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A generalized micromechanics constitutive theory of single crystal with thermoelastic martensitic transformation*

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Abstract Based on the crystallographic theory of martensitic transformation and Hill-Rice's internal variable constitutive theory, a generalized micromechanics constitutive model is established to describe the thermoelastic martensitic transformation and reorientation of single crystal. This model can describe the macroscopic constitutive behavior due to the microstructure changes of forward transformation, reverse transformation and reorientation in single crystal under complex thermodynamic loading condition. The theoretical predictions agree well with the available experiment.

Keywords: micromechanics, constitutive relation, thermoelastic martensitic transformation.

Martensitic transformation is one of the most important transformations in material science. When the shape and volume change produced by the martensitic transformation is accommodated through elastic deformation, this transformation is called thermoelastic martensitic transformation. In the light of the directions of the process and the changes in material microstructures, thermoelastic martensitic transformation can be divided into three kinds: the forward transformation (the transformation from parent phase to martensite), the reverse transformation (the transformation from martensite to parent phase) and the reorientation between different kinds of martensite habit plane variants. These changes in microstructures lead to various macroscopic phenomena such as pseudoelasticity, shape memory effect[1].

With the increasing application of shape memory alloys and structural ceramics, the research on the constitutive relation of these materials attracts interest of the researchers of solid mechanics and a lot of work has been done. For example, Falk[2] applied Landau-Devonshire phenomenological theory to shape memory alloys and obtained one-dimensional stress-strain relations at different temperatures. Sun and Hwang[3] applied micromechanics to investigating the constitutive behavior of transformation plasticity.

In order to understand the transformation constitutive behavior more clearly, it is necessary to study it in a finer scale such as the scale of variants and to absorb more research achievements of physics and materials science. In the present work, the crystallographic theory of martensitic

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transformation and the micromechanics are synthetically employed to investigate the transformation plasticity of the thermoelastic martensitic transformation single crystal.

1 Description of the constitutive element

1.1 Microscopic transformation plastic strain

The martensitic transformation crystallographic theory is one of the most important theories in the field of martensitic transformation in material science. The main content of this theory is that martensitic transformation is realized through an invariant plane strain $\boldsymbol{D}$:

$$\boldsymbol{D} = \boldsymbol{I} + g\boldsymbol{en}, \tag{1}$$

where $\boldsymbol{I}$ is the unit tensor of rank two, $\boldsymbol{e}$ is the displacement direction of the invariant plane, $\boldsymbol{n}$ is the normal of the invariant plane and g, usually taken as a material constant, is the displacement magnitude of the invariant plane per unit length along the normal $\boldsymbol{n}$.

In the light of the crystallographic theory of martensitic transformation, we can determine all the possible kinds of martensite variants with different orientations, i.e. we can determine the invariant plane strain $\boldsymbol{D}_s$ of the sth kind of variants (crystallographically permissive). So, by using small-deformation theory, we can calculate the microstructral transformation strain $\boldsymbol{\varepsilon}_s^{\mathrm{p}}$ corresponding to the formation of the sth kind of variants as

$$\boldsymbol{\varepsilon}_s^{\mathrm{p}} = g\boldsymbol{R}_s = \frac{1}{2}g(\boldsymbol{e}_s\boldsymbol{n}_s + \boldsymbol{n}_s\boldsymbol{e}_s) \quad (s = 1, \cdots, N), \tag{2}$$

where N is the number of the possible kinds of martensite variants.

1.2 The constitutive element and its energies

A representative material sample (constitutive element) with volume V illustrated in fig. 1 is taken from a single crystalline bulk as the subject of study. Temperature T uniformly distributes everywhere in the element and the external macroscopic stress Σ or strain $\boldsymbol{E}$ is applied on the boundary. In order to analyse the elastic strain energy due to the incompatibility of the transformation strain of the variants with each others and the surrounding elastic parent matrix in the constitutive element, a concept of inclusion is used. Inclusions are defined as the very small transformed martensite variants as shown in fig. 1. A lot of micrographs show that a martensite variant appears in a shape of plate or blade, so here we approximate the geometric shape of an inclusion by an oblate spheroid with $a_1 = a_2$, $a_3/a_1 = \rho < 1$, where a_1, a_2 and a_3 are the principal half axes of the spheroid, and from experimental observations[1] we further assume that the short axis of the spheroidal inclusion is normal to the invariant plane of the variant. The value of ρ for all the inclusions is assumed to be a constant while the sizes of the inclusions may be different. So different kinds of variants are represented by inclusions with different orientations of the short axes. A constitutive element is composed of par-

