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A MICROMECHANICAL MODEL FOR THE KINETICS OF MARTENSITIC TRANSFORMATION

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Abstract—Thermomechanical and transformation behaviors of polycrystalline shape memory alloys are studied in the process of stress-induced martensitic transformation from the micromechanical point of view. The microscopic deformation due to transformation is connected to the macroscopic behavior of alloys by introducing two different levels of microstructure in alloys; the microregion as the smallest element and the mesodomain which contains many microregions but is still small compared to the specimen. The thermomechanical constitutive equation and the transformation kinetics are discussed.

1. INTRODUCTION

Extensive metallurgical studies on shape memory alloys have revealed that their "anomalous" behavior under thermomechanical circumstances is due to the martensitic transformation and its reverse transformation (Delaey *et al.*, 1974; Perkins, 1975). The microstructural change associated with the transformation has often been investigated from the thermodynamic point of view (Tong and Wayman, 1975; Ortin and Planes, 1988), while the phenomenological theory explains well the formation of the martensite plates and the self-accommodation process during cooling (Wayman, 1964; Otsuka *et al.*, 1976).

From the engineering point of view the macroscopic behavior of the alloys under the applied thermomechanical load is an important theme to be investigated. The stress–strain–temperature relation, the recovery stress induced during the process and the behavior under cyclic thermomechanical load are some of the topics to be studied from the continuum mechanical point of view (Tanaka *et al.*, 1986; Tanaka, 1990).

The present paper intends to answer the problem of whether such a macroscopic approach is compatible with the microscopic observations. A theoretical chain from the elementary process of "the microregion", which is defined as the smallest microstructure, to the behavior of "the mesodomain", which is a much larger domain and represents a macroscopic behavior of alloys, is explained.

2. MICROSTRUCTURE IN ALLOYS AND KINEMATICS IN MICROREGION

A microregion in a polycrystalline alloy is defined as the smallest microstructural element of the alloy. We introduce the global coordinate system o-$X_1X_2X_3$ attached to the specimen, and the local coordinate system o-$x_1x_2x_3$ characterized by the Eulerian angles ω with respect to the global coordinate (see Fig. 1). The local coordinate system is so defined that the third axis is taken to be normal to the habit plane. The directions of the first two axes lying on the habit plane are determined later.

We then introduce, as illustrated in Fig. 1, a much larger domain in the specimen, a mesodomain, in such a way that it contains a large number of microregions but is still small compared to the size of the specimen.

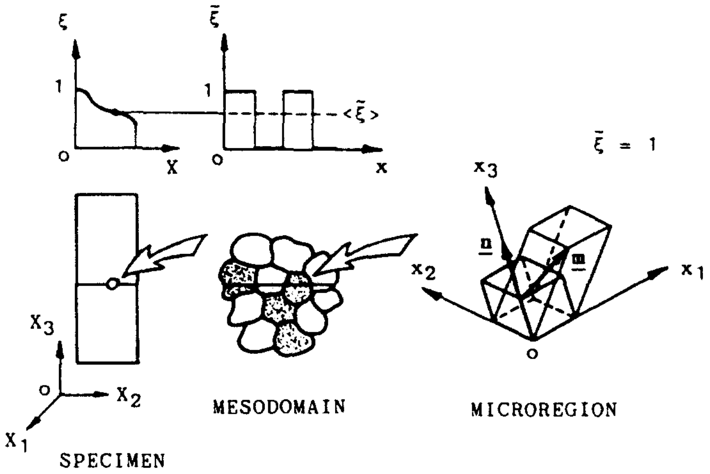

Fig. 1. Microstructures in alloys.

Now we assume that only one state exists at the level of microregion in the process of a martensitic transformation; the non-transformed state or the transformed state; or more directly, the parent phase or the martensite phase.

