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Modeling of the Reorientation Behavior of a Single Crystalline Shape-Memory Alloy by a Micromechanical Approach

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A Helmholtz free energy for a martensitic transformation of a single crystalline shape-memory alloy is obtained by a micromechanical approach. 24 variants of the single crystal are taken into account. In the framework of irreversible thermodynamics, a kinetic relation, a martensitic nucleation criterion and the reorientation criterion of martensitic variants are obtained. These relations are valid for a three-dimensional proportional or non-proportional mechanical loading or a combination of mechanical and thermal loading. Reorientation behavior of a single crystalline shape-memory alloy CuZnAl is simulated. When a tensile load is applied to a thermally-induced martensite, 24 self-accommodated martensitic variants are reoriented to the most favorable variant. In the following unloading and compression load, the most favorable variant in the tensile load is reoriented to the most favorable variant in this loading condition.

Key Words: Irreversible Thermodynamics, Martensitic Variants, Reorientation, Shape Memory Alloy, Single Crystal

1. Introduction

Martensitic phase transformations attract a lot of interest and many phenomena have been discussed and explained in the domain of material science. In the light of modeling the behavior of shape memory alloys (SMA), we can classify several existing models among others in three groups: (a) models based on a non-convex free energy (Ericksen, 1975; Falk, 1980; Müller and Xu, 1991) to describe one-dimensional isothermal pseudo-elastic (super-elastic) behavior and hysteresis phenomenon; (b) phenomenological three-dimensional models based on irreversible thermodynamics (Bondaryev and Wayman, 1988; Graesser and Cozzarelli, 1994) to study pseudo-elastic behavior or reorientation process and (c) micromechanical models of single crystals (Patoor et al., 1987; Sun and Hwang, 1993a, b; Goo and Lexcellent, 1997).

When martensite is thermally induced from
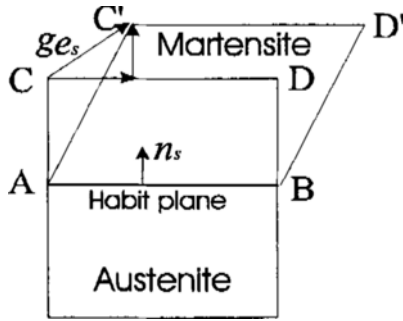
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austenite, self-accommodated martensitic variants are created. The number of the created variants depends on the materials. In case of CuZnAl, 24 martensitic variants of 6 groups of self-accommodated 4 variants are created. When a tensile load is applied to a thermally-induced 24 martensitic variants, 3 variants of each group is reoriented to the most favorable variant of the group. Finally the 6 most favorable variants of 6 groups are reoriented to the most favorable variant with respect to the loading (Sabury et al., 1980). The reorientation behavior is well described experimentally but it is difficult to find a model to simulate the reorientation behavior. In this paper a model to simulate pseudoelastic behavior and reorientation behavior is proposed.

2. Kinematic Relation of Phase Transformation

High temperature phase is designated by austenite, and low temperature phase by martensite. Suppose that two phases have the same Young modulus E, Poisson ratio ν and density ρ. As internal variables, we choose the volume fraction

Fig. 1 Simple shear on the habit plane plus an extension in the direction of the habit plane normal. Austenite ABCD is transformed into martensite ABC'D'.

of each martensitic variant $f_s (s=1, \cdots, N)$ where N is the total number of variants. f_s is defined as $f_s = V_s / V$ where V_s is the volume of variant s. V is the total volume of representative element in study. A variant can be considered to be located in infinite matrix, so solutions obtained in the infinite domain will be applied to this representative element.

According to the phenomenological theory of phase transformation by W. L. R. (Weshsler *et al.*, 1953), the phase transformation of a variant s gives a strain ε_s^p in the variant as follows :

$$\varepsilon_s^p = g R_s = \frac{1}{2} g (e_s \otimes n_s + n_s \otimes e_s) \qquad (1)$$

where e_s is the unit vector in the direction of the displacement of phase transformation, n_s is the normal vector to the habit plane. g is the material constant (Fig. 1) and R_s is the orientation tensor of the variant s.

