Three-dimensional constitutive equations of polycrystalline shape memory alloy

M. TOKUDA ([1]), M. YE ([1]), B. BUNDARA ([2]) and P. SITTNER ([3])

([1]) *Department of Mechanical Engineering,*
Mie University, Kamihama, Tsu 514-8507, Japan

([2]) *JSPS-Post Doctral Fellow from Slovenia*

([3]) *Institute of Physics, Czech Academy of Sciences,*
Na Slovance 2, 180-40 Prague 8, Czech Republic

QUITE UNIQUE and interesting behavior of shape memory alloy (SMA) under complex loading conditions, including the complicated path-dependence, have been observed in systematic experiments by applying some combined loads of axial force and torque to the thin-walled tubular specimen of Cu-based polycrystalline shape memory alloy. A set of constitutive equations is proposed, which can describe the complicated behavior observed in the experiments. The mesoscopic approach is employed in the formulation because the complicated behavior is closely related to the microstructural changes of the material, and the obtained equations show a reasonable agreement with the exprimental results. In the first paper, the process of modelling and the details of the formulated constitutive equations are described, and the comparison between the experimental results and the results evaluated by using the proposed constitutive equations will be shown in the second report.

1. Introduction

SHAPE MEMORY ALLOYS (SMA) were expected to become very important for the engineering applications because of their unique thermo-mechanical properties [1]. Therefore, quite active research and development has been continued in the recent years [2 – 4]. In order to support the engineering applications, the basic and fundamental research work has also been vital; for example, the material development of SMA of better qualities (e.g., the thin-film of SMA [5 – 9]), the development of less expensive SMA and the improvement of their functions and properties (e.g., Fe-based SMA [10, 11]), the experimental research works [12, 13] to investigate the mechanisms of thermo-mechanical properties and their modeling and formulation [14 – 23] appropriate for the prediction of the material

behavior and the design of devices constructed from SMA elements. This paper is concentrated on modeling and formulation of the thermo-mechanical properties of SMA.

The research on the modeling and formulations in the last decades were mostly limited to simple loading conditions (particularly, uniaxial tensile loading), and thus the applications have been considered on the basis of these works. On the other hand, when we take into account the fact that the basic deformation mechanism of SMA is a combination of (1) the temperature (T)-induced martensite phase transformation, and (2) the stress ($\sigma_{ij} : i, j = 1, 2, 3$)-induced martensite phase transformation, various and unknown unique behaviors of SMA are possible. Actually, new engineering applications of SMA can be developed for the multi-axial/complex loading conditions. As an example, the positioning devices or actuators which perform complicated three-dimensional motions themselves by controlling several stress components can be designed. Also, further investigation and clear understanding of new features of SMA will be helpful in the design of future intelligent material systems [24 – 26]. In the literature, however, there are only few reports on the basic research focused on the behavior of SMA under complex loading conditions, experimentally and theoretically as well. From the above mentioned point of view, the authors have continued a series of systematic experiments on the thermo-mechanical behavior of polycrystalline SMA under complex loading conditions, by applying the combined loads of axial force and torque to the thin-walled tubular specimen of Cu-based polycrystalline SMA [27 – 32]. In the experimental part of the research, unique behavior have been obtained. Some phenomena can not be observed by the simple loading experiments. For example,

1. In the proportional deformation tests using the combined loads of axial force and torque, the corresponding deformation is also proportional. That is, the thin-walled tube exhibits the simultaneous torsional and axial (elongation/contraction) deformations under this stress condition[29, 30].

2. Strong and unique path dependence was confirmed. That is, the obtained strain states are different when the stress paths are different, though the current stress states are the same. One special exception is that the zero-stress state corresponds to the zero-strain state, regardless of their paths. That is, the original shape of the specimen is memorized [29, 30].

3. When only the axial force is changed after the combined load of axial force and torque is applied to the thin-walled tube, the tube shows torsional deformation too without any change of torsional loading. The same kind of deformation can be observed under no change of axial force. That is, the axial deformation of a tube can be obtained by changing the torsional loading without any change of axial force. This is also one of the interesting features of SMA under complex loading conditions [29, 30].

4. When a tubular specimen subjected to the torsional loading is heated up to a certain temperature, the torsional deformation induced by the martensite phase transformation decreases monotonically and finally disappears. On the other hand, when the specimen subjected to the reverse torsional load following the forward torsional loading is heated up, the change of torsional deformation was observed to be non-monotonic, that is, the direction of torsional deformation changes during the heating process [32]. The same phenomenon can be expected in the case of tension-compression loading. That is, the specimen will be longer at first and shorter in the next stage during the monotonic heating process.

