Improved Constitutive Modeling for Phase Transformation of Shape Memory Alloys*

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Abstract
This work presented new developments in the constitutive modeling of shape memory alloys (SMAs). As an increasing number of experimental results are being published, it is becoming increasingly difficult to describe complicated SMA behaviors using conventional models. To overcome the shortcomings of existing models, this research proposed two major improvements to the assumed phase transformation function. A more flexible function called logistic sigmoid function has been introduced into the phase transformation function. This improvement affords a better fit to the typical SMA stress-strain relationship. Moreover, a cyclic effect has been considered while developing the new model. The new model is proposed by connecting accumulated strain with the critical phase transformation constants of SMAs. Both improvements were first validated at the material level. Thereafter, structural level validation and application were conducted. Accuracy enhancement may be expected by adopting these new models in SMA-related simulations.

Key words: Computational Mechanics, Shape Memory Alloy, Kinetics of Phase Transformation, Logistic Sigmoid Function, Cyclic Effect, Damping Device

1. Introduction

Reliable, accurate, and efficient computational models are essential for designing shape memory alloy (SMA) devices. Since the discovery of SMAs in the middle of the 20th century, there has been a long-standing interest in the thermo-mechanical constitutive modeling of SMAs. Many constitutive models have been developed in the past 20–30 years; however, with the increasing number of published experimental results, complex and changeful behaviors of SMA have been observed. Experiments have uncovered hitherto unknown crystallographic and mechanical details pertaining to SMA phase transformation; thus far, these details were not considered in conventional models. Moreover, the relatively simple functions in conventional models can no longer well represent those behaviors. Therefore, there is considerable scope for improving the existing models.

Mainstream constitutive models of SMAs can be categorized into two groups: microscopic and macroscopic. Microscopic models focus on molecular- or lattice-particle-level micro-mechanical behavior, whereas macroscopic models are phenomenological models that rely on continuum thermomechanics with internal variables arising from phase transformation. Given that macroscopic models are based on pre-established mathematical functions for describing the phase transformation, they are also called assumed phase transformation kinetics models. These assumed functions are compatible with thermodynamics, but do not directly depend on material constants at the
microscopic level. A large number of material constants used in these models are experimentally determined. Macroscopic models are the most researched models in published literature. Within macroscopic models, the proposals by Tanaka and Nagaki (1) and Boyd and Lagoudas (2) can be categorized as exponential function macroscopic models. Tanaka and Nagaki (1) first proposed the exponential function model assuming that martensite phase transformation is a function of temperature and stress. Boyd and Lagoudas (2) later connected the material constants in Tanaka’s model with phase transformation critical temperature. Another group of macroscopic models is the cosine function group, which was first introduced by Liang and Rogers (3). Later the cosine function model was improved by Brinson (4) by splitting the martensite phase into stress-induced martensite and temperature-induced martensite. Toi et al. (5) further improved the cosine function group by introducing compressive and tensile loading asymmetry. The major difference between cosine function and exponential function models is the shape of the assumed phase transformation function. The abovementioned models have one common feature: for one set of material parameters in temperature-stress phase diagram, the phase transformation route is uniquely defined. Therefore, in this paper we call abovementioned models fixed shape phase transformation models. To avoid this limitation, other types of models with better flexibility such as Ivshin and Pence (6), and Matsuzaki et al. (7) were developed. Related discussion can be found in section 3.

The potential application of SMAs as functional materials requires that the simulation tool have a high degree of accuracy and rich functionality. In this work, our major issues of concern are that the model should provide a good fit to the typical stress-strain relationship of SMAs and support the cyclic effect. According to the experimental evidence in Shaw et al. (8) and Patoor et al. (9), SMA phase transformations occur at different speeds. In the starting and ending regions of the entire phase transformation, transformation speed could be fast in one type of SMA but slow in another. Conventional cosine (3)-(5) or exponential function models (1), (2) with a fixed phase transformation function might be adequate for single-crystal SMAs. Mathematical functions with greater flexibility are required for modeling commonly used polycrystalline SMAs. The logistic sigmoid function is a good replacement for conventional functions.

For actuating materials, common behaviors such as the cyclic effect should be considered in computational models. Experimental results from Tobushi et al. (10) and Lagoudas et al. (11) indicate the decrease in critical phase transformation temperature under cyclic loading. Conventional models consider latent heat (11) or simultaneous plastic deformation (13) as the main cause underlying the cyclic effect. This work takes another point of view by linking accumulated strain, a common cause of the cyclic effect, to critical phase transformation temperature and maximum residual strain, thus aiming to provide physical meaning and simplicity to the cyclic effect model.

In addition to the constitutive modeling improvements, this work presents modeling validations and numerical applications from simulations. The remainder of this paper is organized as follows: Section 2 introduces a constitutive model for SMAs in general. Based on the general model, our improved model based on the use of the logistic sigmoid model is discussed in section 3. The material- and structural-level validations of this model are presented in section 4. Sections 5 and 6 discuss the cyclic effect model, and material level validation and numerical application of this model are presented in section 6.

2. Shape Memory Alloys: Properties and Constitutive Model

2.1. Phases and Phase Transformation in Shape Memory Alloys

In SMAs, the austenite phase is a highly crystallographically symmetrical phase, usually in the cubic crystal structure. In the stress-temperature-phase diagram shown in Fig. 1, the austenite phase structure is presented in the lower right area. The temperature in this
area is higher than the reverse phase transformation finish temperature $A_f$, and the stress is lower than the reverse phase transformation finish stress $\sigma_{A_f}$ (a function of temperature $T$ and slope $C_{A_f}$), which also represents the stable austenitic condition.

