume of this part of material on which the averaging is carried out.

In the paper an internal variable for which the evolution equation could be determined with the aid of L1-model is suggested.

Let us assume that the composition of martensite variants consists of different kinds of variants and different kinds of interfaces pertaining to it. The kinds of interfaces are presented in Fig. 3 in the case of CuAl alloy for which martensite appears in self-accomodating forms [6].

In Fig. 3 a schematic representation of a martensitic plate group with notations from [6] is shown. One self-accomodating group comprises four martensite variants. These variants create different types of interfaces. There are habit type interface, twin type interface and different types of interfaces between austenite

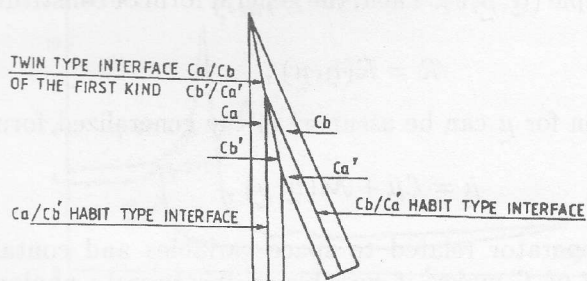


Fig. 3. Schematic representation of a martensite plate group

and martensite. Considered interfaces have different mechanical properties. This fact should be taken into account in mechanical description.

Let us consider a complex of volume V on which averaging takes place. Let $\mathbf{x}_c$ stand for coordinates of the center of the complex. Furthermore, we assume that each kind of interfaces is exactly oriented with the help of a unit vector $\mathbf{n}_m$ perpendicular to it, where m stands for index related to this kind of interfaces.

Let us consider also a system of coordinates with the origin in point $\mathbf{x}_c$. Let $\mathbf{x}_{mj}$ be the position of a point which lies on j -th interface of kind m . Then we can introduce the variable

$$z_{mj} = (\mathbf{x}_{mj} - \mathbf{x}_c) \cdot \mathbf{n}_m = \mathbf{x}_{mj} \cdot \mathbf{n}_m \quad (9)$$

Let us consider an axis in direction $\mathbf{n}_m$ which contains the point $\mathbf{x}_c$. Then the variable z_{mj} means a coordinate on this axis as a point of intersection of the interface and the axis. Let furthermore s_{mj} be the area of mj -th interface in the complex.

We can assume that many different interfaces exist in the complex. They are marked by indices mj . The mj -th interface has a position determined by z_{mj} and area given by s_{mj} . However s_{mj} depends on position z_{mj} and geometry of the complex. Assuming approximately the constant geometry of the complex we can notice that $s_{mj} = s_{mj}(z_{mj})$.

The interfaces can appear and vanish in the complex. It is due to the influx from the outside or efflux into the outside of the interfaces. We consider also the case when the interfaces can be created or annihilated in the complex owing to the deformation. We assume that a new value of j is assigned to each new interface. Let us also introduce the function c_{mj} which is equal 1 if mj -th interface is present in the complex and $c_{mj} = 0$ if that is not satisfied. Then we can define the internal variable for L2-level in the form

$$\eta = \frac{1}{V} \sum_{m \in M} \left(\sum_{j \in J} c_{mj} z_{mj} s_{mj} \right). \quad (10)$$

This variable means the sum of products of coordinates of interfaces and their areas within the complex of volume V . The rate of change of this variable is related to the velocities of interfaces. Values of the velocities and the area of interfaces are just responsible for the amount of dissipation in the complex.

Next let us consider the time derivative of this variable

$$\dot{\eta} = \frac{1}{V} \sum_{m \in M} \left[\sum_{j \in J} c_{mj} \frac{\partial z_{mj}}{\partial t} (s_{mj} + z_{mj} \frac{\partial s_{mj}}{\partial z_{mj}}) \right] = \frac{1}{V} \sum_{m \in M} \left[\sum_{j \in J} c_{mj} A_{mj} \frac{\partial z_{mj}}{\partial t} \right]. \quad (11)$$

The quantity A_{mj} can be calculated from geometrical considerations related to the translation of surfaces in the given complex. In general the range of summation in (11) can vary. It is due to the previously mentioned fact that interfaces can be created and annihilated during the deformation as well as they can flow out and flow into the considered complex.

The formula (11) can be a starting point for determination of the evolution equation for variable η . The internal variable η is constructed on the complex thus it is a more averaged variable than μ . On the other hand, the evolution equation for this variable should depend on a deformation measure expedient for η .

Thus, let us assume that the complex deforms homogeneously. Then its deformation can be described by the Green strain tensor $\mathbf{e}$ as an averaged deformation relative to L1-field of deformation. Evidently in view of all complexes which are considered in the body and assigned to them tensors $\mathbf{e}$ we define by approximation the field of deformation $\mathbf{e}(X)$.

