Finite element simulation of martensitic transition based on thermo-mechanical model

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Abstract
Martensitic phase transition and martensite phase have an important effect on the physical and deformation properties of a material. In this paper, martensitic phase transition in elastic materials is modeled by using thermo-mechanical phenomenological theory. Based on the model proposed, stress-induced martensitic transition in Cu–Zn–Al shape memory alloy is studied by using finite element method. Stress–strain responses of Cu–Zn–Al single crystals under different applied stress rate are simulated by thermo-mechanically coupled calculation. Pseudoelastic deformation, hysteresis of transformation and hardening in stress–strain response are predicted in calculation results. Stress–strain curves determined from numerical simulation have a good agreement with those observed in experiments.

Keywords: Martensitic transition; Finite elements; Thermo-mechanically coupled calculation

1. Introduction
Martensitic transformation is a diffusionless phase transition, in which atoms move cooperatively and often by a shear-like mechanism. When cooling below some critical temperature, parent phase transforms to martensite by shear-like mechanism. When temperature is raised, reverse transformation can take place and martensite can revert to parent phase. The martensitic transformation and the martensite that is formed have a great effect on the physical and deformation properties of material, and determine its possible engineering application [1,2].

There have been research studies on modeling of martensitic transition in elastic material, which could be subdivided into the following a few categories [2]: (1) Ginzburg–Landau or phase field theory; in phase field theory, the formation of a complicated microstructure consisting of austenite and martensitic variants can be described. Besides that, diffuse interfaces between austenite and martensitic variants, as well as between martensitic variants appear as solution of the evolution of equations for the order parameter. (2) Thermo-mechanical phenomenological model; in this model, the volume fraction of martensitic variants is introduced and material with phase transition is treated as composites with varying volume fractions. (3) Elastoplastic models with strain softening applied to the simulation of martensitic transformation; strain softening leads to the formation of domains with localized strains that resemble microstructures observed during phase transitions. In this model, by modeling inhomogeneous deformations, the evolution of martensite is simulated.

In this paper, the evolution of martensite is analyzed by using thermo-mechanical phenomenological theory. The volume fractions of martensitic variants are introduced as internal variables. Constitutive model for martensitic transition is derived from the second law of thermodynamics in the form of Clausius–Duhem inequality. By using this model, stress-induced martensitic transition in Cu–Zn–Al shape memory alloy is analyzed, and stress–strain response at fixed temperature of Cu–Zn–Al single crystals is explored by thermo-mechanically coupled calculation.

2. Model description
2.1. Thermo-mechanical model
In this model, we use the additive decomposition of the total strain, $\varepsilon$, into elastic $\varepsilon_e$ and transformation, $\varepsilon_t$, parts, that is

$$\varepsilon = \varepsilon_e + \varepsilon_t$$ (1)
We consider a representative volume, which is comprised of austenite and martensitic variants. After inducing the volume fraction of each of martensitic variant $\xi_i$, $i = 1, \ldots, m$ as internal variables, the Helmholtz free energy of the volume could be expressed as follows, in which $T$ is the temperature [3]:

$$\psi = \psi(\varepsilon_e, T, \xi)$$

By using the second law of thermodynamics in the form of Clausius–Duhem inequality (Eq. (3)) and taking account of the relation expressed in Eq. (4), we could get

$$\left(\sigma - \frac{\partial \psi}{\partial \varepsilon_e}\right) \cdot \dot{e}_e + \sigma \cdot \dot{e}_i \left(- \frac{\partial \psi}{\partial T} + s\right) T \geq 0$$

$$- \sum_{i=1}^{m} \frac{\partial \psi}{\partial \xi_i} \dot{\xi}_i - \tilde{q} \cdot \nabla \nabla T \geq 0$$

$$\sigma : \dot{e} - (\psi + sT) - q \cdot \nabla T \geq 0$$

$$\psi = \frac{\partial \psi}{\partial \varepsilon_e} \cdot \dot{e}_e + \frac{\partial \psi}{\partial T} \cdot \dot{\xi}_i + \sum_{i=1}^{m} \frac{\partial \psi}{\partial \xi_i} \dot{\xi}_i$$

In Eq. (2), $s$ is the entropy, $\tilde{q}$ the heat flux and $\nabla T$ is the temperature gradient.