The martensite phase is a low-temperature, low-symmetry phase with several variants. Two major variants are: detwinned martensite, which forms at higher stress level (stable when stress is higher than the martensite phase transformation finish stress $\sigma_{M_f}$ or crystallographic reorientation process finish stress $\sigma_{\text{crit.}}$) and twinned martensite, which forms at lower stress levels (stable when stress is lower than crystallographic reorientation process start stress $\sigma_{\text{crit.}}$, temperature is lower than martensite phase transformation finish temperature $M_f$). Compared with austenite, martensite usually has lower stiffness. Detwinned martensite can be transformed from austenite or twinned martensite by applying stress. Therefore, it is called stress-induced martensite. Twinned martensite can be transformed from austenite via a cooling process. Therefore, it is called temperature-induced martensite.

The area between lines $\sigma_{M_f}$ and $\sigma_{A_f}$ is an interim area where mixed phases exist. In area one, martensite phase transformation occurs, whereby high-symmetry austenite transforms to low-symmetry detwinned martensite. In area two, reverse phase transformation occurs, i.e., the backward transformation of the aforementioned martensite phase transformation. Special features of SMAs, such as the shape memory effect, superelasticity, and actuation properties such as high actuation energy and high actuation frequency, are closely related to the phase transformations in these areas.

**2.2. Special Features of Shape Memory Alloys**

The shape memory effect in SMAs is a feature whereby the alloy recovers its original shape after deformation. Even after a large deformation, the seemingly permanent strain can be relieved, and shape recovered, through a heating process. This effect is closely related to phase transformation between the low-stress (austenite, twinned martensite) and high-stress phase groups (detwinned martensite).

Superelasticity is a feature related to original shape recovery. It is different from the shape memory effect, in that it occurs without heating. The effect is only related to austenite–detwinned martensite phase transformations. Owing to the elasticity-like nature of phase transformation, this effect is also called pseudo-elasticity.

**2.3. Phenomenological Model of Shape Memory Alloy**

The stress-strain relation and kinetics of phase transformation for reproducing the special features of SMAs are introduced in this subsection.

- **Incremental form of stress-strain relationship**

The experimental basis of this model is the phenomenological behavior of polycrystalline SMAs. Therefore, crystallographic structural change during martensite phase transformations is considered indirectly in this type of model. The thermomechanical constitutive equation and the kinetics of transformation are derived from the second law of
thermodynamics expressed as the Clausius-Duhem inequality. Apart from the other model, which directly includes variables such as free energy, which are not easily measurable, Brinson proposed a cosine function model with only quantifiable engineering variables and material parameters in its expression. The incremental form of SMAs is as follows:

$$d\sigma = dE \cdot e + E \cdot de + d\Omega \cdot \xi_{s} + \Omega \cdot d\xi_{s} + \theta dT$$  \hspace{1cm} (1)

where $E$ corresponds to the elastic tensor, $\Omega$ is the phase transformation tensor, and $\theta$ is associated with the thermoelastic tensor. In this paper, $\theta dT$ is always ignored due to isothermal condition.

$$E(\xi) = E_{A} + \xi (E_{M} - E_{A})$$  \hspace{1cm} (2)

where $E_{A}$ is the Young’s modulus of the 100% austenite phase, $E_{M}$ is the Young’s modulus of the 100% martensite phase.

$$\Omega(\xi) = -e_{s} E(\xi)$$  \hspace{1cm} (3)

where $e_{s}$ is the maximum residual strain, which can be measured experimentally by unloading 100% detwinned martensite at a temperature lower than the austenite phase transformation start temperature $A_{s}$.

$$\theta(\xi) = -\alpha E(\xi)$$  \hspace{1cm} (4)

where $\alpha$ is the thermoelastic coefficient.

Besides stress $\sigma$ and temperature $T$, internal variable $\xi$ is considered. Martensite phase fraction $\xi$ is divided into two parts: the temperature-induced martensite fraction $\xi_{T}$ and the stress-induced martensite fraction $\xi_{s}$. By rearranging Eq. (1), the incremental form of stress-strain used in finite element simulations becomes the following expression:

$$\Delta \sigma = D_{\sigma} (\Delta \xi + \Delta \xi_{s})$$  \hspace{1cm} (5)

where $\Delta \sigma$ and $\Delta \xi$ are stress and strain increments, respectively, and stiffness $D_{\sigma}$ and $\Delta \xi_{s}$ are defined as follows:

$$D_{\sigma} = \frac{E}{1 - \frac{dE}{d\xi} \frac{d\xi}{d\sigma} - \frac{d\Omega}{d\xi} \frac{d\xi}{d\sigma} \xi_{s} - \Omega \frac{d\xi}{d\sigma}}$$

$$\Delta \xi_{s} = \frac{\left[ \frac{dE}{d\xi} \frac{d\xi}{dT} \xi_{s} + \frac{d\Omega}{d\xi} \frac{d\xi}{dT} \xi_{s} + \Omega \frac{d\xi}{dT} + \theta \right] \Delta T}{E}$$  \hspace{1cm} (6)

Phase transformation kinetics

In SMAs, martensite phase transformation includes martensite phase transformation (from austenite to detwinned martensite) and reverse phase transformation (from detwinned martensite to austenite). The martensite phase transformation is a rate-independent, reversible, crystallographic reorientation process. Because of its diffusionless property, it is a fast, inelastic deformation. Given that martensite phase transformation is a first order transition, both parent and product phases could coexist during the process. The transformation is accompanied by latent heat: forward transformation (Austenite => Martensite) releases heat and reverse transformation (Martensite => Austenite) absorbs heat.