The experimental results under complex loading conditions including the above exposed interesting phenomena could be understood clearly by considering the microscopic behavior of martensite variants. In the present paper, a set of constitutive equations of SMA under the complex (general) thermo-mechanical loading conditions is proposed, which can reproduce the special behavior obtained in the experiments. In the formulation of constitutive equations, the meso-mechanical modeling approach [33] proposed by one of the authors is employed, which can incorporate the multi-layered microstructure of the polycrystalline materials. This meso-mechanical modeling approach was employed for the formulation of inelastic (or plastic) constitutive equations of polycrystalline metallic materials whose main deformation mechanism is slipping (by dislocations) inside the grains, especially under complex/general loading conditions, where the complicated metallurgical dislocation mechanisms controlling the slip deformation are taken account into by using the so-called slip system idea, and the mechanical model of a grain can be obtained as the collection of several slip systems. The interactions among slip systems are assumed in the grain component. The polycrystal model is composed of a large number of crystal grain components and the interactions among grains are determined by using a micromechanical approach. In the present case of polycrystalline SMA, the mechanism of phase transformation is employed instead of the slip mechanism.

In the present report, the derivation of a set of constitutive equations of SMA under complex loading conditions is described. In the following second report, the accuracy/reliability, and applicability of these constitutive equations are discussed by comparing the calculated results with the corresponding experimental ones.

2. Thermo-mechanical model of phase- transformation

The basic phase transformation mechanisms of SMA are the temperature-induced and stress-induced martensite phase transformation. The deformation induced by these martensite phase transformations is considered to be the twin-

type (shear) deformation with a negligibly small change of volume, and controlled by the temperature and the stress tensor [1, 34]. This twin-type (shear) deformation occurs only in the crystallographically determined (easy twin) directions on the crystallographically determined (easy twin) planes. This twin (shear) deformation system with a specific direction and a specific plane is hereafter named the phase transformation system and corresponds to the technical term "slip system" used in the crystal plasticity.

When SMA is subjected to the thermal loading (the change of temperature) only, the martensite phase transformation with the (twin-type) shear strain occurs. However, in this case, no macroscopically significant deformation of crystal grain (as well as the polycrystal composed of these grain components) can be observed. This phenomenon can be explained as follows: in the case of temperature change without any applied external or internal stress, the phase transformation is possible to occur simultaneously in every transformation systems with different orientations, and thus the induced shear (twin) strains cancel each other in the average. On the other hand, in the case of stress-induced phase transformation, the phase transformation occurs in the phase transformation systems with the preferable orientations to the stress state. Thus, only the shear strains with specific directions are summed-up and consequently, the significant macroscopic inelastic deformation can be observed in the crystal components (as well as in the polycrystal).

Our engineering interests are the macroscopic inelastic deformations, the force produced when the deformation is constrained, and their combination. Therefore, only the case when the material is subjected to some stresses is considered in the present paper. The effect of temperature is incorporated as the temperature effect on the shear stress which is necessary for the phase transformation, i.e., on the critical (resolved) shear stress. The typical feature of temperature effect is that the lower is the temperature, the easier the martensite phase transformation will occur (the smaller will be the critical shear stress). That is, the deformation of SMA needs larger stress at higher temperature. This feature of SMA is quite different from that of usual metallic materials with the slip or diffusion mechanism controlled by thermo-activation.

The above-mentioned phase transformation mechanism is determined by using the "shear stress τ – phase transformation) shear strain γ^{PT} – temperature T" relation of the phase transformation system. When the material is of the austenite structure (the parent phase), the mechanical characteristic of this transformation system can be expressed by the loading curve OABC and the unloading curve CDEO shown in Fig. 1, where $\tau_{MS}(T)$, $\tau_{AS}(T)$, and $\tau_{AF}(T)$ are the martensite phase transformation start and finish shear stresses, and the austenite (reverse) phase transformation start and finish shear stresses at the temperature T, respectively. The γ^{PT} is the phase transformation shear strain and γ^{PT}_{max} is the
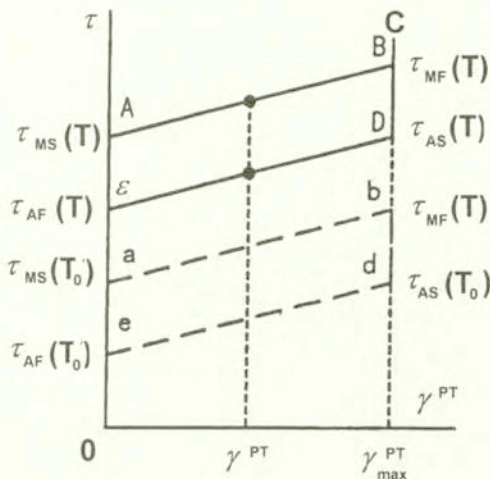
FIG. 1. Typical stress-strain relation of phase transformation system (I).

