Interaction Surface of Phase Transformation Stress by Constitutive Model for Accommodation of Transformation Strain

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The phase transformation behavior of polycrystalline shape memory alloys is investigated by a constitutive model under multi-axial stress states of tension and shear. The constitutive model used here was developed by the authors to describe the accommodation mechanism acting on the phase transformation phenomenon. The transformation occurs in microscopic transformation systems of crystals and is calculated by the constitutive model. The transformation stress is introduced here as an indicator to describe the macroscopic transformation start. Transformation stresses are obtained from calculated stress-strain curves for various loading paths. The interaction surface of macroscopic transformation stresses obtained is revealed to be very similar to the Mises yield surface in the stress space. Discussions are also made on the relation between the equivalent stress and the equivalent transformation strain of Mises type.

Key words: Shape Memory Alloy, Accommodation Mechanism, Constitutive Model, Transformation Stress, Interaction Surface

1. INTRODUCTION

As shape memory alloys have peculiar properties in comparison with other metals, various industrial applications of them are expected. When shape memory alloys are applied to industrial components with high functions, it is indispensable to develop a constitutive model precisely describing the behavior of the materials under various thermo-mechanical conditions. It is essential for a constitutive model of shape memory alloys to describe the accommodation mechanism which acts during phase transformation procedure. There are a lot of constitutive models developed by Tanaka [1], Tokuda [2], Brinson [3] [4], etc. which can successfully describe transformation behavior of shape memory alloys. But most of them are phenomenological ones with internal variables through which accommodation mechanism is reflected in the models indirectly and there are few models that can directly treat the accommodation mechanism which controls transformation behaviors of micro structures of shape memory alloys. The accommodation mechanism automatically chooses transformation planes and directions which should be active so that the internal stress caused by transformation becomes smallest. One of such models that can treat accommodation mechanism directly was developed by the authors [5] [6] where the equal strain assumption is introduced to describe the accommodation behavior in microscopic transformation systems of crystals.

In the present paper, the outline of the constitutive model proposed by the authors is described first and results from sample calculations by the constitutive model are given next in order to demonstrate the ability of the model for describing the deformation behavior of shape memory alloys.

Though it is demonstrated from results of sample calculations that the model is applicable for describing deformation behavior of shape memory alloys, a great

amount of computation is necessary for calculating macroscopic response of the material because the model calculates behaviors of micro structures of a material point at first and then integrate them to describe macroscopic behaviors of the material. It is preferable to develop a macroscopic constitutive model by modifying the present model to reduce the amount of the effort in the computation.

Along this thought, the transformation stress is introduced and defined as an indicator to describe the macroscopic transformation start. The transformation stress can be obtained from the stress-strain curve calculated by the present constitutive model. Plots of transformation stresses obtained from stress-strain curves for different loading paths constitute the interaction surface in the stress space which is very similar in shape to the Mises yield surface used in the plasticity theory. The equivalent stress and the equivalent transformation strain of Mises type which are defined for the macroscopic stress and the macroscopic strain are also introduced and discussed in a view point to develop a macroscopic constitutive model.

2. CONSTITUTIVE MODEL

2.1 Outline of the constitutive model

A constitutive model was proposed by the authors [5] [6] to describe the inelastic behavior of shape memory alloys such as TiNi alloys where the main mechanism of the inelastic behavior is the phase transformation under thermo-mechanical conditions.

In the constitutive model, a material point is treated as an aggregate of many crystal micro grains with arbitrary crystal orientations. Each grain has 24 transformation systems (transformation plane and transformation direction) which are peculiar to the crystal structure of the grain. The equal strain assumption is used in the model to connect the stress-strain relations of the material point to those of micro grains. Namely, the

Fig.1 Equal strain model for micro grains.

Fig.2 Equal strain model for micro grains with sub-elements.

Fig.3 Representation of work hardening of a single crystal.

microscopic strain of each grain is equal to that of the macroscopic strain of the material. And the macroscopic stress is represented as the average of stresses of grains. By using this model, the compatibility of strains of grains is automatically held in the material point. Figure 1 schematically shows the equal strain model. The idea of the equal strain model has been employed before in the modified fraction model for the inelastic (viscoplastic) behavior of metals under high temperatures [7] and also is similar to that employed in the Taylor's model for the plastic behavior of polycrystalline metals [8].