As for the transformation strain $\varepsilon_e$, the following equation exists: $\varepsilon_e = \sum_{i=1}^{m} \varepsilon_i \xi_i$, where $\varepsilon_i$ is the Bain transformation strain that transforms the crystal lattice of the austenite into the crystal lattice of martensitic variant $i$. From the methodology of Lemaître and Chaboche (1997) [3], we must have:

$$\sigma = \frac{\partial \psi}{\partial \varepsilon_e}, \quad s = -\frac{\partial \psi}{\partial T}$$

Eq. (2) then yields the dissipation inequality:

$$\Phi = \sum_{i=1}^{m} \left(\sigma : \varepsilon_u - \frac{\partial \psi}{\partial \varepsilon_e}\right) \dot{\xi}_i - q \cdot \nabla T \geq 0$$

$$= \sum_{i=1}^{m} X_i \dot{\xi}_i - \frac{\tilde{g} \cdot \tilde{q}}{T} \geq 0$$

where $\tilde{g} = \nabla T$, $X_i$ is a thermodynamic force conjugate to the internal variable $\dot{\xi}_i$ and its expression is:

$$X_i = \sigma : \varepsilon_u - \frac{\partial \psi}{\partial \xi_i}$$

2.2. Free energy

In this model, the Helmholtz free energy is assumed to be of the form [4–6]:

$$\psi(\varepsilon_e, T, \xi) = \psi^\varepsilon(\varepsilon_e, T, \xi) + \psi^c(T, \xi) + \psi^P(T, \xi)$$

Here:

(1) $\psi^\varepsilon$ is strain energy, is given by

$$\psi^\varepsilon(\varepsilon_e, T, \xi) = \frac{1}{2} \varepsilon_e : E(\xi) : \varepsilon_e - (T - T_a) A(\xi) : E(\xi) : \varepsilon_e$$

where $\xi = \sum_{j=1}^{m} \xi_j$ is the total volume fraction of martensite, $E(\xi)$ symmetric positive-definite elastic tensor at the reference temperature $T_a$ and $A(\xi)$ is the symmetric thermal expansion tensor at $T_a$.

$\psi^P$ is the energy of transformation, and is given by [2]

$$\psi^P(T, \xi) = \frac{\lambda_0}{T_0} (T - T_0) \xi + g_0 \xi_0 + \sum_{i=1}^{m} \sum_{j=1}^{m} g_{ij} \xi_i \xi_j$$

where $T_0$ is the phase equilibrium temperature and $\lambda_0$ is the latent heat of martensitic transition at $T_0$. Material parameters $g_0$ and $g_{ij}$ characterize the interactions between austenite and martensite and that between martensitic variants, and $g_0 > 0$, $g_{ij} > 0$ and $g_{ij} = 0$. $\xi_0$ is the volume fraction of austenite and $\xi_0 = 1 - \xi = 1 - \sum_{i=1}^{m} \xi_i$. Because the interface between two martensitic variants is an invariant plane, internal stresses and interface energy generated by such variants are all small. Therefore, the contribution to free energy due to the interaction between martensitic variants could be neglected and in Eq. (10) we could assume $g_{ij} = 0$.

(3) $\psi^c$ is the thermal energy, and is given by

$$\psi^c(T, \xi) = c(T - T_a) - cT \ln \left(\frac{T}{T_a}\right)$$

where $c > 0$ is specific heat.

In this paper, we assume that the elastic and thermal expansion properties of the austenite and the martensite are identical and isotropic [2,6], hence Eq. (7) could be reduced to as follows:

$$\psi^c(\varepsilon_e, T, \xi) = \frac{1}{2} \varepsilon_e : E : \varepsilon_e - (T - T_a) A : E : \varepsilon_e$$

2.3. Constitutive equation for stress

From $\sigma = \partial \psi/\partial \varepsilon_e$, and combined Eqs. (8), (10–12), the constitutive equation for stress is derived as follows:

$$\sigma = \frac{\partial \psi}{\partial \varepsilon_e} = E[\varepsilon_e - A(T - T_a)]$$

2.4. Model for phase transition

From Eqs. (6) and (7), the dissipation due to phase transition could be expressed as: $\Phi_i = \sum_{j=1}^{m} X_i \dot{\xi}_j$, in which thermodynamic force $X_i$ conjugate to the internal variable $\xi_i$ is described in Eq. (7).