maximum value of γ^{PT}. In this figure, at the temperature T, the martensite phase transformation in the phase transformation system begins at point A, and the martensite strain γ^{PT} increases with the increase of shear stress τ along the line AB. The increase of γ^{PT} stops at point B at which the martensite phase transformation is completed, and then γ^{PT} does not increase though the shear stress increases (B→ C). In the next step, when the stress is unloaded from the point C, the reverse transformation starts at the point D where the stress is smaller than the stress at B, and this reverse transformation is completed at the point E. The dashed curve in Fig. 1 shows the relation between the shear stress τ and the phase transformation strain γ^{PT} at a different temperature $T_0(< T)$. The dashed loop abde at the temperature T_0 can be obtained by shifting the loop ABDE at the temperature T without any change of its shape. The sub-loading process can be incorporated as follows: As shown in Fig. 2, when the material is unloaded ($d\tau < 0$) at the point P during the martensite phase transformation, the phase transformation strain γ^{PT} does not change and the shear stress reaches the point Q on the reverse transformation line DE. If the unloading ($d\tau < 0$) is continued, the reverse phase transformation begins at the point Q and the shear phase transformation strain γ^{PT} decreases Q→ R→ E). When the material is loaded ($d\tau > 0$) at the point R on the reverse transformation line, the reverse transformation stops and the transformation shear strain γ^{PT} does not change till the stress arrives at the point S on the phase transformation line AB. The detail of sub-loop (or internal loop) PQRS depends on the material and has been still discussed in [35 – 41]. In the present paper, the simplest form has been selected.
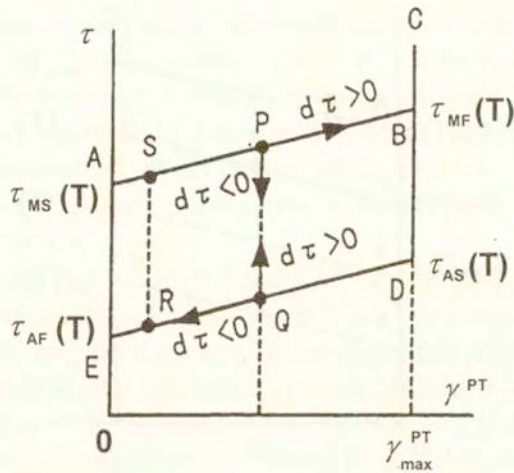
Fig. 2. Typical stress-strain relation of phase transformation system (II).

The relation between shear stress τ and (phase transformation) shear strain γ^{PT}-temperature T mentioned above can be formulated in the following form.

First, when the linear strain hardening rule shown in Figs. 1 and 2 is assumed for simplicity, the critical shear stress for martensite phase transformation $\tau_M(\gamma^{PT}, T)$ at the phase transformation shear strain γ^{PT} and the temperature T is expressed as follows:

$$(2.1) \qquad \tau_M(\gamma^{PT}, T) = \tau_{MS}(T) + H\gamma^{PT},$$

where H is the hardening coefficient (the material constant). The martensite start stress $\tau_{MS}(T)$ is assumed to depend on the temperature T linearly, what has been confirmed both experimentally as well as theoretically (Clausius-Clapeyron equation [1, 34]), and thus,

$$(2.2) \qquad \tau_{MS}(T) = \tau_{OMS} + \beta(T - T_0),$$

where β is the material constant, and τ_{OMS} is the martensite phase transformation (critical) shear stress at the reference temperature T_0 (for example, the room temperature). By using (2.1) and (2.2), $\tau_M(\gamma^{PT}, T)$ can be expressed in the following form:

$$(2.3) \qquad \tau_M(\gamma^{PT}, T) = \tau_{OMS} + \beta(T - T_0) + H\gamma^{PT}.$$

Following (2.3), the martensite phase transformation start function (M-type yield function) F_M is obtained in the following form:

$$(2.4)_1 \qquad F_M = \tau - \left[\tau_{OMS} + H\gamma^{PT} + \beta(T - T_0)\right],$$

where τ is the shear stress resolved on the considered phase transformation system. When the shear stress τ satisfies the equation

$(2.4)_2$ $$F_M = 0,$$

the deformation is as follows:

1. Under the loading condition, that is, for $dF_M = d\tau - \beta dT > 0$, the martensite phase transformation takes place and thus, $d\gamma^{PT} > 0$. In this situation, considering that $d\tau - H d\gamma^{PT} - \beta dT = 0$, from $(2.4)_1$ and $(2.4)_2$

(2.5) $$d\gamma^{PT} = (d\tau - \beta dT)/H,$$

2. Under the neutral loading $dF_M = 0$, or for the unloading $dF_M < 0$, i.e., under the condition $dF_M = d\tau - \beta dT \le 0$, the martensite phase transformation does not occur and the deformation is elastic. Therefore, the increment of phase transformation induced shear strain $d\gamma^{PT}$ is expressed as follows:

(2.6) $$d\gamma^{PT} = 0.$$

The relation between the stress increment $d\tau$ and the strain increment $d\gamma^{PT}$ can be summarized in the following form:

(2.7) $$d\gamma^{PT} = \langle dF_M \rangle \, \langle \gamma_{max}^{PT} - \gamma^{PT} \rangle (d\tau - \beta dT)/H,$$

where
(2.8) $$\langle X \rangle = 1 \quad \text{for} \quad X > 0, \quad \langle X \rangle = 0 \quad \text{for} \quad X \le 0,$$

and γ_{max}^{PT} is the material constant (the maximum phase transformation shear strain); the γ^{PT} can not increase after the phase transformation is completed in the phase transformation system, and $\langle \gamma_{max}^{PT} - \gamma^{PT} \rangle$ in (2.7) is used for this mechanism. As found from (2.3), the γ_{max}^{PT} and the martensite phase transformation finish shear stress $\tau_{MF}(T)$ are related in the following form:

(2.9) $$\tau_{MF}(T) = \tau_{OMS} + \beta(T - T_0) + H\gamma_{max}^{PT}.$$

In what follows, the formulation of the reverse (austenite) phase transformation is considered in the similar way as that mentioned in the case of the martensite phase transformation. According to Fig. 1, the reverse (austenite) phase transformation critical shear stress τ_A is expressed in the linear strain-hardening form:

(2.10) $$\tau_A(\gamma^{PT}, T) = \tau_{OAF} + H\gamma^{PT} + \beta(T - T_0),$$

where τ_{0AF} is the reverse phase transformation (critical) shear stress at the reference temperature T_0. Therefore, the austenite (reverse) phase transformation function (A-type yield function) F_A is

$$(2.11)_1 \qquad -F_A = \tau - \left[\tau_{0AF} + H\gamma^{PT} + \beta(T - T_0)\right],$$

where τ is the (resolved) shear stress on the considered phase transformation system. When the stress state τ satisfies the following equation:

$$(2.11)_2 \qquad\qquad\qquad F_A = 0,$$

the deformation can be classified as follows.

   1. Under the loading condition; $dF_A = -d\tau + \beta dT > 0$, the austenite (reverse) phase transformation occurs, and thus, $d\gamma^{PT} < 0$. From $(2.11)_1$ and $(2.11)_2$, $d\tau - Hd\gamma^{PT} - \beta dT = 0$, and then,

$$(2.12) \qquad\qquad d\gamma^{PT} = (d\tau - \beta dT)/H.$$

   2. Under the neutral loading $dF_A = 0$, or under the unloading condition $dF_A < 0$, that is, in the case of $dF_A = -d\tau + \beta dT \leq 0$, the austenite (reverse) phase transformation does not proceed, and thus, the phase transformation (shear) strain increment $d\gamma^{PT}$ is as follows;

$$(2.13) \qquad\qquad\qquad d\gamma^{PT} = 0.$$

The stress-strain relation explained above can be summarized in the following form;

$$(2.14) \qquad d\gamma^{PT} = <dF_A><\gamma^{PT}> (d\tau - \beta dT)/H,$$

where $<\gamma^{PT}>$ is used to take into account that the reverse transformation stops when the existing phase transformation strain γ^{PT} is included completely by the reverse transformation.

3. Thermo-mechanical model of crystal grain component

   The deformation property (stress-strain-temperature relation) of crystal grain component with the phase transformation systems described in the previous section can be formulated in the following manner.

   The number of phase transformation systems in the crystal grain is assumed to be M (for example, $M = 24$ for the martensite phase transformation of Cu-based SMA used in authors' experiments). When the single crystal grain is in uniform stress state $\sigma_{ij}(i, j = 1, 2, 3)$, the shear stress $\tau(m)$ resolved on the m-th

$(m = 1, 2, .., M)$ phase transformation system can be obtained by the following equation:

$$(3.1) \qquad \tau(m) = \sum_{i,j=1}^{3} \alpha_{(m)ij} \sigma_{ij}.$$

The coefficient $\alpha_{(m)ij}$ in (3.1) is the so-called generalized Schmid factor defined as follows:

$$(3.2) \qquad \alpha_{(m)ij} = \left[s_{(m)i} n_{(m)j} + s_{(m)j} n_{(m)i} \right] / 2,$$

where $s_{(m)i}$ and $n_{(m)i}(i = 1, 2, 3)$ are the unit vector along the shear direction and the unit vector normal to the transformation plane of the m-th phase transformation system, respectively. By using the obtained resolved shear stress $\tau_{(m)}$, the shear strain increment $d\gamma_{(m)}^{\mathrm{PT}}$ of the m-th phase transformation system can be estimated by (2.7) and (2.14) when only the m-th system becomes active. When some systems become active simultaneously in the crystal grain component, the corrections are necessary in order to incorporate the interactions among the phase transformation systems as described below.

2. The critical shear stresses $\tau_{\mathrm{M}(m)}$ and $\tau_{\mathrm{A}(m)}$ for the m-th phase transformation system are affected by a different active transformation system: interactions among the phase transformation systems in a grain. If the isotropic hardening rule is employed for simplicity, the $\tau_{\mathrm{M}(m)}$ and $\tau_{\mathrm{A}(m)}$ are modified as follows:

$$(3.3) \qquad \tau_{\mathrm{M}(m)}(\gamma^{\mathrm{PT}}, T) = \tau_{\mathrm{OMS}} + \beta(T - T_0) + H \sum_{p=1}^{M} \gamma^{\mathrm{PT}}(p),$$

$$(3.4) \qquad \tau_{\mathrm{A}(m)}(\gamma^{\mathrm{PT}}, T) = \tau_{\mathrm{OAF}} + \beta(T - T_0) + H \sum_{p=1}^{M} \gamma^{\mathrm{PT}}(p).$$