When the transformation occurs in a microregion, it deforms as shown in Fig. 1, and a microscopic stress-free strain tensor

$$\tilde{\varepsilon}^* = (\mathbf{m}\otimes\mathbf{n}+\mathbf{n}\otimes\mathbf{m})/2 \tag{1}$$

is observed, where **n** and **m** represent the unit normal to the habit plane, and the vector of motion, respectively. The notation ⊗ stands for the tensor product. Now the first two axes of the local coordinate system which are yet left undetermined are defined such that the vector of motion **m** lies on the x_1, x_3-plane as illustrated in Fig. 1. The microscopic stress-free strain tensor given by eqn (1) now always reads as

$$\tilde{\varepsilon}^*_{13} = \tilde{\varepsilon}^*_{31} = \tilde{\gamma}/2, \quad \tilde{\varepsilon}^*_{33} = \tilde{\varepsilon}, \quad \text{otherwise } \tilde{\varepsilon}^*_{ij} = 0, \tag{2}$$

with respect to the local coordinate system, where $\tilde{\varepsilon}$ and $\tilde{\gamma}$ denote the strain normal to the habit plane, and the shear strain parallel to the habit plane, respectively.

3. ENERGY BALANCE IN A MICROREGION

Thermodynamics of transformation in alloys have revealed that the formation of martensite starts in the parent phase when a so-called "driving force" reaches a threshold value on a habit plane (Tong and Wayman, 1975; Patel and Cohen, 1953). In this study the energy balance is used to derive a transformation condition since the thermodynamical equilibrium should not be assumed during the "catastrophic" transformation process in our microregion.

Just before the transformation the microregion under consideration is subjected to a load stress tensor $\tilde{\sigma}_L$ and a self-equilibrating stress $\tilde{\sigma}_{eq}$ which has been developed due to the interaction of all microregions transformed up to that time with their neighboring material. Since the transformation of the microregion progresses in a "catastrophic" manner, stresses $\tilde{\sigma}_{eq}$ and $\tilde{\sigma}_L$ can be assumed to be unchanged during transformation. The only time-dependent stress $\tilde{\sigma}_n$ is induced due to the interaction of the newly transformed microregion with the surroundings. The strain state $\tilde{\varepsilon}_L$ and $\tilde{\varepsilon}_{eq}$, which corresponds to $\tilde{\sigma}_L$ and $\tilde{\sigma}_{eq}$, respectively, can also be assumed to remain unchanged during transformation. To the stress state $\tilde{\sigma}_n$ a strain tensor

$$\tilde{\varepsilon}_n = \tilde{\varepsilon}_{n,el} + \tilde{\varepsilon}_{n,pl} \tag{3}$$

is related, where the additive decomposition into an elastic and a plastic part is well understood.

If the energy balance equation is formulated just before and after the transformation, and if the equations obtained are subtracted, we arrive at

$$\int (\tilde{\boldsymbol{\sigma}}_{\mathrm{L}}+\tilde{\boldsymbol{\sigma}}_{\mathrm{eq}}+\tilde{\boldsymbol{\sigma}}_{\mathrm{n}}/2):[\tilde{\boldsymbol{\varepsilon}}_{\mathrm{n,el}}+\tilde{\boldsymbol{\varepsilon}}_{\mathrm{n,pl}}+\tilde{\boldsymbol{\varepsilon}}^{*}]\,\mathrm{d}V+\int q\,\mathrm{d}V=\int \Delta e\,\mathrm{d}V+\partial V\Gamma+V\Delta B, \tag{4}$$

where Γ represents an energy "loss" per unit area to produce a new interface, while ΔB stands for an energy "loss" per unit volume during the formation of a martensite variant through such metallurgical processes as the Bain-strain, invariant lattice shear strain and the lattice rotation (see e.g. Wayman, 1964). q is the heat per unit volume supplied from the exterior, while V and ∂V the average volume and surface area of the microregion, respectively.