A martensitic variant is defined by the total quantity of martensite with the same e_s and n_s. The symbol $\otimes$ denotes dyadic product. All vectors and tensors have the same Cartesian reference system fixed in the laboratory. Under the assumption of infinitesimal deformation, the total global strain E is decomposed into elastic strain E^e and phase transformation strain E^p. We do not consider the irreversible plastic deformation due to slip. The global strain E is obtained by the volume average of local strains ε of all variants:

$$E = E^e + E^p = \langle \varepsilon^e \rangle_V + \langle \varepsilon^p \rangle_V = M :$$

$$\Sigma + f \langle \varepsilon^p \rangle_{V_M} = M : \Sigma + g \sum_{s=1}^{N} f_s R_s \qquad (2)$$

where $\langle \ \rangle$, M and f represent the volume average, the elastic compliance tensor and the total volume fraction of martensite, respectively. Σ is the global stress tensor and V_M is the volume of the martensite. The notation : between two tensors denotes the contracted tensor product (A : $B = A_{ijkl} B_{klmn}$, A : $C = A_{ijkl} C_{kl}$ in conventional index notation). If we take into account the thermal dilatation, Eq. (2) is written as:

$$E = M : \Sigma + g \sum_{s=1}^{N} f_s R_s + \alpha (T - T_r) J \qquad (3)$$

where J is the unit tensor of order 2, T_r is the reference temperature, and α is the thermal dilatation coefficient of both phases.

3. Helmholtz Free Energy

When ellipsoidal martensitic variants are produced in the austenite, there are several energies from different origins. Interface energy W^{surf} per unit mass is expressed by:

$$W^{surf} = \frac{\gamma S}{\rho V} \qquad (4)$$

where γ is the surface energy per unit area and S is the total area of interface between martensite and austenite. The value of γ depends greatly on the coherency strain along the austenite-martensite interface. Assuming the interface involves Frank dislocation loops, γ is estimated to be the order of $(5.04 \sim 10.8) \times 10^{-5}$ J/cm^2 (Funakubo, 1987). Conventionally this energy is neglected in SMA but we will keep this term in our general expression. According to the experimental observation of interface (Huo and Müller, 1993) in case of a uniaxial tensile test, the number of interfaces n is maximum near $f = 0.5$, and can be expressed approximately by:

$$n = n_0 f (1 - f) \qquad (5)$$

where n_0 is a constant. Assuming the interface area is proportional to the number of interfaces, the interface energy per unit mass can be expressed by:

$$W^{surf} = \frac{1}{\rho V} \gamma b n_0 f (1 - f) = \frac{A}{\rho} f (1 - f)$$

$$= \frac{A}{\rho} \left(\sum_{s=1}^{N} f_s \right) \left(1 - \sum_{s=1}^{N} f_s \right) \qquad (6)$$

where $A = \gamma b n_0 / V$ is the material constant.

When an ellipsoidal martensitic plate is produced in the austenite, due to the incompatibility of deformations between the variant and its matrix, internal stress takes place. The stress in the plate is given by the Eshelby's solution (Eshelby, 1957). But when there are many plates or many variants, because of interactions among them, we can not directly use the Eshelby's solution. When inclusions are randomly distributed in the matrix, average internal stress was obtained (Mori and Tanaka, 1973). In most SMA, a kind of variant is not distributed throughout a specimen, and double twins (corresponding to double slip in plasticity) are not observed. Thus, when a kind of variant is produced in a domain, other kinds of variants are produced in other domains. In this situation, we can not use the concept of Mori and Tanaka (Mori and Tanaka, 1973). We obtain the average internal stress by the self-consistent formula of K. B. W. (Kroner, 1961; Budiansky and Wu, 1962). Suppose that all plates of a variant have the same form of oblate spheroid with $a_1 = a_2$, $a_3 / a_1 \ll 1$, where a_1, a_2 and a_3 are the principal radii. a_1 and a_2 are on the habit plane, and a_3 coincides with the direction of n_s. According to K. B. W., the difference in strains between the oblate spheroid and its matrix is considered as an eigenstrain (stress-free strain) in the sense of Eshelby. Internal stress σ_s in the variant s can thus be obtained from the Eshelby's solution:

