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A multi-dimensional constitutive model for shape memory alloys

C. LIANG and C.A. ROGERS

Center for Intelligent Material Systems and Structures, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061-0261, U.S.A.

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Abstract. This paper presents a multi-dimensional thermomechanical constitutive model for shape memory alloys (SMAs). This constitutive relation is based upon a combination of both micromechanics and macromechanics. The martensite fraction is introduced as a variable in this model to reflect the martensitic transformation that determines the unique characteristics of shape memory alloys. This constitutive relation can be used to study the complex behavior associated with 2-D and 3-D SMA structures. A simple example using this constitutive model is also presented, which reveals a new and interesting phenomenon of 3-D SMA structures.

Introduction

Based upon the one-dimensional thermomechanical constitutive relation developed by Liang and Rogers [1], a multi-dimensional thermomechanical constitutive model for shape memory alloys is further developed and presented in this paper. Unlike the constitutive model developed by Bondaryev and Wayman [2], this multi-dimensional constitutive model uses a newly introduced internal state variable, the martensite fraction, instead of using the traditional plastic flow theory. This thermomechanical constitutive relation reflects the fundamental characteristics of shape memory alloys, i.e., the phase transformation involved in shape memory effect.

Needless to say, the first concern when developing a multi-dimensional model is whether its one-dimensional version is correct. Previous verification and discussion [3] show that the one-dimensional constitutive model can provide a quantitative prediction and description of the mechanical behavior of shape memory alloys. Based on the one-dimensional constitutive relations for SMAs, design methods for SMA actuators [4] and SMA springs [5] have been developed. Even though most current applications of SMAs as actuators are in wire (or spring) form, a few 3-D SMA components do exist. A good example of these is the SMA pipe coupler [6]. The reason that there are fewer applications of 3-D SMA components is that no practical multi-dimensional constitutive model for SMAs existed until Bondaryev and Wayman [2]. However, Bondaryev and Wayman's multi-dimensional model is only an extension of plasticity theory. Graesser [7] developed a multi-dimensional model for SMAs based on a viscoplastic model. This model is capable of describing the nonlinear and hysteretic behavior of SMAs but fails to include temperature as a primary variable (it assumes non-change uniform temperature distribution), which undoubtedly limits its applications.

Generalized multi-dimensional constitutive relations of SMA

Considering a three-dimensional body, the original coordinate is denoted by $\mathbf{X}$, and the

current deformed configuration is denoted by $\mathbf{x}$. $\mathbf{X}$ stands for $(X_1\ X_2\ X_3)^T$ where the subscripts '1', '2', and '3' represent the X, Y, and Z coordinate axes and the superscript 'T' represents the transpose of matrix. $\mathbf{x}$ can also be written as $(x_1\ x_2\ x_3)^T$. The deformation gradient, $\mathbf{f}$, is given as

$$\mathbf{f} = (\nabla \mathbf{x}^T)^T , \tag{1}$$

where

$$\nabla = \begin{bmatrix} \partial/\partial X_1 \\ \partial/\partial X_2 \\ \partial/\partial X_3 \end{bmatrix} . \tag{2}$$

The Green–Lagrange strain is defined as

$$\bar{\boldsymbol{\varepsilon}} = \frac{\mathbf{f}^T\mathbf{f} - \mathbf{I}}{2} , \tag{3}$$

where $\mathbf{I}$ is a unit tensor.

The 2nd Piola–Kirchhoff (P–K) stress tensor can be derived as

$$\bar{\boldsymbol{\sigma}} = \frac{\rho_0}{\rho} \mathbf{f}^{-1}\boldsymbol{\sigma}(\mathbf{f}^{-1})^T , \tag{4}$$

where ρ_0 is the density in the original configuration and ρ is the density in the current configuration. $\boldsymbol{\sigma}$ is the Cauchy stress tensor. The reasons for using the Green–Lagrange (G–L) strain and 2nd Piola–Kirchhoff stress are: (1) they are invariant under rigid body motion; (2) they are expressed in reference to the original configuration; therefore, it does not matter whether the deformation can significantly change the geometry of the 3-D body; (3) they are energetical conjugates, and (4) the deformation of SMAs can be as high as 8% (maximum recoverable strain), the Green–Lagrange strain can correctly describe the finite deformation of SMA.