It is essential for a constitutive model to describe the accommodation mechanism in the phase transformation process of shape memory alloys. The equal strain model can successfully describe this mechanism. When the equal strain model is applied to transformation systems of each grain and the transformation occurs in one of the transformation systems which is located in the mechanically most favorite orientation to transform, the stress relaxation occurs in that direction and one of other transformation systems becomes to be the most favorite to transform at a next loading step. The accommodation behavior can be described by this mechanism. Moreover it is assumed that each micro grain is composed of many sub-elements which are in equal stress state in the micro grain (equal stress model or series model). And reflecting the structural variations, the critical condition for the transformation of sub-elements of a grain is assumed to be different each other to describe the work hardening in the stress-strain curve (see Fig.3). So the constitutive model mentioned here can be called as a combined model where the equal strain model and the equal stress model are combined. The whole image of the constitutive model is schematically shown in Fig.2.

When the value of the strain (total strain) of a material point is given, the value of stress of the material point can be calculated as below. By the assumption of equal strain, the strain of the grain is equal to the strain of the material point. The elastic strain is obtained by subtraction of the transformation strain from the total strain, and by multiplying the elastic strain with the elastic constant considering the volume fractions of each phase, the stress of each grain is calculated. According to the assumption of the equal stress, the stress thus calculated is applied to all sub-elements of the grain. The resolved shear stress acting on each transformation system of each sub-element is calculated, and when the maximum value of the resolved shear stress becomes larger than the critical value, the sub-element is treated as the transformed one and the intrinsic transformation

strain value is given to the sub-element. Considering the volume fraction of sub-element, the average value of transformation strains of the sub-elements is given as the transformation strain of the grain. The stress of a material point is the average value of stress of all grains. The constitutive relation of a material point is thus calculated.

2.2 Driving force for transformation and its critical value

The start and finish values of the critical shear stress defined at a temperature T_0 for inducing the martensite of a transformation system are denoted as $\tau_{0,MS}$ and $\tau_{0,MF}$. Also, the martensite start and finish temperatures defined at stress free conditions are denoted as M_s and M_f . Assuming the temperature dependence of critical stresses are linear and parallel to each other. The start and finish values of the critical shear stress τ_{MS} and τ_{MF} defined at arbitrary temperature T are described as

$$\tau_{MS} = \tau_{0,MS} + \beta_M (T - T_0) \quad (1).$$

$$\tau_{MF} = \tau_{0,MF} + \beta_M (T - T_0) \quad (2)$$

, where

$$\beta_M = (\tau_{0,MF} - \tau_{0,MS}) / (M_s - M_f) \quad (3)$$

, and also the following conditions are added on τ_{MS} and τ_{MF}

$$\tau_{MS} \geq 0, \quad \tau_{MF} \geq 0 \quad (4).$$

Denoting the resolved shear stress of a transformation system as τ , the condition for starting transformation is written as

$$\tau = \tau_{MS} \quad (5).$$

When the driving stress τ_{DR} for transformation is defined as

$$\tau_{DR} = \tau - \beta_M (T - T_0) \quad (6)$$

, the condition for starting transformation is rewritten as

$$\tau_{DR} = \tau_{0,MS} \quad (7).$$

Each sub-element of the micro grain is assumed to have a different value of the critical shear stress for the transformation each other reflecting the structural variation in the micro grain. Also the transformation in the transformation system of the element is assumed to start and finish at the same instance, the condition for starting and finishing of the transformation is written as

$$\tau_{DR} = \tau_{0,M} \quad (8)$$

, where the following condition is imposed on the value of $\tau_{0,M}$

$$\tau_{0,MS} \leq \tau_{0,M} \leq \tau_{0,MF} \quad (9).$$

For the reverse transformation, similar equations can be obtained by a parallel procedure for the transformation

and are not shown explicitly in the present paper.

To investigate the tension-compression asymmetry [9], the driving stress should be modified as [6]

$$\tau_{DR} = \tau - \beta_M (T - T_0) + a\sigma \quad (10)$$

, where σ is the normal stress acting on the transformation plane and a is a material constant which represents the effect of the normal stress on the transformation and should be adjusted for experimental data.

In order to describe the accommodation behavior in the case of the thermally induced transformation, it is also indispensable to take the effect of the normal stress into the driving stress as eq. (10). Moreover the normal transformation strain as well as the shear transformation strain is necessary to be taken into consideration in such a case [6].