$$\sigma_s = L : (S_s - I) : (\varepsilon_s^p - E^p) = L :$$
$$(S_s - I) : (\varepsilon_s^p - \sum_{t=1}^{N} f_t \varepsilon_t^p) = L : (S_s - I) :$$
$$\varepsilon_s^p - L : (S_s - I) : \sum_{t=1}^{N} f_t \varepsilon_t^p \qquad (7)$$

where L is the elastic stiffness tensor, and S_s is the Eshelby tensor of order 4 of the variant s. The unit tensor I of order 4 is expressed by the Kronecker's symbol given by

$$I_{klpq} = \frac{1}{2} (\delta_{kp} \delta_{lq} + \delta_{kq} \delta_{lp}) \qquad (8)$$

When there is only one kind of variant s, the

obtained internal stress σ_s is the same as that obtained by Mori and Tanaka (1973) as follows:

$$\sigma_s = (1 - f_s) L : (S_s - I) : \varepsilon_s^p \qquad (9)$$

The stored energy W^{int} per unit mass by the internal stress σ_s is obtained (Mura, 1987):

$$W^{int} = -\frac{1}{2\rho V} \int_V \sum_{s=1}^{N} \varepsilon_s^p : \sigma_s dV$$
$$= -\frac{1}{2\rho} \sum_{s=1}^{N} f_s \varepsilon_s^p : L : (S_s - I) :$$
$$\varepsilon_s^p + \frac{1}{2\rho} \sum_{t=1}^{N} \sum_{s=1}^{N} f_s f_t \varepsilon_s^p : L : (S_s - I) : \varepsilon_t^p \quad (10)$$

Let :

$$W_s = -\frac{1}{2} \varepsilon_s^p : L : (S_s - I) : \varepsilon_s^p \qquad (11)$$

and

$$W_{st} = -\frac{1}{2} \varepsilon_s^p : L : (S_s - I) : \varepsilon_t^p \qquad (12)$$

then Eq. (10) is written as:

$$W^{int} = \frac{1}{\rho} \sum_{s=1}^{N} f_s (1 - f_s) W_s - \frac{1}{\rho} \sum_{s=1}^{N} \sum_{\substack{t=1 \\ t \neq s}}^{N} f_s f_t W_{st} \quad (13)$$

The first term on the right-hand of Eq. (13) represents the stored energy by the internal stress of the variant s itself. On the other hand, the second term is the stored energy due to the interaction among variants. The strain energy W^{ext} by the external loading is obtained by:

$$W^{ext} = \frac{1}{2\rho} E^e : L : E^e$$
$$= \frac{1}{2\rho} \left[E - g \sum_{s=1}^{N} f_s R_s - \alpha (T - T_r) J \right] :$$
$$L : \left[E - g \sum_{s=1}^{N} f_s R_s - \alpha (T - T_r) J \right] \quad (14)$$

where L, ρ, α, g and R_s are assumed to be independent of temperature. The specific heat at constant volume c is defined as:

$$c = -T \frac{\partial^2 \Psi}{\partial T^2} = -T \frac{\partial^2 \Psi^T}{\partial T^2} \qquad (15)$$

Assuming the specific heat c is constant, we obtain the free energy per unit volume depending on temperature by integrating Eq. (15). For the austenitic phase it is written as:

$$\Psi_A^T = -c_A T Log(T) + C_1^A T + C_2^A \qquad (16)$$

where c_A is the specific heat of the austenitic

phase. C_1^A and C_2^A are constants. For the martensitic phase it is expressed by:

$$\Psi_M^T = -c_M T Log(T) + C_1^M T + C_2^M \quad (17)$$

where c_M is the specific heat of the martensitic phase. C_1^M and C_2^M are constants. Hence for the two-phase state it is written as:

$$\Psi^T = (1-f)\,\Psi_A^T + f\Psi_M^T = -c_A T Log(T)$$
$$+ C_1^A T + C_2^A + fC^*(T-T_0) + f(c_M - c_A)$$
$$[T_0 Log(T_0) - T Log(T)] \quad (18)$$

where T_0 is the thermal equilibrium temperature defined as $\Psi_A^T(T_0) = \Psi_M^T(T_0)$ and $C^* = (C_1^M - C_1^A)$. Therefore, the specific Helmholtz free energy of the representative element is written as follows:

$$\Psi = W^{ext} + W^{int} + W^{surf} + \Psi^T$$
$$= \frac{1}{2\rho}\left[E - g\sum_{s=1}^{N} f_s R_s - \alpha(T - T_r)J\right] :$$
$$L : \left[E - g\sum_{s=1}^{N} f_s R_s - \alpha(T - T_r)J\right]$$
$$+ \frac{1}{\rho}\sum_{s=1}^{N} f_s(1-f_s)\,W_s - \frac{1}{\rho}\sum_{s=1}^{N}\sum_{\substack{t=1\\t\neq s}}^{N} f_s f_t W_{st}$$
$$+ \frac{A}{\rho}\left(\sum_{s=1}^{N} f_s\right)\left(1 - \sum_{s=1}^{N} f_s\right) - c_A T Log(T)$$
$$+ C_1^A T + C_2^A + fC^*(T-T_0) + f(c_M - c_A)$$
$$[T_0 Log(T_0) - T Log(T)] \quad (19)$$

For the sake of simplicity, we suppose all plates of all variants have the same aspect ratio $\beta = a_3/a_1$. In that case, W_s is a constant independent of variant kinds. In addition, the difference in the specific heat between two phases will be neglected $(c = c_A = c_M)$ because it is difficult to find experimental values.

Global stresses are obtained from the following relation (Lemaitre and Chaboche, 1985):

$$\Sigma = \rho\frac{\partial\Psi}{\partial E} = L : \left[E - g\sum_{s=1}^{N} f_s R_s\right.$$
$$\left. - \alpha(T - T_r)J\right] \quad (20)$$

Thermodynamic forces F_s associated with the variables f_s are defined as:

$$F_s = -\rho\frac{\partial\Psi}{\partial f_s} = gR_s : L : \left[E - g\sum_{s=1}^{N} f_s R_s\right.$$
$$\left. - \alpha(T - T_r)J\right] - (1-2f_s)W_s + 2\sum_{\substack{t=1\\t\neq s}}^{N} f_t W_{st}^*$$
$$- A(1-2f_s) - \rho C^*(T-T_0) \quad (21)$$

where $W_{st}^* = \frac{1}{2}(W_{st} + W_{ts})$ is symmetric on s and t. The Clausius–Duhem inequality is written as follows (Lemaitre and Chaboche, 1985):

$$\sum_{s=1}^{N} F_s \dot{f}_s - \frac{q}{T} grad T \geq 0 \quad (22)$$

where q is the heat flux vector. We suppose each term in Eq. (22) satisfies the inequality:

$$\sum_{s=1}^{N} F_s \dot{f}_s \geq 0 \;;\quad -\frac{q}{T} grad T \geq 0 \quad (23)$$

The heat equation is written as follows (Lemaitre and Chaboche, 1985):

$$\rho c\dot{T} - k\nabla^2 T = \sum_{s=1}^{N} F_s \dot{f}_s + T\left[\frac{\partial\Sigma}{\partial T} :\right.$$
$$\left.\dot{E} - \sum_{s=1}^{N}\frac{\partial F_s}{\partial T}\dot{f}_s\right] \quad (24)$$

where k is thermal conductivity and ∇^2 denotes the Laplacian operator. When the thermal dilatation term, $\alpha(T - T_r)$, is negligible, Eq. (24) is written as:

$$\rho c\dot{T} - k\nabla^2 T = \sum_{s=1}^{N} F_s \dot{f}_s + \rho T C^*\left(\sum_{s=1}^{N} \dot{f}_s\right) \quad (25)$$