The phase transformation equations in this thesis are based on the work of Toi et al., an improved model by Brinson. This transformation model is capable of martensite phase transformation and the corresponding reverse transformation. Stress-induced martensite and temperature-induced martensite have their evolution equations; thus, their volume fractions can be determined separately. The model introduced in this subsection is a general model with limited simulation functions. In phase transformation kinetics, transformation status is determined by Drucker-Prager equivalent stress $\sigma^{DP}$. The variable $\frac{\sigma^{DP}}{1+\beta}$ determines the position in stress-temperature phase diagram in Fig. 1. $\beta$ in $\frac{\sigma^{DP}}{1+\beta}$ is the coefficient to show the asymmetry behavior under compressive and tensile loading.
(i) When \( T > M_s \) and \( C_m(T - M_s) + \sigma_{\text{crit}, f} < \frac{\sigma_{D,P}}{1+\beta} < C_m(T - M_s) + \sigma_{\text{crit}, t} \), martensite phase transformation occurs.

Let \( \sigma_{M_s} = C_m(T - M_s) + \sigma_{\text{crit}, t} \), and \( \sigma_{M_f} = C_m(T - M_s) + \sigma_{\text{crit}, f} \).

For martensite phase fraction,
\[
\xi = \frac{1 - \xi_0}{2} \cos \left( \frac{\pi}{\sigma_{M_f} - \sigma_{M_t}} \left[ \frac{\sigma_{D,P}}{1+\beta} - \sigma_{M_t} \right] \right) + \frac{1 + \xi_0}{2} \tag{8}
\]
\[
\xi_f = \frac{1 - \xi}{1 - \xi_0} \tag{9}
\]

When \( \sigma \geq 0 \), \( \frac{\partial \sigma_{D,P}}{\partial \sigma} = \beta + 1 \)

When \( \sigma \leq 0 \), \( \frac{\partial \sigma_{D,P}}{\partial \sigma} = \beta - 1 \)

(ii) When \( T > A_s \) and \( C_{A_f}(T - A_f) < \frac{\sigma_{D,P}}{1+\beta} < C_{A_t}(T - A_s) \), reverse phase transformation occurs.

For martensite phase fraction,
\[
\xi = \frac{\xi_0}{2} \left[ 1 + \cos \left( \frac{\pi}{\sigma_{A_f} - \sigma_{A_t}} \left[ \frac{C_{A_f}(T - A_f)}{1+\beta} - \sigma_{A_t} \right] \right) \right] \tag{10}
\]
\[
\xi_s = \frac{\xi_0}{2} \tag{11}
\]

When \( \sigma \geq 0 \), \( \frac{\partial \sigma_{D,P}}{\partial \sigma} = \beta + 1 \)

When \( \sigma \leq 0 \), \( \frac{\partial \sigma_{D,P}}{\partial \sigma} = \beta - 1 \)

(iii) Detailed discussion for phase transformation when \( T < M_s \) can be found in companion paper: "Enhanced Computational Modeling of Shape Memory Alloys and Its Applications to Honeycomb Analysis".


The limitation of conventional phenomenological models is obvious. When temperature stays unchanged, given the critical starting stress of phase transformation as well as the finishing stress, according to the transformation kinetics of the abovementioned models, there is only one possible route for changes in the volume fraction of the martensite phase. Similarly, when stress remains unchanged, given the critical starting temperature of phase transformation and the finishing temperature, the uniqueness of the route through which the volume fraction of the martensite phase changes can be determined. However, experimental results contradict the abovementioned. Sharp and abrupt phase transitions at the initiation and completion of phase transformation were reported, which imply that the stress-strain curve could be sharp at the beginning and ending of a phase transformation. Related reports include Patoor et al.\(^{8}\) (single-crystalline SMA) and Shaw and Kyriakides\(^{8}\) (untrained polycrystalline SMA). Contradicting results can be found in Lagoudas et al.\(^{14}\), who described smooth and gradual manner of martensite phase transformation at the beginning and ending part of phase transformation.

Fixed shape transformation hardening functions in conventional models are incapable
of representing SMAs behavior in these experimental findings. In stress-strain curves of single-crystal SMAs, the transformation speed is constant. However, properties of polycrystal SMA are heavily dependent on the properties of each type of crystal as well as its fraction in the polycrystal SMA. Transformation speed can always change. Fixed-shape transformation hardening functions may be able to represent behaviors of single-crystal SMAs, but a shape transformation hardening function is required for polycrystal SMAs. To solve this problem, attempts can be found in several reports. One example is hyperbolic tangent function model proposed by Ivshin and Pence\(^6\) considering isofractional function \(\beta\) as a key variable also attracted attentions. \(\beta\) is a function of stress and temperature which is used to control austenite phase envelop functions. The model structure, assumed variables and phase fraction governing equations are different from the model we will discuss later. Another model follows similar structure as Ivshin and Pence's was proposed by Matsuzaki et al.\(^7\). This model adopted a polynomial function as the governing function of free energy. In the model we will discuss later, similar good fittings have been obtained by using less parameters when compared with Matsuzaki et al's model.