Let V_1, V_2, W_1, W_2 be spaces of functions $\mathbf{h}, (\mathbf{h}, \mu), \bar{\mathbf{h}}, \eta$ correspondingly which are defined on the complex K related to a more averaged model. We assume that there exist functions $G: V_1 \rightarrow W_1$, $G(\mathbf{h}) = \bar{\mathbf{h}}$, $L: V_2 \rightarrow W_2$, $L(\mathbf{h}, \mu) = \eta$. The $\bar{\mathbf{h}}$ and η are counterparts of $\mathbf{h}, \mu$ for L2-model. The time derivative of z_{mj} in (11) is just this quantity which could be calculated on the basis of the L1-model [2÷3]. In general we can assume that

$$\frac{\partial z_{mj}}{\partial t} = Z(\mathbf{h}, \mu). \quad (12)$$

The geometrical quantities A_{mj} also depend on $(\mathbf{h}, \mu)$, therefore, we can assert the general dependance

$$\left(\frac{1}{V} \sum_{m \in M} \sum_{j \in J} c_{mj} A_{mj} \frac{\partial z_{mj}}{\partial t} \right) (\mathbf{h}, \mu) = H(\mathbf{h}, \mu). \quad (13)$$

Then the evolution equation can be expressed in a general form

$$\dot{\eta} = H(G^{-1}(\mathbf{h}), L^{-1}(G^{-1}(\mathbf{h}), \eta)), \quad (14)$$

where L^{-1} is carried out assuming $\mathbf{h}$ to be constant. In practice we can build up the exact form of (14) with the help of numerical calculation on L1-level.

In order to fully describe dissipation within the frame of the L2-model first the free energy should be obtained from L1 description and next this free energy and the remaining constitutive functions should be plotted with variable η .

Let $\bar{\Psi}$, $\bar{\mathbf{t}}$, $\bar{S}$, $\bar{\mathbf{q}}$ stand for the free energy, stress, entropy and heat flux for L2-description. Then the evolution equation for η and constitutive relations should determine the amount of dissipation equal to the total dissipation described by the L1-model. It means that

$$\int \left(\frac{1}{\rho} (\bar{\mathbf{t}} - \rho \partial_{\bar{\mathbf{F}}} \bar{\Psi}) \dot{\bar{\mathbf{F}}} + \frac{1}{\rho} \sum_{\lambda} (\bar{\mathbf{f}}_{\lambda} - \rho \partial_{\bar{\mathbf{w}}_{\lambda}} \bar{\Psi}) \dot{\bar{\mathbf{w}}}_{\lambda} - (\partial_T \bar{\Psi} + \bar{S}) \dot{T} - \partial_{\bar{\mu}} \bar{\Psi} \{ \mathcal{L}_{\bar{\mu}} + \mathcal{M}(\bar{\mathbf{h}}, \bar{\mu}) \} - \right. \\ \left. - \frac{1}{\rho T} \bar{\mathbf{q}} \bar{\mathbf{g}} \right) dV = V \left(\frac{1}{\rho} (\bar{\mathbf{t}} - \rho \partial_{\bar{\mathbf{F}}} \bar{\Psi}) \dot{\bar{\mathbf{F}}} - (\partial_T \bar{\Psi} + \bar{S}) \dot{T} - (\partial_{\eta} \bar{\Psi} \dot{\eta} - \frac{1}{\rho T} \bar{\mathbf{q}} \bar{\mathbf{g}}) \right). \quad (15)$$

4. Final remarks

In the paper a group of internal variables which can describe the dissipation process for L1-level of description is discussed. However detailed identification of their evolution equations creates new rather difficult problems. It is suggested that more advanced methods for calculations perhaps on a yet more fundamental level should be used. In turn, the solution of this problem gives a chance for calculation a dissipation during the martensitic transformation. Then more simple models on L2-level could be constructed and also describe the dissipation.

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Zmienne wewnętrzne w opisie martenzytycznej przemiany fazowej w pojedynczym kryształach

Streszczenie

W pracy rozważa się typy zmiennych wewnętrznych, które powinny być użyte do zamodelowania dysypacji w materiałach podlegających martenzytycznej przemianie fazowej. Problem rozważany jest na dwu poziomach opisu. Pierwszy z nich (L1) związany jest z małą objętością uśredniania. W przypadku takim rozważa się szczegółowe mechanizmy towarzyszące przemianie martenzytycznej. Na tym poziomie opisu wprowadzono trzy typy zmiennych wewnętrznych. Drugi poziom opisu (L2) związany jest z większym stopniem uśredniania. Założono przy tym, że model L1 będzie stanowił teoretyczną podstawę dla modelu L2. Definiuje się zmienną wewnętrzną związaną z opisem L2, dla której równania ewolucji mogłyby być określone za pomocą modelu L1.