4. Constitutive Equations

The variation of the volume fraction of a variant s is due to two origins. One is the martensitic transformation and the other is the reorientation of martensitic variants. Hence the variation rate of the volume fraction of the variant s can be written as (Goo and Lexcellent, 1997):

$$\dot{f}_s = \dot{f}_{s0} + \dot{f}_{s,1} + \cdots + \dot{f}_{s,s+1} + \cdots$$
$$+ \dot{f}_{s,N}, \; s = 1, \cdots, N \quad (26)$$

where $\dot{f}_{s0}$ represents the rate of variation by the phase transformation; $\dot{f}_{s0} > 0$ designates the forward transformation, and $\dot{f}_{s0} < 0$ the reverse transformation. $\dot{f}_{s,t}$ represents the variation rate of f_s by the reorientation from a variant t $(t \neq s)$ to the variant s. If $\dot{f}_{s,t} > 0$, some of the variant t is in the course of reorientation to the variant s. If $\dot{f}_{s,t} < 0$, some of the variant s is in the course of reorientation to the variant t. Thus it follows that

$$\dot{f}_{s,t} = -\dot{f}_{t,s} \quad (27)$$

In phase transformations, dissipation results from frictions on interfaces, defects, plastic deformations, thermal dissipation, etc. . We suppose in the reorientation process, creep phenomenon is negligible. Of course, latent heat does not exist in this process. So we distinguish the dissipation of phase transformation from that of reorientation process. The dissipation rate of the phase transformation $\dot{W}_d^{tr}$ is supposed to be a simple function of the thermodynamic force F_s :

$$\dot{W}_d^{tr} = \pm \sum_{s=1}^{N} \dot{h}_0 F_s \langle \pm (F_s - D_{tr}^{(i)}) \rangle^n \qquad (28)$$

where $\dot{h}_0$ and n are constants, and (i) represents the forward transformation when $i=1$, or the reverse transformation when $i=2$. $+$ of $\pm$ designates the forward transformation, and the reverse transformation. The dissipation of a variant is supposed independent of other variants. A function $\langle H(x) \rangle$ is defined by:

$\langle H(x) \rangle = H(x)$, if $H(x) \geq 0$; $\langle H(x) \rangle = 0$, else   (29)

$D_{tr}^{(i)}$ can be written in a general form:

$$D_{tr}^{(i)} = D_0^{(i)} + D_1^{(i)}(f_s) \qquad (30)$$

where $D_0^{(i)}$ is constant and $D_1^{(i)}(f_s)$ is the hardening term. The dissipation rate $\dot{W}_d^{re}$ due to the reorientation is supposed to be a simple function of $\dot{f}_{s,t}$:

$$\dot{W}_d^{re} = \frac{1}{2} \sum_{s=1}^{N} \sum_{\substack{t=1 \\ t \neq s}}^{N} D_{re}^{(i)} \dot{f}_{s,t} \qquad (31)$$

where $D_{re}^{(i)}$ is written in a general form:

$$D_{re}^{(i)} = D_3^{(i)} + D_4^{(i)}(f_s) \qquad (32)$$

where $D_3^{(i)}$ is constant and $D_4^{(i)}(f_s)$ is the hardening term. $i=1$ represents the reorientation from t to s ; $i=2$ the reorientation from s to t. So we obtain a relation from the equations of mechanical dissipation (Eqs. (28) and (31)):

$$\sum_{s=1}^{N} F_s \dot{f}_s = \pm \dot{h}_0 \sum_{s=1}^{N} F_s \langle \pm (F_s - D_{tr}^{(i)}) \rangle^n$$
$$+ \frac{1}{2} \sum_{s=1}^{N} \sum_{\substack{t=1 \\ t \neq s}}^{N} D_{re}^{(i)} \dot{f}_{s,t} \qquad (33)$$