By treating that the reorientation of transformation will occur when the maximum resolved shear stress in a transformation system of a sub-element become larger by a certain amount than that of the already transformed transformation system in the same sub-element, the reorientation behavior of shape memory alloys can be depicted by the present constitutive model [6].

3. EXAMPLE CALCULATIONS AND DISCUSSION

3.1 Material constants and calculation conditions

Referring to experimental data obtained from uniaxial tensile tests for the shape memory alloy of Ti-50.39at%Ni ($A_f = 334K$, $A_s = 319K$, $M_s = 282K$, $M_f = 262K$) wire at 333K [5], material constants employed for example calculations are as follows.

Young's modulus of austenite $E_a = 65.5GPa$

Young's modulus of martensite $E_m = 14.1GPa$

Poisson's ratio (postulated) $\nu = 0.3$

Martensite start stress $\sigma_{MS} = 302MPa$

Martensite finish stress $\sigma_{MF} = 310MPa$

The start and finish values of critical shear stresses τ_{MS} and τ_{MF} are postulated as

$$\tau_{MS} = \sigma_{MS} / 2, \quad \tau_{MF} = \sigma_{MF} / 2 \quad (11)$$

, where suffix 0 is neglected for brevity.

A micro grain is divided into N sub-elements with equal volume fractions. The value of the critical shear stress for the transformation of i -th sub-element τ_{Mi} is represented as,

$$\tau_{Mi} = \tau_{MS} + (\tau_{MF} - \tau_{MS}) \frac{i-1}{N} \quad (i = 1 \sim N+1) \quad (12).$$

In the present calculations, $N = 1000$ is employed.

The value of the critical shear stress for the reverse transformation of i -th sub-element τ_{Ai} is assumed to be smaller than τ_{Mi} by an amount of τ_C , that is,

$$\tau_{Ai} = \tau_{Mi} - \tau_C \quad (13).$$

τ_C is set to be 50MPa tentatively for the calculation purpose.

The orientations of micro grains are described with Euler angles. Considering the symmetry of the placement of a crystal in the three dimensional space, only angles between 0 and $\pi/2$ are considered in ϕ , θ and ψ . Euler angles are divided by 6 in ϕ , 2 in θ and 3 in ψ respectively for numerical computations in the present case, and total 36 micro grains are placed in each

direction. Considering the finite difference of direction angles, the volume fraction of a grain of each direction is given as

$$\left(\frac{2}{\pi}\right)^2 \{ \cos(\phi - \Delta\phi/2) - \cos(\phi + \Delta\phi/2) \} \Delta\theta\Delta\psi.$$

The intrinsic transformation strains are given for the transformation system with the transformation plane perpendicular to the third coordinate axis and the transformation direction parallel to the first coordinate axis as

$$\tilde{\varepsilon}^* = \begin{bmatrix} 0 & 0 & \tilde{\gamma}/2 \\ 0 & 0 & 0 \\ \tilde{\gamma}/2 & 0 & \tilde{\varepsilon} \end{bmatrix} \quad (14)$$

, and sample values for Cu-Zn-Sn shape memory alloy has been presented in [10] as

$$\tilde{\gamma} = 0.2, \quad \tilde{\varepsilon} = -0.004 \quad (15).$$

Though introducing the normal transformation strain is necessary in order to describe the thermally induced transformation [6], it is not the case for the present study. In the present study, the stress induced transformation will be treated. So, referring to eq. (15), values of

$$\tilde{\gamma} = 0.2, \quad \tilde{\varepsilon} = 0 \quad (16)$$

are employed for simplicity in the present study.

Also, the value of material parameter a shown in eq. (10) is set to be zero and the tension-compression asymmetry is not investigated here.

3.2 Results for single crystal

The transformation behaviors of a single crystal (a micro grain in the constitutive model) are calculated by the constitutive model shown in the previous section. The crystal is treated as one embedded in a polycrystalline and the equal strain model is expected to be applicable. A crystal is put so that a-, b- and c- axis of the crystal coincide with 1-, 2- and 3-axis of the material coordinate respectively. Fig.4 shows a calculated uniaxial stress-strain behavior of a single crystal under external tensile strain. The stress induced transformation behavior in the superelastic regime is successfully depicted in the figure. As shown in Fig. 4, the material exhibits the elastic behavior of the austenite at first, then the transformation begins, and trough the linear hardening regime, the elastic behavior of the martensite emerges at the last stage. Sharp corners are seen around the transition region of the stress strain curve.

