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Finite element calculation of load-biased thermal cycling of shape memory alloy

Sung Young [a], Tae-Hyun Nam [b,*]

[a] School of Mechanical Engineering, Korea University of Technology and Education, Chonan, South Korea
[b] School of Materials Science and Engineering & ERI, Gyeongsang National University, 900 Gazwadong, Jinju, Gyeongnam 660-701, South Korea

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ABSTRACT

Inhomogeneous deformation is one of the essential characters of shape memory alloy. Specimen is composed of many variants which have different strain. There exist a phase interface between two different phases and its mobility will depend on several factors such as curvature and orientation of the interface. The shape memory alloys exhibit hysteresis and one of the main reasons to cause hysteretic behavior is thought to be the internal inhomogeneity. It is thought that the phase interfaces display irregularities in the motion and the resultant state is metastable one which requires a very long relaxation time. In this work, spatially inhomogeneous frictional force to the volume change of the variants is assumed to account for the irregular behavior of the phase transformation. Its effect on the production of the macroscopic strain of a shape memory alloy is investigated using finite element calculation. Load-biased thermal cycling of a shape memory alloy is considered. The numerical result is compared with experimental data of Ti-44.5Ni-5Cu-0.5V (at.%) alloy. A better agreement is obtained for the experimental data when the inhomogeneous friction is assumed.

1. Introduction

The shape memory alloys exhibit interesting thermomechanical behavior due to the solid–solid diffusionless phase transformation between the parent austenite phase and the product martensite phase. This transformation is called martensitic. The martensitic phase transformations are characterized by the fact that the process is athermal, displacive, diffusionless, exhibiting hysteresis, and autocatalytic [1]. In the microscopic point of view, it is thought that there exist inhomogeneities within the solid. Various martensitic variants are observed under a microscope. It is these inhomogeneities which hinder variant rearrangement under external loading. The potential energy barriers are so large that the system remains in a metastable state. The hysteretic character of shape memory alloy is thought to be a kind of non-quasistatic process and the approach to equilibrium proceeds at an extremely slow rate [2].

In the domain wall approach of magnetic materials, the motion of the wall is not smooth but it sticks due to an interaction energy with impurities and imperfections and snaps past if the external field is raised [3]. We think that shape memory materials will show similar phenomena. The mobility of phase interface will be different depending on the neighboring variants and elastic strain energy will develop due to the variant interaction during the martensitic phase transformation. The growth of the variants will exhibit irregular behavior [4].

One of the important phenomena associated with the motion of the phase interface is friction. Energy loss is involved in the stick-slip motion of the interface and the energy will be dissipated by emission of heat or sound. Dislocations will be generated along the trail of the interface. The frictional force is linked to the mobility of the interface.

In this work, the effect of friction on the mechanical behavior of the shape memory alloy was investigated. To account for the irregular nature of the phase transformation, a spatially inhomogeneous frictional field was assumed in the material. Effect of the frictional energy is included in the expression of the potential energy. Continuum finite element calculation was conducted for load-biased thermal cycling of a shape memory alloy. Time histories of the volume fraction of the variants were compared for the case with inhomogeneous and homogenous frictions. It was shown that better agreement with the experimental data can be obtained by assuming inhomogeneous friction field.

* Corresponding author. Tel.: +82 55 7721665; fax: +82 55 7722635.
E-mail addresses: ysy@kut.ac.kr (S. Young), tahynam@gnu.ac.kr (T.-H. Nam).

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2. Modeling of friction

Frictional energy loss occurs with an irreversible interface motion. In the martensitic phase transformation, phase interface exists between two different variants or phases, and the friction acting against the interface motion will depend on several factors. The origins of the friction are the increase of dislocation density at the trail behind the propagating interface or the stick-slip motion of the interface.