Inserting Eqs. (26) and (27) in (33), we obtain the following equation:

$$\sum_{s=1}^{N} \left[\dot{f}_{s0} \mp \dot{h}_0 \langle (F_s - D_{tr}^{(i)}) \rangle^n \right] F_s$$

$$+ \frac{1}{2} \sum_{s=1}^{N} \sum_{\substack{t=1 \\ t \neq s}}^{N} (F_s - F_t - D_{re}^{(i)}) \dot{f}_{s,t} = 0 \qquad (34)$$

This equation can be satisfied for a trivial case $F_s = 0$ (no thermodynamic force) and $\dot{f}_{s,t} = 0$ (no reorientation process). For the equation to be satisfied for any other cases of $F_s \neq 0$ and $\dot{f}_{s,t} \neq 0$, the two terms of the equation should be zero:

$$\dot{f}_s = \pm \dot{h}_0 \langle \pm (F_s - D_{tr}^{(i)}) \rangle^n \qquad (35)$$

and

$$Y_{st} = F_s - F_t - D_{re}^{(i)} = g\,(R_s - R_t) :$$
$$\Sigma + 2 \sum_{n=1}^{N} f_n W_{sn}^* - 2 \sum_{n=1}^{N} f_n W_{tn}^* - D_{re}^{(i)} = 0.$$
$$(s \neq t) \qquad (36)$$

Eq. (35) represents the evolution of the variant s in case of phase transformation. Eq. (36) is the criterion of reorientation between the variants t and s. When $Y_{st} = 0$, some of the variant t is in the course of reorientation to the variant s. In this case, $\dot{f}_{s,t}$ is obtained from the following relations:

$$\dot{Y}_{st} = \dot{F}_s - \dot{F}_t - \dot{D}_{re}^{(i)} = 0 \qquad (37a)$$

$$\dot{f}_s = \dot{f}_{s0} + \sum_{\substack{t=1 \\ t \neq s}}^{K} \dot{f}_{s,t} \qquad (37b)$$

$$\dot{f}_t = \dot{f}_{t0} - \sum_{\substack{m=1 \\ m \neq t}}^{M} \dot{f}_{m,t} \qquad (37c)$$

where K is the number of the variants in the course of reorientation to the variant s and M is the number of the variants to which the variant t is in the course of reorientation. Eq. (37a) is the consistency condition.
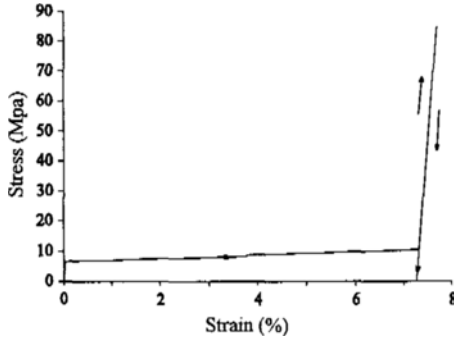
5. Simulation of the Reorientation Behavior

When austenite is transformed to martensite by cooling, 24 self-accommodated variants composed of 6 groups of 4 variants are created. 4 variants of each group are also self-accommodated. According to the experimental observations (Sabury *et al.*, 1980) when a tensile load is applied to the thermally-induced 24 martensitic variants, 3 variants of each group are reoriented to the most favorable variants of the group. In consequence the most favorable variants of each group is reoriented to the most favorable among
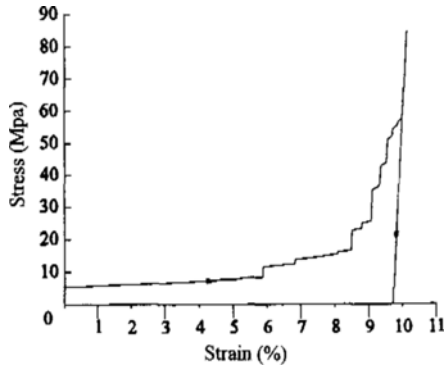
the 24 variants. Sometimes the most favorable variant of a group is reoriented to the most favorable variant of its neighboring group and finally it is reoriented to the most favorable variant among the 24 variants.