The logistic sigmoid function has the flexibility to adjust its curve shape by using only one coefficient. The original logistic sigmoid function is modified to fit the special requirements of transformation hardening. Its adjustable shape makes the logistic sigmoid function a good candidate for being used as a transformation hardening function. The basic form of the improved logistic sigmoid function is as follows:

\[
y = b \cdot \left( \frac{2}{1 + e^{-32ax \pm 16a}} - 1 \right)
\]

\[
b = \frac{1}{1 + e^{-16a}}^{-1}
\]

where coefficient \(a\) is the phase transformation rate coefficient, which is used to control the transition speed of different time phases during transformation. Different from Ivshin and Pence's model, additional variant \(b\) was adapted to enhance flexibility as well as ensure consistence of martensite phase fraction. By implementing this model as the phase transformation hardening function, the kinetics of phase transformation becomes:

(i) When \(T > M_s\) and \(C_{M_s} (T - M_s) + \sigma_{\text{crit.}}^{\text{start}} < \sigma_{\text{crit.}}^{\text{finish}} < C_{M_f} (T - M_f) + \sigma_{\text{crit.}}^{\text{finish}}\), martensite phase transformation occurs.

Let \(\sigma_{M_s} = C_{M_s} (T - M_s) + \sigma_{\text{crit.}}^{\text{start}}, \sigma_{M_f} = C_{M_f} (T - M_f) + \sigma_{\text{crit.}}^{\text{finish}}\).

\[
x = \frac{\sigma_{\text{crit.}}^{\text{finish}} - \sigma_{M_f}}{\sigma_{M_f} - \sigma_{M_s}}
\]

\[
y = b \cdot \left( \frac{2}{1 + e^{-32ax \pm 16a}} - 1 \right)
\]

\[
b = \frac{1}{1 + e^{-16a}} - 1
\]

For martensite phase fraction

\[
\xi_s = \frac{1 - \xi_0}{2} \frac{1}{1 + \xi_0} + \frac{1 + \xi_0}{2}
\]

\[
\xi_T = \frac{1 - \xi_0}{1 - \xi_0}
\]

\[
\xi = \xi_T + \xi_s
\]

Explanation
\[
\frac{\sigma_{\text{DF}}}{1 + \frac{1}{\beta}} \cdot \frac{\sigma_{M_{f}}}{\sigma_{M_{i}}} \text{ in the conventional model is replaced by } x
\]

\[
\cos \left( \frac{\pi}{\alpha_{M} - \sigma_{M_{i}}} \left[ \frac{\sigma_{\text{DF}}}{1 + \frac{1}{\beta}} - \sigma_{M_{f}} \right] \right) \text{ in the conventional model is replaced by } y
\]

(ii) When \( T > A_{s} \) and \( C_{A_{f}}(T - A_{f}) < \frac{\sigma_{\text{DF}}}{1 + \frac{1}{\beta}} < C_{A_{s}}(T - A_{s}) \), reverse phase transformation occurs.

Let \( \sigma_{h_{s}} = C_{A_{s}}(T - A_{s}), \sigma_{h_{f}} = C_{A_{f}}(T - A_{f}) \)

\[
x = \frac{\sigma_{h_{s}} - 1 + \frac{1}{\beta}}{\sigma_{h_{s}} - \sigma_{h_{f}}}
\]

\[
y = b \cdot \left( \frac{2}{1 + e^{-32ax + 16a}} - 1 \right)
\]

\[
b = \frac{1}{2} \frac{2}{1 + e^{-16a}} - 1
\]

For martensite phase fraction

\[
\xi = \frac{\xi_{s}}{2} (1 + y)
\]

\[
\xi_{s} = \frac{\xi_{s}}{2} (1 + y)
\]

\[
\xi_{f} = \frac{\xi_{f}}{2} (1 + y)
\]

Explanation

\[
\frac{\sigma_{h_{s}} - \sigma_{\text{DF}}}{\sigma_{h_{s}} - \sigma_{h_{f}}} \text{ in the conventional model is replaced by } x
\]

\[
\cos \left( \frac{\pi}{\alpha_{M} - \sigma_{M_{i}}} \left[ \frac{\sigma_{h_{s}} - \sigma_{\text{DF}}}{\sigma_{h_{s}} - \sigma_{h_{f}}} \right] \right) \text{ in the conventional model is replaced by } y
\]

Fig. 2  Comparison of cosine function and logistic sigmoid function curve (left). Different phase
transformation kinetics of SMAs obtained by choosing different values of "a" in the logistic sigmoid
function: stress vs. strain (right)

The use of this new phase transformation kinetics may afford high flexibility. In Fig. 2
(left), curves of cosine function and logistic sigmoid function with different coefficient "a" have
been plotted. In fact, curve similar to cosine function can also be achieved using
logistic sigmoid model by properly picking coefficient "a". Fig. 2 (right) presents an
example stress-strain relationship of a typical SMA. Its martensite starting and finishing
stresses are 600 MPa and 1080 MPa, and reverse phase transformation starting and
finishing stresses are 520 MPa and 40 MPa, respectively. In martensite phase
transformation, the phase transformation rate coefficient \( \alpha \) is fixed to 0.9. To demonstrate
the flexibility afforded by the logistic sigmoid model in reverse phase transformation, we
plotted nine examples from \( a = 0.1 \text{–} 0.9 \). To obtain a better fit to the experimental data, we may choose \( a = 0.1 \) for linear phase transformation kinetics, or \( a = 0.9 \) for gradual phase transformations in the starting and finishing regions. This graph clearly demonstrates the capacity of logistic sigmoid function in obtaining a better fit to the stress-strain curve, and with a limit increase in function complexity.