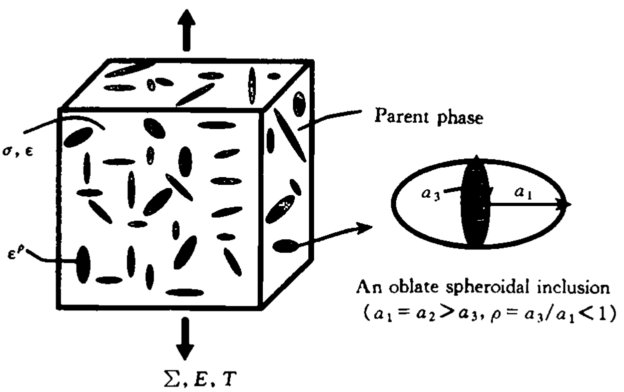

Fig. 1. Illustration of a constitutive element with a lot of inclusions.

ent phase and a large number of inclusions. As the external stress Σ or strain $\boldsymbol{E}$ is homogeneous, the location of an inclusion is considered to be sited stochastically.

Denote the volume occupied by the sth kind of variants ($s = 1, \cdots, N$) by V_s and the corresponding volume fraction by $f_s (= V_s / V)$. The total volume of transformed variants, its volume fraction and the parent phase's volume are $V_i = \sum_{s=1}^{N} V_s$, $f = \sum_{s=1}^{N} f_s$ and $V_p = V - V_i$, respectively[1]. Under applied macroscopic stress Σ and temperature T, the microscopic stress and strain in the element are expressed by $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$. Then there exists the relation between $\boldsymbol{\sigma}$ and Σ,

$$\Sigma = \langle \boldsymbol{\sigma} \rangle_V = \frac{1}{V} \int_V \boldsymbol{\sigma} \mathrm{d} V = \sum_{s=1}^{N} f_s \langle \boldsymbol{\sigma} \rangle_{V_s} + (1 - f) \langle \boldsymbol{\sigma} \rangle_{V_p}, \tag{3}$$

where $\langle \ \rangle$ denotes the volume average over the volume indicated by the subscript. The microscopic and macroscopic strains are assumed to be small and can therefore be decomposed into elastic and plastic parts:

$$\boldsymbol{E} = \langle \boldsymbol{\varepsilon}^{\mathrm{e}} \rangle_V + \langle \boldsymbol{\varepsilon}^{\mathrm{p}} \rangle_V = \boldsymbol{E}^{\mathrm{e}} + \boldsymbol{E}^{\mathrm{p}} = \boldsymbol{M} : \boldsymbol{\Sigma} + \boldsymbol{E}^{\mathrm{p}}, \tag{4}$$

where the thermal strain and stress are neglected for simplicity. We have assumed that the martensite and the parent phase have the same anisotropic constant elastic compliance tensor $\boldsymbol{M}$ in eq. (4). Similarly, the macroscopic plastic strain can be expressed by the microscopic transformation strains:

$$\boldsymbol{E}^{\mathrm{p}} = \langle \boldsymbol{\varepsilon}^{\mathrm{p}} \rangle_V = f \langle \boldsymbol{\varepsilon}^{\mathrm{p}} \rangle_{V_i} = \sum_{s=1}^{N} f_s \boldsymbol{\varepsilon}_s^{\mathrm{p}}. \tag{5}$$

According to the crystallographic theory of martensitic transformation, from eq. (2), we further have

$$\boldsymbol{E}^{\mathrm{p}} = g \sum_{s=1}^{N} f_s \boldsymbol{R}_s. \tag{6}$$

By using Mori-Tanaka mean field theory[4], the transformation-induced internal stress $\bar{\boldsymbol{\sigma}}_s$ in the sth ($s = 1, \cdots, N$) kind of inclusions can be expressed as

$$\bar{\boldsymbol{\sigma}}_s = \boldsymbol{L} : (\boldsymbol{S}_s - \boldsymbol{I}) : \boldsymbol{\varepsilon}_s^{\mathrm{p}} - \boldsymbol{L} : \sum_{t=1}^{N} (\boldsymbol{S}_t - \boldsymbol{I}) : \boldsymbol{\varepsilon}_t^{\mathrm{p}} f_t, \tag{7}$$

where $\boldsymbol{L} = \boldsymbol{M}^{-1}$ is the constant elastic stiffness tensor of the element, $\boldsymbol{I}$ is the identity tensor of rank four and $\boldsymbol{S}$ is the Eshelby tensor determined by elastic constants and the shape parameters (i.e. the orientation and the ratio ρ) of the oblate spheroidal inclusion.