Inserting Eqs. (8), (10–12) into Eq. (7), we obtain

$$X_i = \sigma : \varepsilon_u - \frac{\lambda_0}{T_0} (T - T_0) - g_0 (1 - 2 \xi)$$

which is the driving force for changes in $\xi_i$. Define $\dot{\xi}_ij$ as the rate of the volume fraction $\xi_i$ due to a transition from phase $j$ to $i$, we have the relations [2]

$$\dot{\xi}_i = \sum_{j=0}^{m} \dot{\xi}_ij, \quad \dot{\xi}_ij = -\dot{\xi}_ji, \quad \dot{\xi}_{ii} = 0$$
Then,
\[
\Phi_1 = \sum_{i=1}^{m} X_{i0} \xi_{0i} + \sum_{i=1}^{m} \sum_{j=1}^{m-1} X_{ij} \xi_{ij}
\]  
(15)

where \(X_{i0} = X_i\) is the driving force for the austenite transform to the martensitic variant \(i\) (if \(X_{i0} > 0\)) or for the martensitic variant \(i\) transform to austenite (if \(X_{i0} < 0\)), and

\[X_{ij} = X_i - X_j = \sigma : (\varepsilon_{\text{ij}} - \varepsilon_{\text{ti}})\]  
(16)

is the driving force for the \(j\)th martensitic variant transform to the \(i\)th one (if \(X_{ij} > 0\)) or for the \(i\)th martensitic variant transform to \(j\)th one (if \(X_{ij} < 0\)).

In order to derive the evolution equation for volume fractions, we assume the function \(\Phi_1\) is a positive definitive quadratic form of its variable \(X_{ij}\) [3]. Then we obtain linear evolution equations as follows:

\[\dot{\xi}_{ij} = \lambda_{ij} X_{ij}\]  
(17)

where \(\lambda_{ij}\) are kinetic coefficients and can be determined by comparing calculations and experiments for some non-stationary process. Relations: \(\lambda_{ij} = \lambda_{ji}\) are also obtained, that is, the Onsager reciprocity relations are fulfilled.

In the model, a dissipative threshold is introduced for the driving forces [2,7]. So, only when the driving force exceeds a critical value, the phase transition can take place. Taking account of the relation between heat flux and temperature variations and phase transition are taken account of. Relations:

\[\lambda_{ij} x_{ij} \sigma \] 

is the driving force for the phase transition criterion and kinetic equation for \(\dot{\xi}_{ij}\) as follows:

\[|X_{ij}| > k_{ij} \Rightarrow \dot{\xi}_{ij} = \lambda_{ij} \text{sign}(X_{ij})(|X_{ij}| - k_{ij})\]  
(18)

\[|X_{ij}| \leq k_{ij} \Rightarrow \dot{\xi}_{ij} = 0\]

where \(k_{ij}\) is the given dissipative threshold for \(X_{ij}\).

2.5. Heat equation

From the first law of thermodynamics, we have the relation

\[\dot{e} = \sigma : \dot{\varepsilon} + r - \text{div} \tilde{q}\]  
(19)

where \(e\) is the inner energy and \(r\) is the heat supply. At the same time, from \(\varepsilon = \psi + T\dot{s}\), we obtain \(\dot{e} = \dot{\psi} + T \dot{s} + T\dot{s}\). Inserting this relation and Eq. (4) into Eq. (19) results in

\[\sigma : \dot{\varepsilon} + \sum_{i=1}^{m} \frac{\partial \psi}{\partial \xi_i} \dot{\xi}_i + T \dot{s} = \sigma : \dot{\varepsilon} + r - \text{div} \tilde{q}\]  
(20)

From the second equation in Eq. (6) and the expression for free energy (Eq. (8)), the following equation is derived:

\[s = A \cdot E : \varepsilon_e - \frac{\lambda_0}{T_0} \xi + c \ln \left( \frac{T}{T_a} \right)\]  
(21)