4.1. Material Level Validation: Stress-strain Fitting Using Logistic Sigmoid Function Model

The experimental part of material validation was conducted by Nitinol Devices & Components, Inc. A uniaxial tension test was performed on a circular SMA wire. By fixing one end of this wire, a forced displacement was applied. As a result, we obtained a stress-strain curve containing a full cycle of loading and unloading. This curve is represented by the green dotted line in Fig. 3.

Auricchio and Taylor\(^{(15)}\) and Toi et al.\(^{(5)}\) attempted to fit this stress-strain relation. However, a good fit of this relation has not been obtained thus far. Owing to the intrinsic problems in the exponential model used by Auricchio and the cosine model used by Toi, it is difficult to fit the martensite phase transformation and reverse phase transformation.

A relative linear stress-strain relationship was observed during martensite phase transformation. This behavior is not easy to fit using the conventional model. When the cosine function model is used, an intermediate phase transformation occurs once the specimen enters its phase transformation region. Therefore, when using conventional models to fit this relatively linear stress-strain relation, the phase transformation region (region between phase transformation starting stress (temperature) and finishing stress (temperature)) must be very small. As an improvement, the logistic sigmoid model is able to describe the slow and gradual phase transformations in the starting and finishing regions of the entire phase transformation process. Conventional cosine functions ignore phase transformations in the starting and finishing regions in describing linear phase transformations, which could be a major cause of fitting error.

Conventional models could not represent any sudden increase in stress in the finishing region of martensite phase transformations. When using the conventional model, the behavior over the entire phase transformation is determined by phase transformation starting stress (or temperature) and phase transformation finishing stress (or temperature), in an isothermal (or isostress) case. A smooth and almost linear stress-strain relation followed by a sudden stress increase can only be represented by a model with greater flexibility such as the logistic sigmoid model.

In the reports by Auricchio and Taylor\(^{(15)}\) as well as by Toi et al.\(^{(5)}\), similar stress-strain curves could be found between martensite phase transformation (loading) and reverse phase transformation (unloading). The similarity is due to an intrinsic property of the cosine and exponential function models. However, experimentally, a different behavior could be observed in reverse phase transformation.

In Fig. 3, for the sake of comparison, fitting with the cosine function model while using the same material parameters as the logistic sigmoid function model is shown as well. This is a good example of how similarity between forward and reverse phase transformations is inevitable when using the cosine function model. Only the logistic sigmoid model could fit the different behaviors of forward and backward phase transformations.

Therefore, a good fit was obtained using the logistic sigmoid model. Details of the material constants are listed Table 1. The phase transformation rate coefficient \( \alpha \) is determined by the transformation rates in each region of each phase transformation. Owing to a sudden stress increase in the finishing part of the martensitic phase transformation, \( a = 0.9 \) is used for martensite phase transformation. For fitting the smooth, large reverse
transformation stress-strain curve, a moderate \( a = 0.4 \) was selected.

This successful fitting of a complex stress-strain relationship validates the use of the logistic sigmoid function model for phase transformation. The flexibility of the logistic sigmoid model endows it with the capacity of representing SMA behavior with different phase transformation rates. Therefore, this model can be used to describe SMA behavior with high accuracy and considerably low error in stress-strain fitting.

![Fig. 3](image)

Table 1. SMA material constants under uniaxial loading

<table>
<thead>
<tr>
<th>Material constants</th>
<th>( E_A = 5.5 \times 10^4 \text{MPa} )</th>
<th>( M_f = -67.5^\circ\text{C} )</th>
<th>( C_M = 8.0\text{MPa/}^\circ\text{C} )</th>
<th>( \varepsilon_L = 0.052 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( E_M = 2.0 \times 10^4 \text{MPa} )</td>
<td>( M_s = -32.5^\circ\text{C} )</td>
<td>( C_A = 8.0\text{MPa/}^\circ\text{C} )</td>
<td>( \alpha )</td>
</tr>
<tr>
<td>( \theta = 0.55\text{MPa/}^\circ\text{C} )</td>
<td>( A_s = -30.7^\circ\text{C} )</td>
<td>( \sigma_{\text{crit.}}^{\text{start}} = 0\text{MPa} )</td>
<td>( \sigma_{\text{crit.}}^{\text{finish}} = 0\text{MPa} )</td>
<td>( \beta = 0.15 )</td>
</tr>
<tr>
<td>( \beta = 0.15 )</td>
<td>( \alpha = 15.7^\circ\text{C} )</td>
<td>( \sigma_{\text{crit.}}^{\text{finish}} = 0\text{MPa} )</td>
<td>( \sigma_{\text{crit.}}^{\text{finish}} = 0\text{MPa} )</td>
<td></td>
</tr>
</tbody>
</table>

4.2. Structural Level Validation: Four-point Bending of an SMA Beam

Structural level validation of the logistic sigmoid function model was conducted by comparing the simulation results with the results of Auricchio’s SMA beam four-point bending experiment. In their bending test, a SMA circular beam (wire) similar to that used in uniaxial testing was tested. The diameter of this wire was 1.49 mm, and its length was 20 mm. Two points which forces are applied on divide this beam into three equally long parts.