By using eq. (7), in the case of material being isotropic, the total elastic strain energy W per unit volume of the constitutive element can be expressed as

$$W = \frac{1}{2} \Big(\boldsymbol{E} - \sum_{s=1}^{N} \boldsymbol{\varepsilon}_s^{\mathrm{p}} f_s \Big) : \boldsymbol{L} : \Big(\boldsymbol{E} - \sum_{s=1}^{N} \boldsymbol{\varepsilon}_s^{\mathrm{p}} f_s \Big) + W_i \sum_{s=1}^{N} f_s - \sum_{s=1}^{N} \sum_{t=1}^{N} f_s f_t W_{st}, \tag{8}$$

where

$$W_i = W_s = -\frac{1}{2} \boldsymbol{\varepsilon}_s^{\mathrm{p}} : \boldsymbol{L} : (\boldsymbol{S}_s - \boldsymbol{I}) : \boldsymbol{\varepsilon}_s^{\mathrm{p}}, \tag{9}$$

$$W_{st} = -\frac{1}{4} \big[\boldsymbol{\varepsilon}_s^{\mathrm{p}} : \boldsymbol{L} : (\boldsymbol{S}_t - \boldsymbol{I}) : \boldsymbol{\varepsilon}_t^{\mathrm{p}} + \boldsymbol{\varepsilon}_t^{\mathrm{p}} : \boldsymbol{L} : (\boldsymbol{S}_s - \boldsymbol{I}) : \boldsymbol{\varepsilon}_s^{\mathrm{p}} \big]. \tag{10}$$

As all the parent-martensite and martensite-martensite interfaces are coherent for martensitic

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1) In i is used as a subscript indicating relevance to "inclusion", instead of an index of variants.

transformation, the surface energy change is ignored during transformation.

The total change in chemical free energy ΔG_{chem} for unit volume of the constitutive element is

$$\Delta G_{\mathrm{chem}}(T) = \frac{\Delta G}{V}\sum_{s=1}^{N} V_s = \Delta G\sum_{s=1}^{N} f_s = k(T - T_0)\sum_{s=1}^{N} f_s, \tag{11}$$

where $\Delta G = G_{\mathrm{m}}(T) - G_{\mathrm{p}}(T)$ and $G_{\mathrm{p}}(T)$, $G_{\mathrm{m}}(T)$ are chemical free energy per unit volume of parent and martensite phases, respectively. T_0 is the equilibrium temperature of the two phases and k is a positive constant.

The complementary free energy Ψ of the constitutive element per unit volume can be formulated as

$$\begin{aligned}\Psi(\Sigma, T, f_1, \cdots, f_N) &= -(W + \Delta G_{\mathrm{chem}} - \Sigma : \boldsymbol{E}) = \frac{1}{2}\Sigma : \boldsymbol{M} : \Sigma \\ &\quad + \Sigma : \sum_{s=1}^{N} \boldsymbol{\varepsilon}_s^{\mathrm{p}} f_s - (W_i + \Delta G)\sum_{s=1}^{N} f_s + \sum_{s=1}^{N}\sum_{t=1}^{N} f_s f_t W_{st}.\end{aligned} \tag{12}$$

The total energy dissipation W_{d} of the unit volume of constitutive element is the summation of the energy dissipation $W_{\mathrm{d}}^{\mathrm{tr}}$ per unit volume of constitutive element during the forward and/or reverse transformation and the energy dissipation $W_{\mathrm{d}}^{\mathrm{re}}$ per unit volume of constitutive element during the reorientation. We assumed that $W_{\mathrm{d}}^{\mathrm{tr}}$ is proportional to the accumulated volume fraction of transformation $f_{\mathrm{cu}}^{\mathrm{tr}} = (\sum_{s=1}^{N}\int_0^{f_{s0}} |\,\mathrm{d}f_{s0}\,|$, where f_{s0} is the part of the volume fraction of the sth kind of variants induced by transformation) and $W_{\mathrm{d}}^{\mathrm{re}}$ is proportional to the accumulated volume fraction of reorientation $f_{\mathrm{cu}}^{\mathrm{re}} = \frac{1}{2}\sum_{s=1}^{N}\sum_{\substack{t=1 \\ t\neq s}}^{N}\int_0^{f_{st}} |\,\mathrm{d}f_{st}\,|$, where $f_{st}(s \neq t)$ is the part of the volume fraction of the sth kind of variants reoriented from tth kind of variants). So we have