2. The phase transformation can not proceed any more after the phase transformation covers the whole area of the grain component. That is, the following equation in the volume fraction $\xi_{(m)}$ of the m-th $(m = 1.2, .., M)$ phase transformation system has to be considered:

$$(3.5) \qquad \sum_{m=1}^{M} \xi_{(m)} \leq 1.$$

By considering the relation $\xi_{(m)} = \gamma_{(m)}^{\mathrm{PT}} / \gamma_{\max}^{\mathrm{PT}}$, the phase transformation stops when the following equation is satisfied:

$$(3.6) \qquad \sum_{m=1}^{M} \gamma_{(m)}^{\mathrm{PT}} = \gamma_{\max}^{\mathrm{PT}}.$$

By incorporating the above two corrections, the relation between the increment of resolved shear stress $d\tau_{(m)}$ and the increment of phase transformation shear strain $d\gamma_{(m)}^{\mathrm{PT}}$ can be obtained as follows:

$$(3.7) \qquad d\gamma_{(m)}^{\mathrm{PT}} = \left\langle dF_{X(m)} \right\rangle \left\langle \gamma_{\max}^{\mathrm{PT}} - \sum_{p=1}^{M} \gamma_{(p)}^{\mathrm{PT}} \right\rangle G\left(\gamma_{(m)}^{\mathrm{PT}}\right) \cdot \left(d\tau_{(m)} - \beta dT \right) \Big/ H.$$

In this equation,

$$(3.8)_1 \qquad F_{X(m)} = F_{\mathrm{M}(m)}, \quad G\left(\gamma_{(m)}^{\mathrm{PT}}\right) = 1, \quad \text{when } F_{\mathrm{M}(m)} = 0,$$

$$(3.8)_2 \qquad F_{X(m)} = F_{\mathrm{A}(m)}, \quad G\left(\gamma_{(m)}^{\mathrm{PT}}\right) = \left\langle \gamma_{(m)}^{\mathrm{PT}} \right\rangle, \quad \text{when } F_{\mathrm{A}(m)} = 0,$$

$$(3.8)_3 \qquad F_{X(m)} = 0, \quad G\left(\gamma_{(m)}^{\mathrm{PT}}\right) = 1, \quad \text{when } F_{\mathrm{M}(m)} \neq 0, \quad F_{\mathrm{A}(m)} \neq 0,$$

where

$$(3.8)_4 \qquad F_{\mathrm{M}(m)} = \tau_{(m)} - \left[\tau_{0\mathrm{MS}} + H \sum_{p=1}^{M} \gamma_{(p)}^{\mathrm{PT}} + \beta(T - T_0) \right],$$

$$(3.8)_5 \qquad -F_{\mathrm{A}(m)} = \tau_{(m)} - \left[\tau_{0\mathrm{AF}} + H \sum_{p=1}^{M} \gamma_{(p)}^{\mathrm{PT}} + \beta(T - T_0) \right].$$

On the other hand, the phase transformation (deviatoric) strain increment de_{ij}^{PT} of the crystal grain component can be obtained as follows:

$$(3.9) \qquad de_{ij}^{\mathrm{PT}} = \sum_{m=1}^{M} \alpha_{(m)ij} d\gamma_{(m)}^{\mathrm{PT}}.$$

Therefore, if (3.7) is employed in (3.9),

$$(3.10) \qquad de_{ij}^{\mathrm{PT}} = \sum_{m=1}^{M} \alpha_{(m)ij} \left\langle dF_{X(m)} \right\rangle \left\langle \gamma_{\max}^{\mathrm{PT}} - \sum_{p=1}^{M} \gamma_{(p)}^{\mathrm{PT}} \right\rangle$$
$$\cdot G\left(\gamma_{(m)}^{\mathrm{PT}}\right) \left(d\tau_{(m)} - \beta dT \right) \Big/ H.$$

By considering the incremental form of (3.1),

$$(3.11) \qquad d\tau_{(m)} = \sum_{i,j=1}^{3} \alpha_{(m)ij} d\sigma_{ij},$$

the relations among the increment of phase transformation strain de_{ij}^{PT}, the increment of stress $d\sigma_{ij}$, and the increment of temperature dT for the crystal grain component can be obtained in the following form.

$$(3.12)_1 \qquad de_{ij}^{\mathrm{PT}} = \sum_{m=1}^{M} \alpha_{(m)ij} \left\langle dF_{X(m)} \right\rangle \left\langle \gamma_{\max}^{\mathrm{PT}} - \sum_{p=1}^{M} \gamma_{(p)}^{\mathrm{PT}} \right\rangle$$

$$\cdot G\left(\gamma_{(m)}^{\mathrm{PT}}\right) \sum_{k,l}^{3} \alpha_{(m)kl} d\sigma_{kl} - \beta dT \Bigg) \bigg/ H,$$

$$(3.12)_2 \qquad d\gamma_{(m)}^{\mathrm{PT}} = \left\langle dF_{X(m)} \right\rangle \left\langle \gamma_{\max}^{\mathrm{PT}} - \sum_{p=1}^{M} \gamma_{(p)}^{\mathrm{PT}} \right\rangle G\left(\gamma_{(m)}^{\mathrm{PT}}\right)$$

$$\cdot \left(\sum_{i,j=1}^{3} \alpha_{(m)ij} d\sigma_{ij} - \beta dT \right) \bigg/ H,$$

with the conditions:

$$(3.12)_3 \qquad F_{X(m)} = F_{\mathrm{M}(m)}, \ G\left(\gamma_{(m)}^{\mathrm{PT}}\right) = 1, \quad \text{when } F_{\mathrm{M}(m)} = 0,$$

$$(3.12)_4 \qquad F_{X(m)} = F_{\mathrm{A}(m)}, \ G\left(\gamma_{(m)}^{\mathrm{PT}}\right) = \left\langle \gamma_{(m)}^{\mathrm{PT}} \right\rangle, \quad \text{when } F_{\mathrm{A}(m)} = 0,$$

$$(3.12)_5 \qquad F_{X(m)} = 0, \ G\left(\gamma_{(m)}^{\mathrm{PT}}\right) = 1, \quad \text{when } F_{\mathrm{M}(m)} \neq 0, \ F_{\mathrm{A}(m)} \neq 0,$$

where

$$(3.12)_6 \qquad F_{\mathrm{M}(m)} = \tau_{(m)} - \left[\tau_{\mathrm{0M}} + H \sum_{p=1}^{M} \gamma_{(p)}^{\mathrm{PT}} + \beta(T - T_0) \right],$$

$$(3.12)_7 \qquad - F_{\mathrm{A}(m)} = \tau_{(m)} - \left[\tau_{\mathrm{0M}} + H \sum_{p=1}^{M} \gamma_{(p)}^{\mathrm{PT}} + \beta(T - T_0) \right],$$

$$(3.12)_8 \qquad \tau_{(m)} = \sum_{i,j=1}^{3} \alpha_{(m)ij} \sigma_{ij}.$$

As it can be found from the set of Eq. $(3.12)_{1-7}$, the obtained stress-strain-temperature relations are of a form of the theory whose internal variables are

the phase transformation strain $\gamma_{(m)}^{\text{PT}} (m = 1, 2..., M)$. When we recall $M = 24$ for the martensite phase transformation and the corresponding reverse phase transformation, the deformation of a single crystal grain component is found to be controlled by 24 internal variables.

The increment of total strain $d\varepsilon_{ij}$ of the crystal grain component is as follows:

$$(3.13) \qquad d\varepsilon_{ij} = d\varepsilon_{ij}^{e} + d\varepsilon_{ij}^{\text{PT}} + d\varepsilon_{ij}^{\text{T}},$$

where $d\varepsilon_{ij}^{e}$, $d\varepsilon_{ij}^{\text{PT}}$ and $d\varepsilon_{ij}^{\text{T}}$ are the elastic part, phase transformation part, and thermal part of (total) strain increment $d\varepsilon_{ij}$, respectively. The elastic and thermal parts can be described as follows, when the material is assumed to be elastically and thermally isotropic,

$$(3.14) \qquad d\varepsilon_{ij}^{e} = ds_{ij}/2G + \delta_{ij}\sigma/3K,$$

$$(3.15) \qquad d\varepsilon_{ij}^{\tau} = \beta\delta_{ij}dT,$$

where δ_{ij} is the Kronecker delta, s_{ij} and σ are the deviatoric and volumetric parts of stress tensor σ_{ij}, respectively, G is the shear modulus, K is the bulk modulus, β is the coefficient of thermal expansion.

The conclusion of this section is that the stress-temperature relation of the grain component is given by a set of Eqs. $(3.12)_{1-7}$, (3.13) – (3.15) whose form is of the internal variable type.

4. Thermo-mechanical model of the polycrystal

When the stress-strain-temperature relation of a polycrystal is derived on the basis of stress-strain-temperature relation of its crystal grain component, the interactions among grain components have to be reconsidered. That is, each grain component has its own stress and strain depending on its own orientation in the polycrystal because each grain has the anisotropy related with the phase transformation system: thus the complicated interactions among grains appear in order to satisfy the compatibility condition of strain as well as the equilibrium condition of stress in the polycrystal. Thus the non-uniform stress and strain distributions appear even if the applied load is quite simple, for example, the uniaxial tension of a solid bar. The effect of non-uniform strain and stress distributions on the mechanical properties of polycrystalline materials are very important, especially when the strain or stress path is complex (e.g., non-proportional stress/strain history including the arbitrary change of temperature). This kind of interaction effect would be even more significant in the case of SMA than the polycrystalline metallic materials whose deformation mechanism is the dislocation slip. For example, as described in Sec. 2, the phase transformation can occur by the change

of temperature without any stress, but the significant deformation can not be observed in this case, because the produced phase transformation shear strain cancel each other. On the other hand, if the material is in some state of stress, only the preferable phase transformation system becomes active, and significant phase transformation strain can be observed even if the stress is rather small (due to the temperature effect). That is, the produced internal (residual) stress may have a significant effect on the macro-deformation of polycrystalline materials. This effect of internal or residual stress is quite interesting for the design of two-way shape memory properties of SMA, and thus the effect of residual stress or internal stress are quite interesting from the engineering application as well as the micromechanic points of view. Also, the internal stress may have an important role on the path dependent behavior when the polycrystalline material is subjected to a complex loading path. This is one of the main reasons why the meso-mechanical technique [33] was employed for the derivation of constitutive equations in this research work.