Let us decompose the difference of the free energy per unit volume Δe as follows:

$$\Delta e = \Delta e_{\mathrm{e}}+\Delta e_{\mathrm{c}}+\Delta e_{\mathrm{h}}+\Delta e_{\mathrm{p}}, \tag{5}$$

where Δe_{e} represents the thermoelastic energy difference, Δe_{c} the chemical energy difference, Δe_{h} the heat stored in the interval and Δe_{p} the plastic part, or more directly the energy due to dislocation production. Since we clearly observe the relations

$$\int \Delta e_{\mathrm{e}}\,\mathrm{d}V=\int (\tilde{\boldsymbol{\sigma}}_{\mathrm{L}}+\tilde{\boldsymbol{\sigma}}_{\mathrm{eq}}+\tilde{\boldsymbol{\sigma}}_{\mathrm{n}}/2):\tilde{\boldsymbol{\varepsilon}}_{\mathrm{n,el}}\,\mathrm{d}V,$$

$$\int (\Delta e_{\mathrm{h}}+\Delta e_{\mathrm{p}})\,\mathrm{d}V=\int (\tilde{\boldsymbol{\sigma}}_{\mathrm{L}}+\tilde{\boldsymbol{\sigma}}_{\mathrm{eq}}+\tilde{\boldsymbol{\sigma}}_{\mathrm{n}}/2):\tilde{\boldsymbol{\varepsilon}}_{\mathrm{n,pl}}\,\mathrm{d}V+\int q\,\mathrm{d}V, \tag{6}$$

eqn (4) is finally written as

$$V\Delta G_{\mathrm{c}}=\int \Delta e_{\mathrm{c}}\,\mathrm{d}V=\int (\tilde{\boldsymbol{\sigma}}_{\mathrm{a}}+\tilde{\boldsymbol{\sigma}}_{\mathrm{n}}/2):\tilde{\boldsymbol{\varepsilon}}^{*}\,\mathrm{d}V-\partial V\Gamma-V\Delta B, \tag{7}$$

where ΔG_{c} presents the difference of chemical energy per unit volume of the microregion, and $\tilde{\boldsymbol{\sigma}}_{\mathrm{a}}=\tilde{\boldsymbol{\sigma}}_{\mathrm{L}}+\tilde{\boldsymbol{\sigma}}_{\mathrm{eq}}$ is the actual stress tensor in the microregion before the transformation.

Energy balance (7) may be rewritten as

$$\Delta G=-\Delta B,\quad \Delta G=\Delta G_{\mathrm{c}}-(\tilde{\boldsymbol{\sigma}}_{\mathrm{a}}+\tilde{\boldsymbol{\sigma}}_{\mathrm{n}}/2):\tilde{\boldsymbol{\varepsilon}}^{*}-(\partial V/V)\Gamma, \tag{8}$$

where the term $\tilde{\boldsymbol{\sigma}}_{\mathrm{a}}:\tilde{\boldsymbol{\varepsilon}}^{*}=\tilde{\sigma}_{\mathrm{a}}\tilde{\varepsilon}+\tilde{\tau}_{\mathrm{a}}\tilde{\gamma}$ with $\tilde{\sigma}_{\mathrm{a}}=\tilde{\sigma}_{\mathrm{a}33}$ and $\tilde{\tau}_{\mathrm{a}}=\tilde{\sigma}_{\mathrm{a}31}$ represents the interaction energy with the actual stress (Patel and Cohen, 1953), while $\tilde{\boldsymbol{\sigma}}_{\mathrm{n}}:\tilde{\boldsymbol{\varepsilon}}^{*}/2$ is the energy due to interaction with the other microregions. The quantity ΔG defined by the second part of eqn (8) is a generalized form of the driving force discussed by metallurgists.

In order to measure the extent of transformation in a microregion ω which is subjected to $(\tilde{\boldsymbol{\sigma}}_{\mathrm{a}}, T)$, the micro-fraction $\tilde{\xi}=\tilde{\xi}(\tilde{\boldsymbol{\sigma}}_{\mathrm{a}}, T, \omega)$ is introduced through

$$\tilde{\xi}=\begin{cases}1 & \text{for}\quad \Delta G=-\Delta B,\\ 0 & \text{for}\quad \Delta G>-\Delta B.\end{cases} \tag{9}$$

In Fig. 1 a distribution of $\tilde{\xi}$ along a horizontal line in the mesodomain is illustrated schematically. When ΔG reaches a threshold value $-\Delta B$ on a habit plane ω, the martensitic transformation occurs in the microregion ω, and the microregion is labelled by $\tilde{\xi}=1$ under this local agency (σ_a, T). For a habit plane on which $\Delta G > -\Delta B$ holds, no transformation yet begins, and the microregion is labelled as $\tilde{\xi} = 0$.