24 transformation systems are considered in the calculation. In the transformation procedure of the calculation, it is observed the $(2\bar{1}\bar{1})$ - $[1\bar{1}1]$ transformation system acts at first following $(2\bar{1}\bar{1})$ - $[111]$, $(2\bar{1}1)$ - $[1\bar{1}\bar{1}]$, (211) - $[1\bar{1}\bar{1}]$ in order and this series of 4 transformation systems is repeated. This fact is regarded as a thing corresponding to the experimentally observed phenomenon [11] that diamond-like figures composed from four different variants are observed at the phase transformed region of specimens. This may be considered to be a proof that the constitutive model can successfully predict the accommodation behavior in the phase transformation of shape memory alloys.

3.3 Results for polycrystalline

The polycrystalline material is treated as an aggregate of single crystals with different crystal orientations.

Because the orientation of a crystal at a material point is probabilistic matter, the probabilistic average of the stress value of each crystal with a different crystal orientation gives the (macroscopic) stress of a material point. In the present calculations, the material is assumed to be isotropic and the crystal orientation is uniformly distributed in the 3-dimensional space.

Figure 5 shows the result for a polycrystalline shape memory alloy under uniaxial tension. On the contrary to the result for a single crystal shown in Fig. 4, the stress-strain curve is smooth where transition regions are smoothly connected. The reason why the stress-strain curve for a polycrystalline becomes smooth is considered that the polycrystalline material is composed of many crystals with different orientations and contains a large number of transformation systems having various transformation directions. It is also revealed that the microscopic phase transformation starts earlier than the macroscopically detected starting point on the macroscopic stress-strain curve and lasts beyond the macroscopically detected finishing point. This situation will be the same for the stress-strain curve provided from experiments. That is, the true starting and finishing point of transformation cannot be obtained from the stress-strain curve obtained by experiments. This fact corresponds with the indication made by Brinson [12] in his work on the microscopic observation.

Another example is shown in Fig.6 where the superelastic behavior of a shape memory alloy is calculated under loading and unloading conditions.

4. INTERACTION SURFACE OF TRANSFORMATION STRESS

4.1 Transformation Stress

As shown in chapters 2 and 3, the response of shape memory alloys under the various loading of combined mechanical and thermal loadings can be analyzed by using the proposed constitutive model. But there are some difficulties in the actual calculation procedure. An enormous amount of the computation is needed for calculating the deformation of shape memory alloys. That is, the transformation behavior of very large number ($24 \times \text{number of sub-elements} \times \text{number of micro grains}$) of transformation systems should be calculated.

To avoid this difficulty and develop a new constitutive model dealing with macroscopically defined quantities, the transformation stress is introduced here and the property of it is investigated.

The transformation stress is defined as a stress indicator for starting the macroscopic transformation and determined on the stress-strain curve as shown in Fig.5. The transformation stress is obtained as the stress at the intersection of an extension line of elastic portion of stress-strain curve and a tangent line of the dominant transformation portion of the stress-strain curve.

4.2 Interaction surface of transformation stress

Calculations are conducted for several multi-axial cases of the combined loading of the axial strain and the shear strain and stress-strain curves are obtained for each loading case. According to the procedure mentioned in section 4.1, transformation stresses are obtained from calculated stress-strain curves for each loading case. The

Fig.4 Uniaxial stress-strain curve for single crystal of Ti-Ni shape memory alloy in the superelastic regime.

Fig.5 Stress-strain curve for polycrystalline under uniaxial tension loading.

Fig.6 Superelastic behavior of polycrystalline shape memory alloy under loading and unloading condition

plots of transformation stresses in the stress space constitute a curved surface called as the interaction surface. Fig. 7 shows the interaction surface (curve) of transformation stresses and the Mises yield surface for comparison. It is clear that the interaction surface of transformation stresses is very similar to the Mises yield surface used in the plasticity theory.

4.3 Equivalent stress and equivalent transformation strain

As it is revealed that interaction surface of the transformation stress is very similar to that of Mises yield surface, it seems hopeful to investigate the applicability of the equivalent stress and the equivalent strain of Mises type to the theory of transformation.