The above mentioned interaction among grain can be taken into account by using the well-developed mechanics of inhomogeneous solids. The typical models proposed on the basis of inhomogeneous solid mechanics are the KBM model [43, 44] (self-consistent model) and eigen-strain model [45, 46]. Both of them are based on the inclusion theory developed by ESHELBY [42]. According to the inclusion theory, the stress and strain distributions in the inclusions are uniform and have a quite simple linear relation with the applied load, when the spherical or ellipsoidal anisotropic inclusion is embedded in an isotropic elastic matrix. Therefore, the stress and strain distributions are uniform in the inclusions, and thus, the complicated stress and strain distributions around the grain boundaries in the case of a polycrystal can not be incorporated directly. There exists no convenient (simple) model which can incorporate the distributions of stress and strain in each grain component. This kind of effect has been investigated by using the finite element analyses. However, it is very difficult to incorporate this effect in the compact constitutive equations. Moreover, this grain boundary effect has been investigated by using the electron microscopy as well as the computer analysis (e.g., FEM analysis, molecular dynamic analysis, etc.). However, so many unknown problems are still left for futher consideration.

Among two convenient and simple theories of inhomogeneous solid mechanics metioned above, the eigen-strain theory is rather effective, e.g., in the deformation course of materials reinforced by dispersed particles, and on the other hand, the KBW model is effective in the case of, for example, the polycrystal composed of many grain components where the characteristics of grain component are as follows:

1. the grain component has its orientation described by the generalized Schmid factor,

2. the grain component has a limit of transformability described by Eq. (3.5), and thus the size, shape and location of the grain in the polycrystal are not considered in the model, though the volume fraction is taken into account. In this case, the following equation can be obtained for SMA with the phase transformation mechanism.

$$(4.1) \qquad s_{ij}^{(k)} - S_{ij} = \alpha G \left(e_{ij}^{\mathrm{PT}(k)} - E_{ij}^{\mathrm{PT}} \right),$$

where $s_{ij}^{(k)}$ is the deviatoric stress component of the k-th grain component embeded in the polycrystal, S_{ij} is the averaged (macroscopic) deviatoric stress $\left[S_{ij} = \text{average} \left(s_{ij}^{(k)} \right) \right]$, $e_{ij}^{\mathrm{PT}(k)}$ is the (deviatoric) phase transformation strain components of the k-th grain, E_{ij}^{PT} is the averaged (macroscopic) phase transformation $\left[E_{ij}^{\mathrm{PT}} = \text{average} \left(e_{ij}^{(k)} \right) \right]$, G is the averaged shear modulus of polycrystal. The coefficient α in (4.1) is still being discussed in the case of inelastic matrix and it is not the material constant, in general. However, the coefficient α is assumed to be constant in the engineering applications, for simplicity. The proposed values are as follows:

$\alpha = 0$ (for stress constant model, the so-called Maxwell model),

$\alpha = 0.2$ (for modified KBW model by Berveiller-Zaoui [47]),

$\alpha = 1.0$ (for KBW original model [43]),

$\alpha = 2.0$ (for strain constant model, the so-called Voigt model),

$\alpha = \infty$ (for inelastic strain constant model; Taylor model),

In the final stage of this paper, one simple example of consitutive equations of SMA incorporating the interaction among grains in the polycrystal is demonstrated in a closed form. Here the stress constant model ($\alpha = 0$) is selected as an example. That is,

$$(4.2) \qquad \sigma_{ij}^{(k)} = \Sigma_{ij} = S_{ij} + \delta_{ij}\Sigma.$$

where S_{ij} and Σ are the deviatoric and volumetric parts of stress Σ_{ij}, respectively, and δ_{ij} is the Kroncker delta. In this case, the total strain increment $d\varepsilon_{ij}^{(k)}$ of the k-th grain component in the polycrystal model can be described as follows:

$$(4.3) \qquad d\varepsilon_{ij}^{(k)} = d\varepsilon_{ij}^{e(k)} + d\varepsilon_{ij}^{\mathrm{PT}(k)} + d\varepsilon_{ij}^{\mathrm{T}(k)}$$

$$= ds_{ij}^{(k)}/2G + \delta_{ij}d\sigma^{(k)}/3K + \beta\delta_{ij}dT + d\varepsilon_{ij}^{\mathrm{PT}(k)}$$

$$= dS_{ij}/2G + \delta_{ij}d\Sigma/3K + \beta\delta_{ij}dT + \sum_{m=1}^{M} \left[\alpha_{(m)ij}^{(k)} \left\langle dF_{X(m)}^{(k)} \right\rangle \right.$$

$$(4.3) \qquad \cdot \left\langle \gamma_{\max}^{\text{PT}} - \sum_{p=1}^{M} \gamma_{(p)}^{\text{PT}(k)} \right\rangle G^{(k)}\left(\gamma_{(m)}^{\text{PT}}\right) \cdot \left(\sum_{k,l=1}^{3} \alpha_{(m)kl}^{(k)} dS_{kl} - \beta dT \right) \Big/ H \Bigg]$$

[cont.]