$$W_{\mathrm{d}} = W_{\mathrm{d}}^{\mathrm{tr}} + W_{\mathrm{d}}^{\mathrm{re}} = D^{\mathrm{tr}} f_{\mathrm{cu}}^{\mathrm{tr}} + D^{\mathrm{re}} f_{\mathrm{cu}}^{\mathrm{re}} = D^{\mathrm{tr}}\sum_{s=1}^{N}\int_0^{f_{s0}} |\,\mathrm{d}f_{s0}\,| + \frac{1}{2}D^{\mathrm{re}}\sum_{s=1}^{N}\sum_{\substack{t=1 \\ t\neq s}}^{N}\int_0^{f_{st}} |\,\mathrm{d}f_{st}\,|, \tag{13}$$

where D^{tr} and D^{re} can be considered as the generalized frictional resistances to the p-m and the m-m interface motions, respectively, and they are assumed to be material constants.

2 Constitutive relation for forward and reverse transformations in stress space

In this section, we only consider the processes of forward and reverse transformations in macroscopic stress space and the constitutive relation will be established in the stress space.

According to the internal variable constitutive theory[5], by the derived analytic expression of the complementary free energy $\Psi(\Sigma, T, f_1, \cdots, f_N)$, we can immediately conclude the thermodynamic state of the constitutive element is completely defined by the variables Σ, T, $f_1, \cdots, f_N$, in which Σ and T are macroscopic state variables and $f_1, \cdots, f_N$ are obviously the internal variables describing the microstructure change of material during transformation.

2.1 Transformation yielding condition

Denote the thermodynamic force conjugated to the internal variable f_s by F_s. Then

$$F_s = \frac{\partial \Psi}{\partial f_s} = \Sigma : \boldsymbol{\varepsilon}_s^{\mathrm{p}} - (W_i + \Delta G) + 2\sum_{t=1}^{N} f_t W_{st}. \tag{14}$$

When the transformation proceeds $(\dot{f}_s \neq 0)$, the second law of thermodynamics requires (with noting time rate d( )/dt denoted by ($\dot{}$))

$$\dot{\Psi}\,|_{\Sigma,T} = \sum_{s=1}^{N} \frac{\partial \Psi}{\partial f_s}\dot{f}_s = \sum_{s=1}^{N} F_s \dot{f}_s \geqslant 0, \tag{15}$$

where " = " in the above last inequality holds only for the ideal non-dissipative process (frictionless p-m interface motion). Under the condition of forward and/or reverse transformations, we have

$$f_{st} = 0,\ \text{and}\ f_s = f_{s0}(s = 1,\cdots,N;\ t = 1,\ \cdots,s-1,\ s+1,\cdots,N). \tag{16}$$

In the processes of forward and/or reverse transformations, the energy dissipation rate $\dot{W}_{\mathrm{d}}$ is (by eq. (13))

$$\dot{W}_{\mathrm{d}} = \dot{W}_{\mathrm{d}}^{\mathrm{tr}} = D^{\mathrm{tr}}\dot{f}_{\mathrm{cu}}^{\mathrm{tr}} = D^{\mathrm{tr}}\sum_{s=1}^{N} |\dot{f}_s|. \tag{17}$$

Since $\dot{\Psi}\,|_{\Sigma,T}$ must be equal to $\dot{W}_{\mathrm{d}}$ (according to thermodynamics), we have

$$\sum_{s=1}^{N} F_s\dot{f}_s = D^{\mathrm{tr}}\sum_{s=1}^{N} |\dot{f}_s|. \tag{18}$$

Because relation (18) is suitable to any possible combinations of $(\dot{f}_1, \dot{f}_2, \cdots, \dot{f}_N)$, we have

$$\begin{cases} F_s = \pm D^{\mathrm{tr}} & \text{if} \quad \dot{f}_s \neq 0, \\ \dot{f}_s = 0 & \text{if} \quad -D^{\mathrm{tr}} < F_s < D^{\mathrm{tr}}, \end{cases} \qquad (s = 1,\cdots,N), \tag{19}$$

where " + " stands for the forward transformation of the sth kind of variants with $\dot{f}_s > 0$ and " − " stands for the reverse transformation of the sth kind of variants with $\dot{f}_s < 0$. Substituting eq. (14) into the first part of eq. (19), we obtain the forward and reverse transformation yield functions for the sth $(s = 1,\cdots,N)$ kind of martensite variants as

$$Y_s(\Sigma, T, f_1,\cdots,f_N) = \Sigma : \boldsymbol{\varepsilon}_s^{\mathrm{p}} - (W_i + \Delta G) + 2\sum_{t=1}^{N} W_{st}f_t \mp D^{\mathrm{tr}} = 0, \tag{20}$$

where " − " stands for the forward transformation and " + " for reverse transformation. Because the volume of the lattice changes during transformation (usually tr$\boldsymbol{R}_s \neq 0$), this yield condition for forward and reverse transformation has the characteristics of pressure sensitivity.