4. CONSTITUTIVE EQUATIONS IN A MICROREGION

When the material behavior is limited within the elastic range, the constitutive equation in a microregion can be written in the transformed state as

$$\tilde{\varepsilon} - \tilde{\varepsilon}^* - \tilde{\varepsilon}_T = \tilde{\mathbf{I}} : \tilde{\sigma}, \quad \tilde{\varepsilon}_T = \tilde{\alpha}(T - T_0) \tag{10}$$

where $\tilde{\varepsilon}$ means the strain tensor induced in the microregion, and $\tilde{\varepsilon}_T$ stands for the thermal expansion term with a thermal expansion tensor $\tilde{\alpha}$. And $\tilde{\mathbf{I}}$ and T_0 represents the elastic compliance tensor and the reference temperature, respectively. The current stress tensor $\tilde{\sigma}$ in the microregion is equivalent to $\tilde{\sigma}_L + \tilde{\sigma}_{eq} + \tilde{\sigma}_n$.

It is worth noting here that the first part of eqn (10) can be rewritten in the global coordinate system as

$$\varepsilon - \varepsilon^* - \varepsilon_T = \mathbf{I} : \sigma, \tag{11}$$

where the stress and strain tensors with respect to the global coordinate system are given with the help of the orthogonal transformation tensor $\mathbf{Q}(\omega)$ as follows:

$$\sigma_a = \mathbf{Q} \cdot \tilde{\sigma}_a \cdot \mathbf{Q}^T, \quad \varepsilon = \mathbf{Q} \cdot \tilde{\varepsilon} \cdot \mathbf{Q}^T, \quad \varepsilon^* = \mathbf{Q} \cdot \tilde{\varepsilon}^* \cdot \mathbf{Q}^T,$$
$$\varepsilon_T = (\mathbf{Q} \cdot \tilde{\alpha} \cdot \mathbf{Q}^T)(T - T_0). \tag{12}$$

The transformation between the elastic compliance tensors $\tilde{\mathbf{I}}$ and $\mathbf{I}$ with respect to the local and global coordinate systems, respectively, is also understood as usual.

5. AVERAGING PROCESS

Let us first define over a mesodomain an average value $\langle f \rangle$ of an arbitrary microscopic quantity $f(\omega)$ evaluated in a microregion ω by the formula

$$\langle f \rangle = \frac{\int g(\omega) f(\omega)\, \mathrm{d}\omega}{\int g(\omega)\, \mathrm{d}\omega}. \tag{13}$$

The weighting function $g(\omega)$ represents the distribution density function characterizing the crystallographic axes of the microregions.

The extent of transformation in the mesodomain is measured by the macrofraction ξ defined by

$$\xi = \langle \tilde{\xi} \rangle = \frac{\int g(\omega) \tilde{\xi}\, \mathrm{d}\omega}{\int g(\omega)\, \mathrm{d}\omega}, \quad 0 \leqslant \xi \leqslant 1. \tag{14}$$

Figure 1 illustrates a distribution of the macro-fraction ξ along a line in the specimen.

Now by taking an average of eqn (11) we obtain

$$\mathbf{E}-\mathbf{E}_c-\mathbf{E}_T = \langle \mathbf{l}:\boldsymbol{\sigma}\rangle = \mathbf{L}:\boldsymbol{\Sigma},$$

$$\mathbf{E} = \langle \boldsymbol{\varepsilon}\rangle,\quad \mathbf{E}_c = \langle \boldsymbol{\varepsilon}^*\rangle = \frac{\displaystyle\int g(\omega)(\mathbf{Q}\cdot\bar{\boldsymbol{\varepsilon}}^*\cdot\mathbf{Q}^T)\tilde{\xi}\,\mathrm{d}\omega}{\displaystyle\int g(\omega)\,\mathrm{d}\omega},$$