Young and Nam [5] derived an expression of the potential energy of each variant incorporating the effect of the frictional energy loss. If the mechanical and thermal equilibriums are achieved, according to the second law of thermodynamics, the lost work is nonnegative for the increment of the volume fraction $\Delta\eta_a$ at each material point.

$$\overline{T}\Delta s_{\mathrm{total}} = -\Delta g_{\mathrm{total}} - \sum_{a=1}^{M}\Delta\eta_a(u_a - \overline{T}s_a - \overline{\mathbf{P}}:\mathbf{F}^e\mathbf{F}_a\mathbf{F}^{-1}) = -\sum_{a=0}^{M} = \Delta\eta_a g_a \geq 0 \quad (1)$$

The subscript a denotes the index of the variant. $\overline{T}\Delta s_{total}$ is equal to the lost work which is dissipated by friction and rate-dependent effects, $\overline{T}\Delta s_{\mathrm{total}} = \overline{T}\Delta s_{\mathrm{fric}} + \overline{T}\Delta s_{\mathrm{rate}}$. Each term of the right hand side is assumed to be nonnegative.

To get an expression for the energy loss by the friction, a planar interface is considered. If the interface area between phases a and b is A_{ab}, and the frictional force per unit area is f_{ab}, and the distance the interface moves is Δx_a in the outward perpendicular direction to the variant a at the interface, then the dissipated energy will be

$$\begin{aligned}\overline{T}\Delta s_{\mathrm{fric}} &= \frac{1}{2V}\sum_{a,b=0}^{M} f_{ab}\left[\Delta V_a^{ab}\right]A_{ab}\Delta x_a \\ &= \frac{1}{2V}\sum_{a,b=0}^{M} f_{ab}\left[\Delta V_a^{ab}\right]\Delta V_a^{ab} \\ &= \frac{1}{2}\sum_{a,b=0}^{M} f_{ab}|\Delta\eta_a^{ab}|\end{aligned} \quad (2)$$

where $[g]$ equals to +1 or -1 depending on the sign of the variable, f_{ab} is not negative and $f_{ab} = f_{ba}$ and $f_{aa} = 0$, and each term in the summation is counted twice so that the total is divided by 2. Only the frictional force associated with the volume change of the variant is considered in this study. ΔV_a^{ab} denotes the volume increment of the variant a by the transformation between a and b variants. Expanding the summation,

$$\begin{aligned}\overline{T}\Delta s_{fric} &= \frac{1}{2}(f_{01}|\Delta\eta_0^{01}| + f_{02}|\Delta\eta_0^{02}| + \cdots + f_{0M}|\Delta\eta_0^{0M}|) \\ &+ \frac{1}{2}(f_{10}|\Delta\eta_1^{10}| + f_{12}|\Delta\eta_1^{12}| + \cdots + f_{1M}|\Delta\eta_1^{1M}|) \\ &+ \cdots\end{aligned} \quad (3)$$

If the inequality of the second law

$$\overline{T}\Delta s_{\mathrm{rate}} = -\Delta g_{\mathrm{total}} - \overline{T}\Delta s_{fric} \geq 0 \quad (4)$$

holds for each pairwise transformation, the following inequality can be written for any variant pair ab

$$-\Delta\eta_a^{ab}g_a - \Delta\eta_b^{ab}g_b - \left(\frac{1}{2}f_{ab}|\Delta\eta_a^{ab}| + \frac{1}{2}f_{ab}|\Delta\eta_b^{ab}|\right) \geq 0 \quad (5)$$

or

$$-\Delta\eta_a^{ab}\left(g_a + \frac{1}{2}f_{ab}\left[\Delta\eta_a^{ab}\right]\right) - \Delta\eta_b^{ab}\left(g_b + \frac{1}{2}f_{ab}\left[\Delta\eta_b^{ab}\right]\right) \geq 0 \quad (6)$$

Regarding the term $(g_a + 1/2(f_{ab}[\Delta\eta_a^{ab}]))$ as an effective potential energy, $\overline{g}_a$, the second law imposes a restriction that the sum of the products of the potential energy $\overline{g}_a$ and the increment of the volume fraction should be nonpositive for each transformation pair. Friction has a detrimental effect to the phase transformation, since the value of the potential energy increases by the friction.