A schematic of the experimental setup is shown in Fig. 4. The beam is supported at two ends. At the left end, the beam is supported and fixed in the horizontal direction. At the right end, the beam is simply supported without any other constraint. Room temperature during testing was 20°C. SMA material parameters are listed in Table 1. This experiment records two parameters: load force \( F \) and vertical displacement of the midspan.

For simulation, Euler-Bernoulli cubic beam element and the beam-layered approach were adopted. Beam elements in this simulation are subdivided into ten layers along the vertical direction. The displacement, strain, stress, and martensite phase fraction of each layer are visible in this simulation. Six elements were used for meshing in this simulation. No apparent difference was found in the simulation when the beam was subdivided into 60 elements.

![Fig. 4](image)
The calculated and experimental load-displacement curves are plotted in Fig. 5. Identical material parameters were used in simulations using the logistic sigmoid function and cosine function. Both simulations yield comparatively good results for the loading part, whereby martensite phase transformations occur. However, for the unloading portion, the results obtained were different from the experiment results. Similar mismatches were also reported by Auricchio et al.\(^{15}\) and Toi et al.\(^{5}\). Detailed comparisons between the logistic sigmoid function model and the conventional model (cosine function model) are as follows:

In martensite phase transformation, apparent martensite phase transformation starting stresses are different. However, theoretically, the martensite phase transformation starting stress is 420 MPa for both models. In the load-displacement curve, the stiffness change point of the logistic sigmoid function model is higher than that of the cosine function model. This is because of the gradual phase deformation in the logistic sigmoid model, when \(a = 0.9\). The good fit with the stress-strain relation is represented in the load-displacement curve.

An abrupt increase in stress toward the finishing region of martensite phase transformation was observed. This behavior may also be considered as an increase in stiffness toward the finishing region of martensite phase transformation. This behavior corresponds to an increase in stress in the stress-strain relationship shown in Fig. 3. Because of a good fit in terms of stress increase using the logistic sigmoid function model, stiffness increase was observed in the second part of martensite phase transformation, as shown in Fig. 5. For comparison, no such behavior was observed in the simulation result of the cosine function model. Stiffness decreases over the entire martensite phase transformation.

For reverse phase transformation, better fitting in elastic region was observed when using the logistic sigmoid model. The result obtained using the logistic sigmoid model presents a more identifiable curve at the beginning of reverse phase transformation, followed by a smaller stiffness value during phase transformation. This behavior fits the experimentally determined behavior better than the result obtained using the cosine function model. The reason for these different behaviors could be traced back to their stress-strain relationship, shown in Fig. 3.

According to SMA material constants, finishing critical stress of reverse phase transformation is 34.4 MPa for both two models. However, reverse phase transformation finishing stress in Fig. 3 and load in Fig. 5 are different. In the logistic sigmoid model, \(a = 0.4\) is chosen to represent the big unloading curve. This choice leads to significant difference between the results obtained using these two models. With the cosine function model, reverse phase transformation is completed at almost exactly 34.4 MPa. However, with the logistic sigmoid model, phase transformation is almost complete at 100 MPa. This result is much closer to experimental result than that obtained using the cosine function model.

By using the layered beam approach stress, very detailed strain and martensite phase
distribution along the radial direction could be obtained. The element right beside the left loading point was studied extensively. The stress-strain relation of each layer in this element and its martensite phase fraction change are plotted in Fig. 6.

Fig. 6 Detailed equivalent stress and martensite phase fraction information obtained by using layered approach: stress-strain relationship in each layer (left), martensite phase fraction change (right)

5. Proposed Model: Cyclic Effect Model Dependent on Accumulated Strain

The cyclic effect is one of the most important recent topics in SMAs. Ideally, SMAs completely recover their original shape. However, experiments show different behavior. After every loading cycle, a small residual strain is observed. As the cyclic loading continues, partial recovery of the inelastic strain increases until it reaches saturation. A stable stress-strain loading curve is observed thereafter. This type of cyclic behavior can be observed in several experimental reports including those by Tobushi et al.\(^{(10)}\), Auricchio and Sacco\(^{(12)}\), and Patoor et al.\(^{(9)}\).

Researchers are trying to embed the cyclic effect behavior support into their respective computational models\(^{(1),(11)-(13)}\). Tanaka\(^{(1)}\) considered this effect as unfinished reverse phase transformation, in which the martensite phase remains even after stress reaches the critical finishing stress of reverse phase transformation \(\sigma_{AF}\). Given that the martensite and austenite phases have different Young’s moduli, usually the difference is as large as three times. The absence of a difference in stiffness values in the elastic region at the beginning of each cycle does not support this hypothesis. Lagoudas\(^{(11)}\) assumed simultaneous plastic deformation during phase transformation and introduced a minor hysteresis loops in his model. This hypothesis has a physical meaning because slip at grain boundary, defect, and dislocation does cause plastic deformation even at relatively low stress levels. However, some parameters used in this model cannot be obtained directly. Furthermore, this model is too complicated to be implemented and is very computationally intensive. The cyclic model proposed by Auricchio\(^{(12)}\) uses phase-transformation-induced latent heat as the main reason underlying the cyclic effect. Latent-heat-induced temperature change of specimen could influence phase transformation critical stresses such as reverse transformation start and finish critical stresses \(\sigma_{A_s}, \sigma_{A_f}\) and martensite transformation start and finish critical stresses \(\sigma_{M_s}, \sigma_{M_f}\). A physically reasonable dominant factor is one advantage of this model. Absorption of thermal energy during reverse transformation could lower the stress level requirement for unloading, which agrees with the experimental results. However, release of latent heat during martensite phase transformation leads to increased stress level in loading, which is in contrast with the experimental results.