Inserting this equation and Eq. (1) into Eq. (20), and taking account of the relation between heat flux and temperature expressed in Fourier’s law: \(\text{div} \tilde{q} = -k \Delta T\), we obtain the heat equation as follows:

\[-\sigma : \sum_{i=1}^{m} \varepsilon_{\text{ui}} \dot{\xi}_i + \sum_{i=1}^{m} \frac{\partial \psi}{\partial \xi_i} \dot{\xi}_i + cT - T_0 \frac{\lambda_0}{T_0} \xi = r + k \Delta T\]  
(22)

where \(k\) is the coefficient of thermal conductivity. Combined with Eq. (7), the heat equation reduces to:

\[cT - k \Delta T = \sum_{i=1}^{m} X_i \dot{\xi}_i + T_0 \frac{\lambda_0}{T_0} \dot{\xi}_t - r\]  
(23)

3. Application to single crystal of Cu–Zn–Al shape memory alloy

In shape memory alloy, martensitic transition could be induced by the application of stress. Stress-induced martensitic transition that takes place at a temperature above the austenite finish temperature \(T_f\) always leads to a pseudoelastic response of shape memory material. Studies on mechanical behavior of single crystals of shape memory alloy not only make a better understanding of the characteristic of martensitic transition, but also give much fundamental information on the mechanism of mechanical behavior of polycrystalline shape memory material.

There have been research studies on the mechanical behavior of single crystal, such as the studies by Otsuka et al. on Cu–Al–Ni single crystals and Mueller and Xu on Cu–19.0 Zn–7.0Al (wt%) single crystals [8,9]. The investigations by Rodriguez and Brown on Cu–Al–Ni found that there are apparent temperature variations in specimens (about 17°C under nearly adiabatic condition) during the tests because of the exothermic and endothermic nature of austenite-to-martensite and martensite-to-austenite transformations [10]. The temperature variations also result in apparent hardening in stress–strain curve, as observed by Lexcellent et al. [11].

In this section, Cu–25.63Zn–4.2Al (wt%) shape memory alloy is studied by using the thermo-mechanically coupled model. By using the finite element method, the stress-induced martensitic transitions in single crystals are explored and the mechanical behaviors under cycling load at fixed temperature are simulated. In calculations, the interactions between temperature variations and phase transition are taken account of.

3.1. Material parameters in thermo-mechanical model

According to experimental results, only one martensitic variant can be obtained from single crystals if an axial tensile stress is applied to the sample along an arbitrary axis other than symmetry axis. Moreover, for a single crystal under tensile and compression loading, the habit planes of martensitic variants transformed are different [11]. Therefore, the simulation of phase transition under tensile and compression loading are performed respectively, and the value of \(m\), which denotes the numbers of martensitic variants in the model, is equal to one: \(m = 1\). Then the model for phase transition reduces to as follows:

\[X = \sigma : \varepsilon_t - \frac{\lambda_0}{T_0} (T - T_0) - g_0(1 - 2\xi)\]  
(24)
Table 1
Material constant of samples A and B

<table>
<thead>
<tr>
<th>Sample</th>
<th>E (MPa)</th>
<th>ρ (kg/m³)</th>
<th>c (J/kg·°C)</th>
<th>ε̇ (tension)</th>
<th>ε̇ (compression)</th>
<th>Mₛ (°C)</th>
<th>Aₛ (°C)</th>
<th>g₀ (MJ/m³)</th>
<th>λ₀/T₀ (MJ/K m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>20,000</td>
<td>8228</td>
<td>393</td>
<td>0.09455</td>
<td>−0.076</td>
<td>30.0</td>
<td>28.5</td>
<td>0.181</td>
<td>0.178</td>
</tr>
<tr>
<td>B</td>
<td>50,814</td>
<td>8228</td>
<td>393</td>
<td>0.06652</td>
<td>−0.047</td>
<td>20.0</td>
<td>16.0</td>
<td>0.083</td>
<td>0.185</td>
</tr>
</tbody>
</table>

In calculations, we take coefficient of thermal expansion α = 25 × 10⁻⁶ K⁻¹ [12], and other material parameters for different single crystalline samples are listed in Table 1 [11].

According to the experimental results, the kinetic coefficient λ in Eq. (25) is determined as: λ = 0.0005. At the same time, for simplicity, we take k₀ = 0 in Eq. (25).