The equivalent stress and the equivalent transformation strain of Mises type are defined for the present cases of calculation as

$$\begin{aligned}\sigma_{eq} &= \sqrt{\sigma_{33}^2 + 3\sigma_{31}^2} \\ \varepsilon_{eq}^{tr} &= \int d\varepsilon_{eq}^{tr} \\ d\varepsilon_{eq}^{tr} &= f_s f_g \tilde{\gamma} / \sqrt{3}\end{aligned}\quad (17)$$

,where σ_{eq} , ε_{eq}^{tr} , $d\varepsilon_{eq}^{tr}$, f_s , f_g and $\tilde{\gamma}$ denote the equivalent stress, the equivalent transformation strain, the increment of it, the volume fraction of sub-element, the volume fraction of micro grain and the inheinsic shear strain of the transformation respectively.

Figure 8 shows the relations between the equivalent stress and the equivalent transformation strain for loading cases of 0, 45 and 90 degree in α which represents the loading direction in the strain space as

$$\tan \alpha = \varepsilon_{31} / \varepsilon_{33}.$$

It is clear from the figure that stress-strain curves for different loading cases almost coincide with each other in the relations between the equivalent stress and the equivalent transformation strain.

It may be concluded from these results that an invariant theory in the plasticity will be also effective for the macroscopic transformation theory of shape memory alloys.

5. CONCLUSIONS

The constitutive model which has been proposed by the authors before and can describe the accommodation behavior of the transformation of shape memory alloys is briefly described. And by sample calculations it is demonstrated that this model is applicable for describing the deformation behavior of shape memory alloys under various loading conditions.

It is pointed out from the stress-strain curve obtained for a polycrystalline that the microscopic phase transformation starts earlier than the macroscopically detected starting point on the stress-strain curve and lasts beyond the macroscopically detected finishing point. This situation will be the same for the stress-strain curve provided from an experiment. That is, the true starting and finishing point of transformation cannot be obtained from the stress-strain curve.

But the transformation stress macroscopically determined from the stress-strain curve may be more important for describing the macroscopic material behavior of shape memory alloys. The transformation stress is defined here as the transformation start stress which is determined on the stress-strain curve macroscopically. It is discovered that transformation stresses obtained from calculated stress-strain curves for various loading conditions form the interaction surface in the stress space which is very similar to the Mises yield surface used in the plasticity theory.

Also the relation between the equivalent stress and the equivalent transformation strain of Mises type is examined. It is pointed out that stress-strain curves for various loading paths are coincide with each other in the relation between the equivalent stress and the equivalent transformation strain.

These findings will be useful for developing a new macroscopic constitutive model for shape memory alloys.

Fig.7 Interaction surface of transformation stresses and Mises yield surface.

Fig.8 Relation between equivalent stress and equivalent transformation strain.

References

- [1] K. Tanaka, H. Tobushi and S. Miyazaki, "Properties of Shape Memory Alloys", 1st ed., Yokendo, Tokyo (1993) pp62-122.
- [2] M. Tokuda, Y. Men, B. Bundara, P. Sittner, *Trans. JSME.*, **A**, **65**-631, 491-497 (1999).
- [3] L. C. Brinson, *J Intelligent Material Systems and Structures.*, **4**, 229-242 (1993).
- [4] M. Panico and L. C. Brinson, *J Mech Phys Solids.*, **55**, 2491-2511 (2007).
- [5] A. Suzuki, H. Shibutani, T. Yamamoto, T. Sakuma, H. Baba, *Proc. 57th conf. of JSMS.*, 205-206 (2008).
- [6] A. Suzuki, W. Araki, H. Shibutani, T. Yamamoto, T. Sakuma, *Proc. Conf. on Strength of Materials (M&M2008)*, JSME., OS1001 (2008).
- [7] A. Suzuki, *Proc. of the International Conf. on Creep '86*, 471-476 (1986).
- [8] G. I. Taylor, *J. Inst. Metals.*, **62**, 307-324 (1938) pp.307-324.
- [9] R. R. Adharapurapu, F. Jiang, K. Vecchio, G. T. Gray III, *Acta Materialia.*, **54**, 4609-4620 (2006).
- [10] K. Tanaka, H. Tobushi and S. Miyazaki, "Properties of Shape Memory Alloys", 1st ed., Yokendo, Tokyo (1993) p86 and p94.
- [11] K. Ohtsuka, et al., "Shape Memory Alloys", 1st ed., Ed. by H. Funakubo, Sangyo Tosho, Tokyo (1984) pp22-23.
- [12] L. C. Brinson, I. Schmidt and R. Lammering, *J Mech Phys Solids.*, **52**, 1549-71 (2004).

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