The cyclic effect model used in this paper is a phenomenological model. Without the complexity of previous models, this model is able to represent cyclic behavior during a cyclic loading process. The model connects accumulated strain to several material parameters such as martensite phase transformation start and finish temperatures \(M_s\) and \(M_f\), reverse phase transformation start and finish temperatures \(A_s\) and \(A_f\), respectively, as well as maximum residual strain \(\varepsilon_{L}\). The accumulated strain \(e\) is expressed as follows:
where $\dot{e}_{eq}$ is von Mises equivalent strain velocity. Different from Lagoudas et al.\textsuperscript{(11),(13),(14)} which picked phase volume fraction as key factor to estimate cyclic effect behavior, we chose equivalent strain in this case to represent cyclic effect both during phase transformation and during elastic loading. By proper choosing coefficients in this model, we can even assign weight to each process (phase transformation and elastic loading). The connection between accumulated strain, $e$, and martensite phase transformation start and finish temperatures $M_s$ and $M_f$, as well as reverse phase transformation start and finish temperatures $A_s$ and $A_f$ are expressed as

$$M_s(e) = M_s(0) + \alpha_{M_s} \left( 1 - \exp \left( -\beta_{M_s} e \right) \right)$$

$$M_f(e) = M_f(0) + \alpha_{M_f} \left( 1 - \exp \left( -\beta_{M_f} e \right) \right)$$

$$A_s(e) = A_s(0) + \alpha_{A_s} \left( 1 - \exp \left( -\beta_{A_s} e \right) \right)$$

$$A_f(e) = A_f(0) + \alpha_{A_f} \left( 1 - \exp \left( -\beta_{A_f} e \right) \right)$$

where $M_s(0)$, $M_f(0)$, $A_s(0)$, and $A_f(0)$ are phase transformation critical temperatures. $\alpha_{M_s}$, $\alpha_{A_s}$ and $\beta_{M_s}$, $\beta_{A_s}$ are experimentally determined material constants. The maximum residual strain is divided into two coefficients, $\varepsilon_L^M$, the maximum residual strain during martensite phase transformation, and $\varepsilon_L^A$, the maximum residual strain during reverse phase transformation. $\varepsilon_L^M$ and $\varepsilon_L^A$ are expressed as follows:

$$\varepsilon_L^M(e) = \varepsilon_L(0) + \alpha_L^M \left( 1 - \exp \left( -\beta_L^M e \right) \right)$$

$$\varepsilon_L^A(e) = \varepsilon_L(0) + \alpha_L^A \left( 1 - \exp \left( -\beta_L^A e \right) \right)$$

where $\varepsilon_L(0)$ is called the initial maximum residual strain. $\alpha_L^M$, $\beta_L^M$, $\alpha_L^A$, and $\beta_L^A$ are material parameters that can be obtained by fitting stress-strain curves from material testing. The cyclic-effect-supported computational model can be derived by substituting equations (21)–(26) in the kinetics of phase transformation.

6. Numerical Implementation of Cyclic Effect Model

6.1. Material level Validation: SMA Wire Under Cyclic Uniaxial Tension

A cyclic uniaxial tension test was conducted by Tobushi\textsuperscript{(10)}. NiTi (Ti: 55.3 wt%) SMA wire produced by Furukawa Electric Co., Ltd. was used in this experiment. Diameter of this wire was 0.75 mm. The SMA specimen was placed in an environment with a constant temperature of 80°C. Loading and unloading at this temperature were repeated 100 times. Strain rate during this process was constant at 2%/min.

In each loading cycle, unloading starts once strain reaches 8% in the loading process. Experimental results from these tests were re-plotted in Fig. 7. To more clearly express this behavior, representative stress-strain relations of cycle Nos. 1, 2, 5, 10, 20, 50, and 100. Three major effects could be observed from the experimental results: (1) Residual strain increases as cyclic loading continues; (2) Critical phase transformation starting and finishing stresses decrease as cyclic loading continues; (3) Changes in material parameters converge as cyclic loading continues.

To represent this cyclic behavior, initial material parameters are selected so that they fit the stress-strain behavior in the first cycle. The material parameters used for validation are listed in Table 2. Through appropriate selection of coefficients in the cyclic effect model, similar behavior could be represented using the simulation program. Cycle Nos. 1, 2, 5, 10, 20, 50, and 100 are plotted in Fig. 7 for the clear expression. Three major cyclic effects were observed in the simulation result.
Fig. 7 Qualitative material-level validation: experimental data from Tobushi (above), simulation data using cyclic effect model (below)