$$\mathbf{E}_T = \langle \boldsymbol{\varepsilon}_T\rangle = \langle \mathbf{Q}\cdot\tilde{\boldsymbol{\alpha}}\cdot\mathbf{Q}^T\rangle(T-T_0),\quad \boldsymbol{\Sigma} = \langle\boldsymbol{\sigma}\rangle, \tag{15}$$

where $\mathbf{E}$ stands for the macroscopic strain tensor, which is related to the macroscopic displacements through the strain-displacement relation, while $\mathbf{E}_c$ is the macroscopic stress-free strain tensor due to transformation, and $\mathbf{E}_T$ is the macroscopic strain tensor due to thermal expansion. When the transformation is complete in the whole mesodomain, $\mathbf{E}_c$ has an extreme value $\mathbf{E}_c^*$.

The global stress tensor $\boldsymbol{\Sigma}$ corresponding to the macroscopic strain tensor $\mathbf{E}$ is given by

$$\boldsymbol{\Sigma} = \langle\boldsymbol{\sigma}\rangle = \langle\boldsymbol{\sigma}_L\rangle + \langle\boldsymbol{\sigma}_{eq}+\boldsymbol{\sigma}_n\rangle = \langle\boldsymbol{\sigma}_L\rangle. \tag{16}$$

Many different schemes exist to give an effective elastic moduli tensor $\mathbf{L}$ in eqn (15), and to simulate a "global" stress ($\boldsymbol{\Sigma}$)–strain ($\mathbf{E}$) relation (Patoor *et al.*, 1987; Hutchinson, 1970; Tanaka and Fischer, unpublished).

6. KINETIC EQUATION OF MACROFRACTION ξ

Under an incremental loading ($\mathrm{d}\boldsymbol{\sigma}$, $\mathrm{d}T$) that corresponds to the global thermomechanical increment ($\mathrm{d}\boldsymbol{\Sigma}$, $\mathrm{d}T$), the number $\mathrm{d}N$ of the microregions transforming to martensite phase per unit volume of parent phase may be assumed to be (Magee, 1968):

$$\mathrm{d}N = -k\langle \mathrm{d}\Delta G\rangle,\quad \mathrm{d}\Delta G \leqslant 0, \tag{17}$$

with $k > 0$ as a proportionality constant. The change in macrofraction $\mathrm{d}\xi$ is now given by

$$\mathrm{d}\xi = [V\bar{V}(1-\xi)\,\mathrm{d}N]/\bar{V} = V(1-\xi)\,\mathrm{d}N = -kV(1-\xi)\langle \mathrm{d}\Delta G\rangle \tag{18}$$

with the average volume of mesodomain $\bar{V}$.

Since the self-equilibrating stress state $\boldsymbol{\sigma}_{eq}$ may approximately be described by a hydrostatic compression stress state $-p\xi\mathbf{I}$ with unity tensor $\mathbf{I}$ (Johansson, 1937; Nilan, 1967), it follows from eqns (17) and (18), together with the second part of eqn (8), a final governing equation for the macrofraction ξ:

$$\left(\frac{1}{1-\xi}+kVp\mathbf{I}:\mathbf{E}_c^*\xi\right)\mathrm{d}\xi = -kV\left\langle\frac{\partial\Delta G_c}{\partial T}\right\rangle \mathrm{d}T + kV\xi\mathbf{E}_c^*:\mathrm{d}\boldsymbol{\Sigma}. \tag{19}$$

The solution $\xi(\boldsymbol{\Sigma}, T)$, the transformation kinetics, describes the progress of the macroscopic transformation. We could derive as the simplest case the transformation kinetics employed by Tanaka and Sato (1985):

$$\xi = 1-\exp\,[A(M_s-T)+\mathbf{B}:\boldsymbol{\Sigma}],\quad A = -kV\left\langle\frac{\partial\Delta G_c}{\partial T}\right\rangle,\quad \mathbf{B} = -kV\mathbf{E}_c^*. \tag{20}$$

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