The strain increment dE_{ij} of the polycrystal model can be expressed by the following equation:

$$(4.4) \qquad dE_{ij} = \sum_{k=1}^{K} V^{(k)} \Bigg\{ dS_{ij}/2G + \delta_{ij}d\sum/3K + \beta\delta_{ij}dT$$

$$+ \sum_{m=1}^{M} \Bigg[\alpha_{(m)ij}^{(k)} \left\langle dF_{X(m)}^{(k)} \right\rangle \cdot \left\langle \gamma_{\max}^{\text{PT}} - \sum_{p=1}^{M} \gamma_{(p)}^{\text{PT}(k)} \right\rangle G^{(k)}\left(\gamma_{(m)}^{\text{PT}}\right)$$

$$\cdot \left(\sum_{k,l=1}^{3} \alpha_{(m)kl}^{(k)} dS_{kl} - \beta dT \right) \Big/ H \Bigg] \Bigg\}$$

where $V^{(k)}$ is the volume fraction of the k-th grain component. Therefore,

$$(4.5) \qquad dE_{ij} = \sum_{k=1}^{K} V^{(k)} \Bigg\{ \sum_{m=1}^{M} \Bigg[\alpha_{(m)ij}^{(k)} \left\langle dF_{X(m)}^{(k)} \right\rangle$$

$$\cdot \left\langle \gamma_{\max}^{\text{PT}} - \sum_{p=1}^{M} \gamma_{(p)}^{\text{PT}(k)} \right\rangle G^{(k)}\left(\gamma_{(m)}^{\text{PT}}\right) \cdot \left(\sum_{k,l=1}^{3} \alpha_{(m)kl}^{(k)} dS_{kl} - \beta dT \right) \Big/ H \Bigg] \Bigg\}$$

$$+ dS_{ij}/2G + \delta_{ij}d\sum/3K + \beta\delta_{ij}dT,$$

where

$$(4.6) \qquad \gamma_{(p)}^{\text{PT}(k)} = \int d\gamma_{(p)}^{\text{PT}(k)},$$

and

$$F_{X(m)}^{(k)} = F_{\text{M}(m)}^{(k)}, \quad \text{if } F_{\text{M}(m)}^{(k)} = 0,$$

$$(4.7)$$

$$F_{X(m)}^{(k)} = F_{\text{A}(m)}^{(k)} = 0, \quad \text{if } F_{\text{A}(m)}^{(k)} = 0,$$

where

$$F_{\text{M}(m)}^{(k)} = \tau_{(m)}^{(k)} - [\tau_{\text{OM}} + H\gamma_{(m)}^{\text{PT}(k)} + \beta(T - T_0)],$$

$$(4.8)$$

$$-F_{\text{A}(m)}^{(k)} = \tau_{(m)}^{(k)} - [\tau_{\text{OA}} + H\gamma_{(m)}^{\text{PT}(k)} + \beta(T - T_0)].$$

A set of Eqs. (4.4) – (4.8) is an example of a set of constitutive equations constructed on the basis of a mesoscopic approach. In this approach, the simplest models are selected for each structural levels. It is possible to use more complicated but elegant and more accurate models for all structures and interactions between them. When we select the model of a structure, it is very important to consider the balance of reliability/accuracy among the selected models as well as the computer capacity according to the engineering needs.

Finally, it should be noted that the proposed constitutive equations can be described symbolically in a form of internal variable theory, where internal variables are $\gamma_{(m)}^{\mathrm{PT}(k)}$, in a following manner.

$$dE_{ij} = \sum_{k,l=1}^{3} F_{ijkl}\left(S_{pq}, \Sigma, T : \gamma_{(m)}^{\mathrm{PT}(n)}\right) dS_{kl}$$

$$+ F_{ij}\left(S_{ij}, \Sigma, T : \gamma_{(m)}^{\mathrm{PT}(n)}\right) d\Sigma + F_{ij}^{\mathrm{T}}(S_{pq}, \Sigma, T : \gamma_{(m)}^{\mathrm{PT}(k)})dT,$$

(4.9)

$$d\gamma_{(m)}^{\mathrm{PT}(k)} = \sum_{p,q=1}^{3} H_{(m)pq}^{(k)}(S_{ij}, \Sigma, T : \gamma_{(m)}^{\mathrm{PT}(k)})dS_{pq}$$

$$+ H_{(m)}^{(k)}\left(S_{ij}, \Sigma, T : \gamma_{(m)}^{\mathrm{PT}\,(k)}\right) d\Sigma + H_{(m)}^{\mathrm{T}\,(k)}\left(S_{ij}, \Sigma, T : \gamma_{(m)}^{\mathrm{PT}\,(k)}\right) dT.$$

5. Concluding remarks

The thermo-mechanical models selected for each structural level are quite simple and can be treated without any computer. For example, the inhomogeneous solid mechanical model was developed long ago, and these models were capable of solving so many important engineering problems without the aid of computer.

In our opinion, even if the macroscopic behavior is quite complex depending on the history of thermo-mechanical loading, this complicated behavior can be reproduced by a combination of some simple mechanisms corresponding to each structural level. That is, if the materials are considered to be a kind of thermo-mechanical system composed of simple mechanical components (materials), the complicated behavior can be reproduced.

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