2.2 Stress-strain relation

According to the internal variable theory, the macroscopic plastic strain rate $\dot{\boldsymbol{E}}^{\mathrm{p}}$ of the constitutive element is

$$\dot{\boldsymbol{E}}^{\mathrm{p}} = \sum_{s=1}^{N} \frac{\partial^2 \Psi}{\partial \Sigma \partial f_s}\dot{f}_s = \sum_{s\in\{S_a\}} \boldsymbol{\varepsilon}_s^{\mathrm{p}} \quad z\dot{f}_s, \tag{21}$$

where $\{S_a\}$ denotes the set of active kinds of variants with $\dot{f}_s \neq 0$. Each $\dot{f}_s (\neq 0)$ can be determined by the corresponding consistency condition

$$\dot{Y}_s = \frac{\partial Y_s}{\partial \Sigma} : \dot{\Sigma} + \frac{\partial Y_s}{\partial T}\dot{T} + \sum_{t\in\{S_a\}} \frac{\partial Y_s}{\partial f_t}\dot{f}_t = 0 \tag{22}$$

as

$$\dot{f}_s = -\frac{1}{2}\sum_{t\in\{S_a\}} W_{st}^{-1}(\boldsymbol{\varepsilon}_t^{\mathrm{p}} : \dot{\Sigma} - k\dot{T}),\ (s \in \{S_a\}). \tag{23}$$

Finally, the incremental stress-strain relation is

$$\dot{\boldsymbol{E}} = \dot{\boldsymbol{E}}^{\mathrm{e}} + \dot{\boldsymbol{E}}^{\mathrm{p}} = \boldsymbol{M} : \dot{\Sigma} - \frac{g^2}{2}\sum_{s\in\{S_a\}} \boldsymbol{R}_s \sum_{t\in\{S_a\}} W_{st}^{-1}\left(\boldsymbol{R}_t : \dot{\Sigma} - \frac{k}{g}\dot{T}\right). \tag{24}$$

In the above equations, the rational $\dot{f}_s (s = 1, \cdots, N)$ is guaranteed by the following loading condition.

For any given sth($s = 1, \cdots, N$) kind of variants, under the condition of $\sum_{t=1}^{N} f_t < 1$, if

$$\begin{aligned} &\Sigma : \boldsymbol{\varepsilon}_s^{\mathrm{p}} - (W_i + \Delta G) + 2\sum_{t=1}^{N} W_{st} f_t - D^{\mathrm{tr}} = 0, \\ &- \sum_{t \in \{S_a\}} W_{st}^{-1}(\boldsymbol{\varepsilon}_t^{\mathrm{p}} : \dot{\Sigma} - k\dot{T}) > 0 \ (s \in \{S_a\}), \end{aligned} \tag{25}$$

then

$$\dot{f}_s > 0. \tag{26}$$

On the other hand, under the condition of $f_s > 0$, if

$$\begin{cases} \Sigma : \boldsymbol{\varepsilon}_s^{\mathrm{p}} - (W_i + \Delta G) + 2\sum_{t=1}^{N} W_{st} f_t + D^{\mathrm{tr}} = 0, \\ - \sum_{t \in \{S_a\}} W_{st}^{-1}(\boldsymbol{\varepsilon}_t^{\mathrm{p}} : \dot{\Sigma} - k\dot{T}) < 0 \ (s \in \{S_a\}), \end{cases} \tag{27}$$

then

$$\dot{f}_s < 0. \tag{28}$$

At any other occasions, we have

$$\dot{f}_s = 0. \tag{29}$$

2.3 Discussions

2.3.1 The yield surface of the forward transformation and its evolution. According to eq. (19), the yield surface of the forward transformation is described by the envelope of the following N surfaces in stress space:

$$g\Sigma : \boldsymbol{R}_s = k(T - T_0) + W_i - 2\sum_{t=1}^{N} W_{st} f_t + D^{\mathrm{tr}} \quad (s = 1, \cdots, N). \tag{30}$$