$D_{re}^{(i)}$ in the criterion of reorientation is assumed to be a function of f_s:

$$D_{re}^{(i)} = \pm D_{re}^0 + \lambda (f_s - f_s^{mem}) \qquad (38)$$

(a)

(b)

Fig. 2 (a) Reorientation behavior of 4 martensitic variants, $(\alpha_1, \alpha_2, \alpha_3) = (30°, 30°, 30°)$.
(b) Reorientation behavior of 24 martensitic variants, $(\alpha_1, \alpha_2, \alpha_3) = (30°, 30°, 30°)$.

where D_{re}^0 and λ are constants and f_s^{mem} is the volume fraction of the variant s when the applied loading changes its loading direction. $+$ of the $\pm$ is for the reorientation from the variant t to s and $-$ of the $\pm$ is for the reorientation from the variant s to t. The consistency condition of reorientation (Eq. (37a)) between the variant s and t is written as:

$$\dot{Y}_{st} = g(\boldsymbol{R}_s - \boldsymbol{R}_t) : \dot{\Sigma} + 2\sum_{n=1}^{N} \dot{f}_n W_{sn}^*$$

$$- 2\sum_{n=1}^{N} \dot{f}_n W_{tn}^* - \lambda \dot{f}_s = 0. \quad s \neq t \qquad (39)$$

Using Eqs. (37), (38) and (39), we can simulate the behavior of reorientation of martensitic variants. Simulated results are shown in Figs. 2 $\sim$5 and the used parametric values are shown in Table 1. $(\alpha_1, \alpha_2, \alpha_3)$ are the angles between the applied tensile loading and the three axes of the single crystal, $[1\ 0\ 0]$, $[0\ 1\ 0]$, $[0\ 0\ 1]$, respectively. The used habit plane normal directions $\boldsymbol{n}_s$ and phase transformation directions $\boldsymbol{e}_s$ are near $\{2\ 7\ \bar{8}\}$ and $\langle 2\ \bar{9}\ 8 \rangle$ respectively (Patoor et al., 1987).

Figure 2(a) shows the reorientation behavior of a self-accommodated group of 4 martensitic variants with $(\alpha_1, \alpha_2, \alpha_3) = (30°, 30°, 30°)$. About 7% of strain is obtained when 3 martensitic variants are reoriented to the most favorable variant in the group. Figure 2(b) shows the reorientation behavior of a self-accommodated 24 martensitic variants with $(\alpha_1, \alpha_2, \alpha_3) = (30°, 30°, 30°)$. Figure 3(a) and 3(b) show the reorientation behavior of a self-accommodated group of 4 variants and 24 variants with $(\alpha_1, \alpha_2, \alpha_3) = (45°, 45°, 45°)$. The obtained strains are less than those of Fig. 2. That means the maximum strain obtained by the reorientation of martensitic variants depends much on the angles $(\alpha_1, \alpha_2, \alpha_3)$. Figure 4 shows the reor-

Table 1 Used values of the parameters for the simulation.