As a special case, if the frictional energy loss can be written by

$$\overline{T}\Delta s_{fric} = f_0|\Delta\eta_0| + f_1|\Delta\eta_1| + \cdots + f_M|\Delta\eta_M| \quad (7)$$

where f_a is nonnegative, the following inequality can be written.

$$\begin{aligned}\overline{T}\Delta s_{\mathrm{rate}} &= -\sum_{a=0}^{M}\Delta\eta_a g_a - (f_0|\Delta\eta_0| + f_1|\Delta\eta_1| + \cdots + f_M|\Delta\eta_M|) \\ &= -\Delta\eta_0(g_0 + f_0[\Delta\eta_0]) - \Delta\eta_1(g_1 + f_1[\Delta\eta_1]) \\ &- \cdots - \Delta\eta_M(g_M + f_M[\Delta\eta_M]) \geq 0\end{aligned} \quad (8)$$

Then the effective potential energy will be $\overline{g}_a = (g_a + f_a[\Delta\eta_a])$

For the transformation from variant a to b, the following exponential relation is assumed using the effective potential energy difference.

$$\dot{\eta}_b^{ab} = \eta_a a_{ab} e^{-B(\overline{g}_b - \overline{g}_a)} - \eta_b a_{ba} e^{-B(\overline{g}_a - \overline{g}_b)} \quad (9)$$

The first term is nucleation of phase $b$from a, and the second term is the reverse one. Since it is a transformation between two variants, we always have $\dot{\eta}_a^{ab} = -\dot{\eta}_b^{ab}$ so that the sum of the volumes of a and b variants will be conserved. a_{ab} is a reference rate constant, which is assumed the same as a_{ba}. Driving force for the transformation is the difference of the effective potential energies, $\overline{g}_a - \overline{g}_b$. The parameter B is a rate sensitivity parameter; if the value is large, small driving force will be enough to cause rapid transformation, and the inequality (6) will be approximately satisfied. Since the signs of $\Delta\eta_a^{ab}$ and $\Delta\eta_b^{ab}$ are opposite, the driving force in (9) will be

$$\begin{aligned}\overline{g}_a - \overline{g}_b &= \left(g_a + \frac{1}{2}f_{ab}\left[\Delta\eta_a^{ab}\right]\right) - \left(g_b + \frac{1}{2}f_{ab}\left[\Delta\eta_b^{ab}\right]\right) \\ &= g_a - g_b + f_{ab}\left[\Delta\eta_a^{ab}\right]\end{aligned} \quad (10)$$

Substituting (10) into (9)

$$\begin{aligned}\dot{\eta}_b^{ab} &= \eta_a a_{ab} e^{-B(g_b - g_a + f_{ab}[\Delta\eta_b^{ab}])} - \eta_b a_{ab} e^{-B(g_a - g_b + f_{ab}[\Delta\eta_a^{ab}])} \\ &= \eta_a a_{ab} e^{-f_{ab}B} e^{-B(g_b - g_a)} - \eta_b a_{ab} e^{-f_{ab}B} e^{-B(g_a - g_b)} \\ &= \eta_a \overline{a}_{ab} e^{-B(g_b - g_a)} - \eta_b \overline{a}_{ab} e^{-B(g_a - g_b)}\end{aligned} \quad (11)$$

Since the friction f_{ab} is positive, the rate constant a_{ab} will be reduced to a new value $\overline{a}_{ab}$ by the factor of $e^{-f_{ab}B}$ due to the friction. The overall transformation rate for variant a will be given by the sum of all combinations.

$$\dot{\eta}_a = \sum_{b=0}^{M}\dot{\eta}_a^{ab} \quad (12)$$

3. Numerical results and discussion

To evaluate the effect of friction first, the constitutive behavior was examined by using a simple numerical example. Transformation between austenite and single martensitic variant is considered, and an axial stress is applied to the material at the temperature 350 K above the equilibrium temperature 320 K. The tensile transformation strain of the martensite is 0.1, and the other material parameters are $B = 4 \times 10^{-5}$ and $a_{01} = 2 \times 10^{-4}$ where the subscript 0 and 1 denote austenite and martensite, respectively. Two cases of friction,$f = 0$ MPa and $f = 0.633$MPa, are considered. Fig. 1 contains comparison of the calculation results. The width of the hysteresis becomes larger with the higher friction; the stress for the forward transformation is larger, and the threshold stress for the reverse transformation is lower.

Next, as a more general problem, load-biased thermal cycling of Ti-44.5Ni-5Cu-0.5V (at.%) is considered. An experimental result is shown in Fig. 2. B2–B19' transformation occurred during the tests