Table 2. SMA material constants under uniaxial cyclic loading

<table>
<thead>
<tr>
<th>Material constants</th>
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<tbody>
<tr>
<td>$E_A = 4.14 \times 10^4$MPa</td>
<td>$M_F = -45^\circ C$</td>
</tr>
<tr>
<td>$E_M = 1.14 \times 10^4$MPa</td>
<td>$M_S = -42^\circ C$</td>
</tr>
<tr>
<td>$\theta = 0.55$MPa/$^\circ C$</td>
<td>$A_F = -10^\circ C$</td>
</tr>
<tr>
<td>$\beta = 0.15$</td>
<td>$A_F = 17^\circ C$</td>
</tr>
<tr>
<td>$\beta_{M_S} = 1.0 \times 10^{-6}$</td>
<td>$\alpha_{AF} = 10$</td>
</tr>
<tr>
<td>$\alpha_M = 10$</td>
<td>$\alpha_{AF} = 10$</td>
</tr>
<tr>
<td>$\alpha_L = 0$</td>
<td>$\beta_{AF} = 1.0 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Thus, the cyclic effect model used in this section expressed qualitatively similar results compared with the experimental results. Error was limited, and could be eliminated by proper determination of coefficients in the cyclic effect model. This brings up the major limitation of this model: too many coefficients need to be determined by fitting experimental stress-strain curves. However, this demerit originates from the flexibility afforded by this model.

6.2. Application: Multi Cycle Loading on SMA-braced Frame Structure

One of SMAs’ major potential applications is in damping devices. SMAs have different loading route during loading and unloading, which leads to hysteresis. Mechanical movement drives phase transformation and is transformed into thermal energy.

As shown in Fig. 8, the SMA-braced structure is a three-story truss-beam mixed structure. The bottom joints of this structure are fixed in all directions. A push over force is applied toward the right at the left end of the top beam. Each floor of this structure is 13 ft in height. Steel columns and beams are represented as solid lines. The six dotted lines in Fig. 8 represent hybrid SMA braces. Their shapes are the same as those in Walter Yang’s simulation, which are in accordance with the standard put forth by the American Society of
Civil Engineers (ASCE).

The detailed structure of this hybrid damping device is presented in the middle panel of Fig. 8. Outer components, which are marked black, are high-stiffness steel components. Grey components in the center are strut components. A strut is a type of high-stiffness steel with low yield stress, and is usually used as a damping material. Red wires around strut components are made of an SMA. The figure on the right is a simplified FEM model of the hybrid damping device. To avoid singularity when using this free joint, multi-element SMA brace in finite element simulation and the static condensation method were adopted.

Two effects are expected from simulation: (1) hysteresis effect, i.e., the effect that absorbs mechanical energy; and (2) re-centering effect, i.e., the ability to recover the original shape after large deformation. The SMA as well as the strut could exhibit hysteresis behavior. Considering the high cost of SMA, it is more cost-efficient to use strut as the major damping material. Given that hysteresis behavior in strut is due to permanent plastic deformation, only the SMA with a superelasticity effect could exhibit the re-centering effect. Therefore, this hybrid device was designed after considering functionality and cost performance. Its multi-cycle behaviors are discussed as follows:

Two simulations are included in this section: the simulation considering cyclic effect and that neglecting the cyclic effect. Material parameters used in the simulation considering the cyclic effect are listed in Table 2. Critical temperatures of phase transformation such as $\gamma_0$, $\gamma_1$, $\alpha_0$, and $\alpha_1$ are considered as functions of accumulated strain $e$.

As can be seen in Fig. 9, both simulations show good agreement with the simulation result by Walter Yang. Furthermore, because the martensite phase has lower stiffness compared with the austenite phase, results obtained using the present model could be considered more reasonable. When considering the cyclic effect, the structure reaches a stable status after only five cycles. For the simulation that does not consider cyclic effect, the stable status was not reached even after 20 cycles. This is an interesting discovery closely related to the damping capacity of the hybrid SMA damping device.

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This behavior is also represented from their phase fraction change shown in Fig. 10. Martensite phase transformation and reverse transformation occur in every loading cycle when the cyclic effect is ignored. Martensite phase transformations in SMA components Nos. 4, 5, and 6 continue in every cycle of push over loading. However, in the simulation considering the cyclic effect, reverse phase transformation never occurs after five cycles. All SMA components inside braces become 100% martensite phase. In other words, they are all elastic material after five cycles, as can be observed in Fig. 11. The hysteresis behavior after five cycles is ascribed to the plastic deformation of strut components. Therefore, simulation using the cyclic effect model is considered to show less damping capacity than that neglecting the cyclic effect.

Fig. 10  Martensite phase fraction change in each SMA component: simulation considering cyclic effect (left), simulation without considering cyclic effect (right). All components are transformed into pure martensite after the first five loading cycles.

Fig. 11  Stress-strain curve under loading in 2nd floor SMA component: simulation with(left) and without(right) considering cyclic effect. SMA component turns elastic after the first four cycles.

7. Summary and Conclusions

This work proposed two major improvements to the conventional SMA computational model. To describe complex and changeful stress-strain relations in different types of SMAs, the logistic sigmoid function was introduced to the kinetics of phase transformation. Without modifications to the successful numerical framework in the conventional model, this improvement could provide greater flexibility. Material- and structural-level validations have proved the model's availability. Better performances in uniaxial loading and four-point bending simulations were observed compared with other models.

The use of SMAs is highly expected as functional material in actuators, sensors, and damping devices. However, change in material properties under cyclic loading is an issue that cannot be ignored. The cyclic effect model dependent on accumulated strain was developed and validated under cyclic uniaxial loading. The numerical example of damping devices in frame structure shows lower damping capacity when considering the cyclic effect.

Based on this validated model, interesting findings have been made under cyclic loading. Further applications are expected as future works.
References