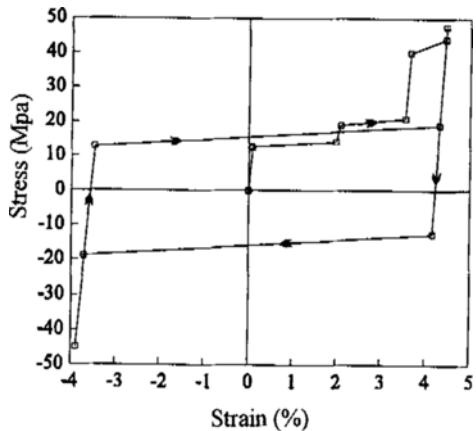|	$(\alpha_1, \alpha_2, \alpha_3)$ in degree	E (MPa)	ν	D_{re}^0 (MJ/m³)	λ (MJ/m³)	α_3/α_1	g
Fig. 2	(30, 30, 30)	20000	0.3	1.0	1.0	10^{-6}	0.206
Fig. 3	(45, 45, 45)	20000	0.3	1.0	1.0	10^{-6}	0.206
Fig. 4	(20, 20, 20)	20000	0.3	1.0	0.5	10^{-6}	0.206
Fig. 5	(10, 20, 30)	20000	0.3	1.0	0.5	10^{-6}	0.206
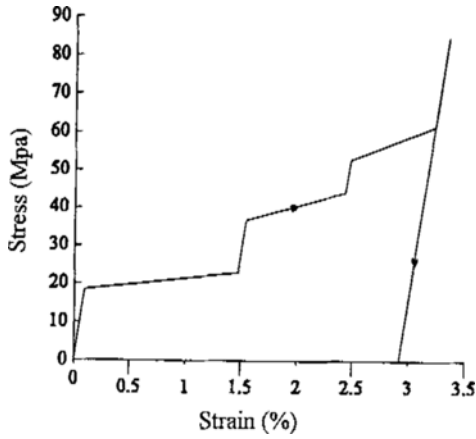
(a)
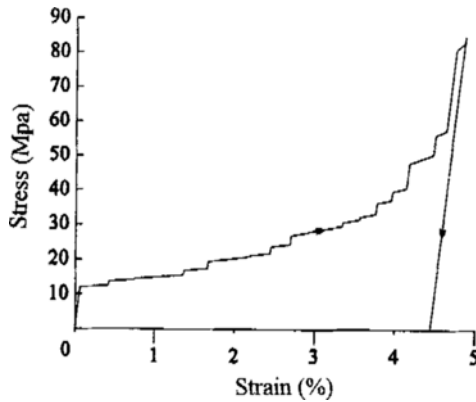
(b)

Fig. 3 (a) Reorientation behavior of 4 martensitic variants, $(\alpha_1, \alpha_2, \alpha_3) = (45°, 45°, 45°)$.
(b) Reorientation of 24 martensitic variants, $(\alpha_1, \alpha_2, \alpha_3) = (45°, 45°, 45°)$.

Fig. 4 Reorientation behavior of 4 martensitic variants $(\alpha_1, \alpha_2, \alpha_3) = (20°, 20°, 20°)$.
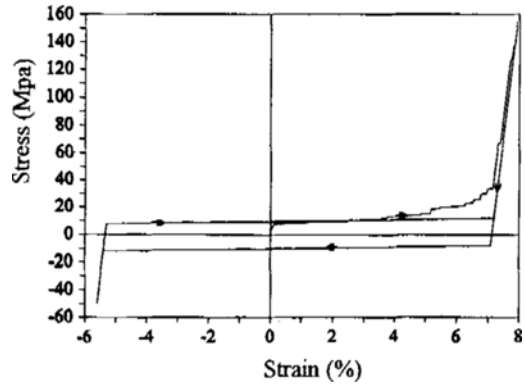
Fig. 5 Reorientation behavior of 24 martensitic variants, $(\alpha_1, \alpha_2, \alpha_3) = (10°, 20°, 30°)$.

ientation of a self-accommodated 4 martensitic variants with $(\alpha_1, \alpha_2, \alpha_3) = (20°, 20°, 20°)$ under a loading, unloading and reloading. Figure 5 shows the reorientation of a self-accommodated 24 martensitic variants with $(\alpha_1, \alpha_2, \alpha_3) = (10°, 20°, 30°)$, under a loading, unloading and reloading. In case of 24 variants the curve is nearly continuous but in case of 4 variants the curve is stepwise.

6. Conclusion

In the phase transformation of shape memory alloys, the simulation of reorientation of martensitic variants and two-way memory effect is not easy. The reorientation behavior of martensitic variants of a single crystalline shape memory alloy was successfully simulated by a micro-mechanical approach. When a tensile load is applied to 24 martensitic variants, 23 variants are reoriented to the most favorable variant. This behavior is consistent with experimental observation (Sabury *et al.*, 1980). Under the compressive loading after unloading, the most favorable variant under the tensile load is reoriented directly to the most favorable variant with respect to the compressive load.

Using a self-consistent method, we can simulate the reorientation behavior of polycrystalline shape memory alloys.

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