Eq. (30) represents a hyperplane with $\boldsymbol{R}_s$ as normal in stress space. This indicates that the yield surface is constructed by the N intersecting hyperplanes in stress space and it has vertex structure. Eq. (30) also indicates that the sth kind of martensite variants begin to appear or grow up when $g\Sigma : \boldsymbol{R}_s - k(T - T_0)$, the combination of applied stress and temperature, reaches a critical value, which is not only dependent on $\boldsymbol{R}_s$ and volume fraction f_s but also on other kinds of transformed variants, i.e. the loading history.

At the beginning of the forward transformation, $f_s = 0 (s = 1, \cdots, N)$. From eq. (30), we can draw a conclusion that the first transformed kind of variants is the one for which the external work is the biggest. If there is no external force and the transformation is induced by the change of temperature, the starting transformation temperature M_s is the same for different kinds of variants. This is consistent with the experimental fact that all kinds of martensite variants can be observed in the specimen during pure cooling.

As eq. (30) shows there exists a coupling term $2\sum_{t=1}^{N} f_t W_{st}$ in the yield function. This means the yield hyperplanes for different kinds of variants are interrelated. So the evolution of the yield surface is very complex during the transformation. In the simple case of proportional loading process, if only one kind of martensite variants appears, which is usually observed in practice, we can prove that the constitutive response is a softening one at the beginning of the transformation. In uniaxial tensile experiment, the softening character displays minus slope in the stress-strain curve during transformation. This phenomenon has been verified in some monocrystalline shape memory alloys, for example, the appearance of γ'_1 in Cu-Al-Ni single crystal[6].

2.3.2 The effect of the inclusion shape. The curve of W_i with the change of the inclusion shape parameter ρ from 0 to 1 is drawn in fig. 2, where the material constants are from Cu-based shape memory alloys[7]. Fig. 2, shows that with the decrease of ρ from 1 to 0, W_i decreases monotonically. When $\rho = 0$ (corresponding to a penny-shaped flat ellipsoid), $W_i = 0$. Eq. (30) indicates that W_i is a kind of the energy barrier that the external work must overcome to form martensite inclusions. The smaller the ρ is, the smaller the W_i is and more easily the martensite inclusions can form . So it is not difficult to explain why martensite variants usually appear in very thin plates of blades as shown in a large number of micrograghs.

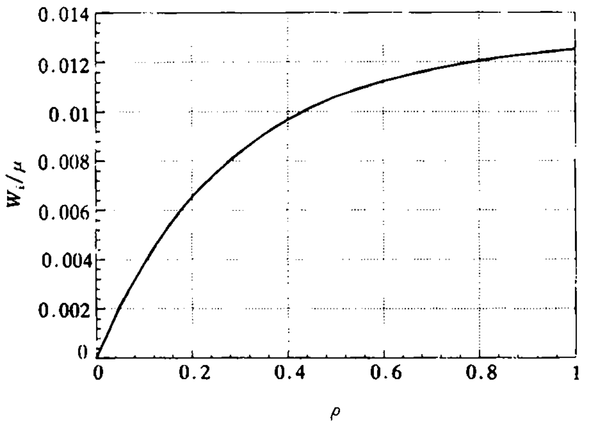

Fig. 2. The effect of the inclusion shape parameter ρ on the elastic strain energy W_i.

For the case where only one kind of martensite variant appears in the material under uniaxial tension, the curves of tangential modulus $K_{\tan}$ with respect to ρ for different kinds of variants with orientation R are shown in fig. 3. As we have just demonstrated, in most materials, martensite variants usually appear in very thin plates or blades, i.e. ρ is close to zero. So the stress-strain curve is approaching elastic-perfectly plastic with $\rho \rightarrow 0$. A lot of experimental stress-strain curves in monocrystalline shape memory alloys under uniaxial tension are coincident with this prediction (see, for example, the experiment result shown in fig. 4[8]). In this experiment, only one kind of variants was observed.