### 3.2. FEM simulation results

Because only one martensitic variant can be obtained in single crystals, two-dimensional model is used in calculation to diminish calculation time, which is rectangle with dimension of 25 mm × 5 mm. In calculation, the constant stress rates in experiment are realized by displacement boundary conditions: displacements in x and y direction of left side of model are restrained, and right side move with a constant velocity in x positive direction (tensile loading) or in x negative direction (compressive loading), and then move with the same velocity in reversed direction to realize unloading after displacement reach its maximum value. As for thermal boundary condition, we take ambient temperature and initial temperature of specimen as 62°C according to experiment. Moreover, because ends of specimen are gripped during experimental process and convection condition of them are worse, for simplicity, we only apply convection conditions on two sides of model in y direction in calculation and the convection coefficient taken is k = 160.0 W/K m² [11].

All the FEM calculations are carried out by using finite element computer program FEPG. This software can automatically
generate complete finite element source code based on model equations.

In order to examine the effect of heat generation and conduction, calculations are carried out for three different applied stress rates (respectively, are \( \dot{\sigma} = 0.1, 1.0 \) and \( 2.0 \) MPa/s).

The tensile stress–strain curve of sample A calculated is shown in Fig. 1. In Fig. 2, evolution of the contours of the martensite volume fraction at representative instances (a–l) keyed to Fig. 1, during the forward and reverse transformations for the test at the lowest stress rate is shown. Besides that, Fig. 3 shows contours of the temperature at the same representative instances during the forward and reverse transformations. The relation between the temperature of center point of sample A and strains under different applied stress rates is shown in Fig. 4. The compressive stress–strain curve of sample A, the tensile and compressive stress–strain curves of sample B calculated are, respectively, shown in Figs. 5–7.
4. Discussion

From the calculated results, we could find that the evolution of the relation between stress and strain under loading could be divided into three stages. When loading, we could observe stress increase with strain and the relation between them satisfies Hook's law. This stage is linked to elastic deformation of austenite; the second stage: when stress reaches a critical value (threshold stress of martensite appearance: $\sigma_{\text{th,AM}}$), austenite-to-martensite transition takes place and strain increase under almost constant stress with a small hardening, that is, deformation exhibits pseudoelastic characteristics; after martensitic transition is finished, stress increase with strain and this stage is linked to elastic deformation of martensite.

As for the evolution of the relation between stress and strain under unloading, similar analysis could be performed: at first, elastic deformation of martensite takes place, when stress reaches a critical value (threshold stress of austenite appearance: $\sigma_{\text{th,MA}}$), martensite transform to austenite, and deformation takes place under almost constant stress due to the transition. After martensite completely disappeared, elastic deformation of austenite is present.

By comparing threshold stresses of martensite appearance and austenite appearance, it could be found that $|\sigma_{\text{th,MA}}| < |\sigma_{\text{th,AM}}|$, that is, phase transition has hysteresis. By comparing the stress–strain curves calculated under different stress rates, it could be found that the width of hysteresis loop is increase with the stress rate.

The calculated results also show that when stress rate is small (0.1 MPa/s), the hardening response of stress–strain curve is also very small, and the hardening increases with the applied stress rate. Because we set $k = 0$ and $A = \text{constant}$ (see Eqs. (24) and (25)) in our calculations, the hardening response is entirely due to thermal effects associated with the phase transformations. When the applied stress rate is small, there is enough time for heat transfer between sample and its surroundings, so the temperature variation of sample is also small (see Fig. 4). Therefore, strain hardening during phase transition is very small. However, when applied stress rate is high, because there is not enough time for heat transfer between sample and its surroundings, the temperature variation of sample is high (see Fig. 4). Therefore, there is an apparent hardening in stress–strain curve. After compared with the experimental results by Lexcellent et al., the stress–strain curves calculated have a good agreement with them.

5. Conclusion

In this paper, martensitic transition in elastic materials is modeled by using thermo-mechanical theory. Based on the model proposed, stress-induced martensitic transition in Cu–Zn–Al single crystals is studied by using finite element method. The stress–strain responses of single crystals under different applied stress rates are simulated by thermo-mechanically coupled calculation.

(1) Due to stress-induced martensitic transition, pseudoelastic stress–strain responses are obtained by calculation. Moreover, hysteresis of phase transition is predicted and the width of hysteresis loop increases with the applied stress rate.

(2) Because of temperature variations caused by the exothermic and endothermic nature of martensitic forward and reverse transformations, stress–strain curve show a hardening response and the hardening increased with the applied stress rate.

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References