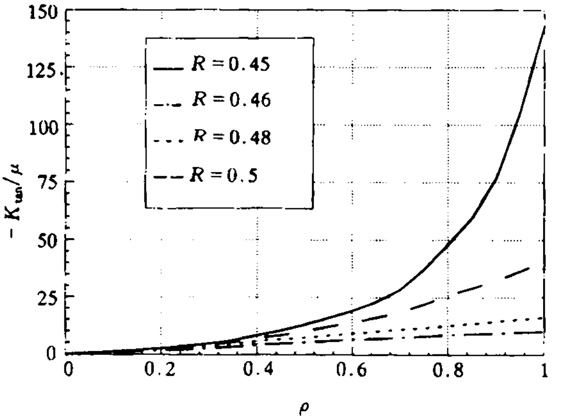

Fig. 3. The effect of the inclusion shape parameter ρ on the tangential modulus $K_{\tan}$ under uniaxial tension.

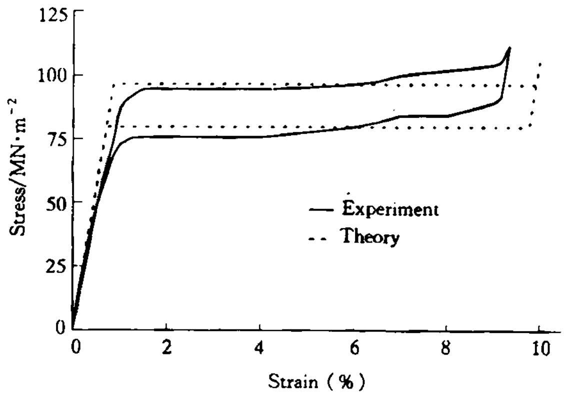

Fig. 4. Theoretical stress-strain curve compared with the experimental curve of Cu-Zn monocrystal[8].

3 Generalized constitutive relation in strain space

Now we have established the forward and/or reverse transformations of single crystals in stress space and discussed it in detail. However, it does not involve the microstructural change of reorientation, which is also a very important microstructural transition in thermoelastic martensitic transformation. Besides, in some special cases such as one kind of variants appearing under uniaxial tension, this model is a softening one in stress space. The uniqueness of the solution cannot be guaranteed. Thus, we further derive a generalized constitutive model in strain space, which can describe the forward transformation, reverse transformation and reorientation simultaneously. Due to the limit of space, only the result is shown as follows1).

3.1 Yielding conditions

The forward and reverse transformations yield conditions Y_{s0} for the sth ($s=1,\cdots,N$) kind of martensite variants and the reorientation conditions Y_{st} for the tth ($t=1,\cdots,s-1,s+1,\cdots,N$) kind of variants to be reoriented to the sth ($s=1,\cdots,N$) are expressed by

$$\begin{aligned} Y_{s0}(\boldsymbol{E},T,f_1,\cdots,f_N) &= \boldsymbol{\varepsilon}_s^{\mathrm{p}} : \boldsymbol{L} : \boldsymbol{E} - \sum_{n=1}^{N} Q_{sn} f_n - (W_i + \Delta G) \mp D^{\mathrm{tr}} \\ &= 0 \quad (s = 1,\cdots,N), \end{aligned} \tag{31}$$

$$\begin{aligned} Y_{st}(\boldsymbol{E},T,f_1,\cdots,f_N) &= (\boldsymbol{\varepsilon}_s^{\mathrm{p}} - \boldsymbol{\varepsilon}_t^{\mathrm{p}}) : \boldsymbol{L} : \boldsymbol{E} - \sum_{n=1}^{N} (Q_{sn} - Q_{tn}) f_n - D^{\mathrm{re}} = 0 \\ &(s = 1,\cdots,N;\ t = 1,\cdots,s-1,\ s+1,\cdots,N). \end{aligned} \tag{32}$$

Because the volume of the lattice changes during transformation (usually $\mathrm{tr}\boldsymbol{\varepsilon}_s^{\mathrm{p}} \neq 0$), the yield conditions for forward and reverse transformations are related to the volume deformation of the constitutive element. On the other hand, as $\mathrm{tr}\boldsymbol{\varepsilon}_s^{\mathrm{p}} = \mathrm{tr}\boldsymbol{\varepsilon}_t^{\mathrm{p}}$, the yield condition for the reorientation has nothing to do with the volume deformation of the constitutive element. The yield surface for the forward transformation, reverse transformation and reorientation consists of $N \times (N+1)$ hyperplanes in strain space.

3.2 Stress-strain relation in strain space

According to internal variable theory, the macroscopic stress rate $\dot{\boldsymbol{\Sigma}}$ of the constitutive element is

$$\dot{\boldsymbol{\Sigma}} = \boldsymbol{L} : \dot{\boldsymbol{E}} - \sum_{s=1}^{N} \frac{\partial F_s}{\partial \boldsymbol{E}} \dot{f}_s = \boldsymbol{L} : \dot{\boldsymbol{E}} - \boldsymbol{L} : \sum_{s=1}^{N} \boldsymbol{\varepsilon}_s^{\mathrm{p}} \quad \dot{f}_s, \tag{33}$$

where $\dot{f}_s$ ($s=1,\cdots,N$) is classified into

$$\dot{f}_s = \dot{f}_{s0} + \sum_{t \in \{B_s\}} \dot{f}_{st} - \sum_{\substack{t \\ s \in \{B_t\}}} \dot{f}_{ts} \quad (s = 1,\cdots,N). \tag{34}$$

$\{B_s\}$ is the set $\{t;t \neq s \text{ and } \dot{f}_{st} > 0\}$ of the active kinds of variants which are reoriented to the sth kind of variants. The volume fraction rates $\dot{f}_n$ must satisfy the following consistency equations

$$\boldsymbol{\varepsilon}_s^{\mathrm{p}} : \boldsymbol{L} : \dot{\boldsymbol{E}} - k\dot{T} = \sum_{n=1}^{N} \left[Q_{sn} \dot{f}_{n0} + \sum_{q \in \{B_n\}} (Q_{sn} - Q_{sq}) \dot{f}_{nq} \right] \quad (s \in \{A\}), \tag{35}$$

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1) Yan Wenyi, Micromechanics constitutive researches for transformable materials and transformation localization analysis, *Ph.D. Thesis*, Beijing: Tsinghua University, 1995.

$$(\boldsymbol{\varepsilon}_s^{\mathrm{p}} - \boldsymbol{\varepsilon}_t^{\mathrm{p}}) : \boldsymbol{L} : \dot{\boldsymbol{E}} = \sum_{n=1}^{N} (Q_{sn} - Q_{tn}) \dot{f}_{n0}$$

$$+ \sum_{n=1}^{N} \sum_{q \in \{B_n\}} (Q_{sn} - Q_{tn} - Q_{sq} + Q_{tq}) \dot{f}_{nq} \quad (s = 1, \cdots, N;\ t \in \{B_s\}). \tag{36}$$

Through the solution of the set of eqs. (35) and (36), we can obtain each $\dot{f}_{n0}(n \in \{A\})$ and $\dot{f}_{nq}$ $(q \in \{B_n\},\ n = 1, \cdots, N)$. The rational $\dot{f}_{n0}$ is guaranteed by the condition: $\dot{f}_{n0} > 0$ for the forward transformation of the nth kind of variants and $\dot{f}_{n0} < 0$ for the reverse transformation for the nth kind of variants. The rational $\dot{f}_{nq}$ must satisfy: $\dot{f}_{nq} > 0$ is $q \in \{B_n\}$; otherwise, $\dot{f}_{nq} = 0$.

After calculation $\dot{f}_s(s = 1, \cdots, N)$ from eq. (34), we can obtain the macroscopic stress rate $\dot{\boldsymbol{\Sigma}}$ by using eq. (33) and the macroscopic plastic strain rate $\dot{\boldsymbol{E}}^{\mathrm{p}}$, which is expressed as

$$\dot{\boldsymbol{E}}^{\mathrm{p}} = \sum_{s=1}^{N} \boldsymbol{\varepsilon}_s^{\mathrm{p}} \dot{f}_s. \tag{37}$$

4 Comparison with experiments

The above theory is applied to the uniaxial tension of Cu-Zn single crystal shape memory alloy. All the material parameters used in this model are completely adopted from the experimental research[8]. The theoretical predictions are compared with the experiment.

From the above model, under their experiment condition, we can determine that the kind of martensite variants with normal $[-0.732, 0.141, -0.666]$ will appear in the sample and the critical stress is $\Sigma_{11}^{cr} = 96.5$ MPa, which are consistent well with the variants observed in their experiment with normal $[-0.78, 0.12, -0.62]$ and the critical stress 94.7 MPa. Besides, under their experiment condition, we can prove that only a kind of martensite variants appears in the sample during loading-unloading cycling. This is also consistent with the experimental observation. The theoretical stress-strain curve and experiment curve are compared in figure 4.

5 Conclusion

By combining the crystallographic theory with micromechanics analysis and the internal variable theory, the constitutive model for the forward and reverse transformation plasticity of single crystal is established in stress space. Then it is extended to the strain space for the general case which includes reorientation. When quantitatively applied in uniaxial tension, the theoretical predictions agree well with the experimental.

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