The first and the second laws of thermodynamics can be written in the current configuration as

$$\begin{cases} \rho\dot{U} - \mathrm{tr}(\boldsymbol{\sigma}\mathbf{v}) + \mathrm{div}\,\mathbf{q}_{\mathrm{sur}} - \rho q = 0 \\ \rho\dot{S} - \rho q^{-1}T + T^{-1}\,\mathrm{div}\,\mathbf{q}_{\mathrm{sur}} - T^{-2}\mathbf{q}_{\mathrm{sur}} \cdot \mathrm{grad}\,T \geqslant 0 , \end{cases} \tag{5}$$

where tr( ) denotes the trace operator, and 'div' and 'grad' are the divergence and gradient operator in the current configuration, respectively. T is the temperature, S the entropy, q the heat generated by internal heat sources, $\mathbf{q}_{\mathrm{sur}}$ the heat transferred from surroundings, and U the internal energy. $\mathbf{v}$ is the deformation velocity tensor defined by $\dot{\mathbf{f}}\mathbf{f}^{-1}$. Rewriting the first and the second law of thermodynamics in the original configuration yields:

$$\begin{cases} \rho_0\dot{U} - \mathrm{tr}(\bar{\boldsymbol{\sigma}}\dot{\bar{\boldsymbol{\varepsilon}}}) + \mathrm{Div}\,\mathbf{Q} - \rho_0 q = 0 \\ \rho_0\dot{S} - \rho_0 q^{-1}T + T^{-1}\,\mathbf{Q} - T^{-2}\,\mathbf{Q} \cdot \mathrm{Grad}\,T \geqslant 0 , \end{cases} \tag{6}$$

where 'Div' and 'Grad' are the divergence and gradient operator in the original reference, respectively. **Q** is defined as

$$\mathbf{Q} = \frac{\rho_0}{\rho} \mathbf{f}^{-1} \cdot \mathbf{q}_{\text{sur}} \,. \tag{7}$$

The general state variable, Λ, is defined as

$$\Lambda \equiv (\bar{\varepsilon}_{ij},\, T,\, \xi) \quad \begin{cases} i = 1, 2, 3 \\ j = 1, 2, 3 \,, \end{cases} \tag{8}$$

where ξ is the martensite volume fraction, an internal variable introduced to describe the phase transformation involved in the mechanical behavior of SMAs. Martensitic transformations are governed by the Helmholtz free energy. According to Müller [8], thermodynamics behind the phase transformation can be described as: 'the energy, E, tries to minimize by pulling all particles into the depths of the potential wells, and the entropy attempts to maximize by distributing the particles evenly over the available range of shear lengths. In this competition, it is the free energy,

$$\Phi(\Lambda) = U - ST \,, \tag{9}$$

that achieves a minimum'. The free energy is the summation of the non-chemical energy, such as the strain energy and the thermal energy, and the chemical free energy. In other words, it is the overall strain energy that affects the phase transformation rather than the individual strain and stress components. From the experimental study conducted by Kajeshita et al. [9], the hydrostatic pressure has a small influence on the phase transformations. The deformation, along with phase transformation, is mainly of a shear nature. This point is also supported by the actual physics behind martensitic phase transformation, i.e., the deformation associated with both the martensitic and reverse transformations is shear detwining and twining. The strain energy that affects the phase transformation should be the distortion energy. The transformation function or criteria for an SMA component subjected to multi-dimensional forces derived by Bondaryev and Wayman [2] also indicates that the phase transformation begins when the distortion strain energy is greater than a certain chemical free energy.

Based on finite strain J_2 deformation theory [10], the distortion strain energy, U_d, for finite strain may be expressed as

$$U_d = \frac{1}{2G} J_2 = \frac{1}{2} \bar{\sigma}_{\text{eq}} \bar{\varepsilon}_{\text{eq}} \,, \tag{10}$$

where G is the shear modulus, J_2 the second invariant of stress deviator tensor given in terms of 2nd Piola–Kirchhoff stress, $\bar{\sigma}_{\text{eq}}$ the equivalent 2nd Piola–Kirchhoff stress, and $\bar{\varepsilon}_{\text{eq}}$ the equivalent Green–Lagrange strain. It is necessary to assume that SMA is incompressible. Therefore, the general state variable may be expressed in terms of the equivalent G–L strain as

$$\Lambda \equiv (\bar{\varepsilon}_{\text{eq}},\, T,\, \xi) \,. \tag{11}$$

The equivalent G–L strain, $\bar{\varepsilon}_{\text{eq}}$, and equivalent P–K stress, $\bar{\sigma}_{\text{eq}}$, are defined by

$$\bar{\varepsilon}_{eq} = \tfrac{1}{3}\sqrt{2}[(\bar{\varepsilon}_{11} - \bar{\varepsilon}_{22})^2 + (\bar{\varepsilon}_{22} - \bar{\varepsilon}_{33})^2 + (\bar{\varepsilon}_{33} - \bar{\varepsilon}_{11})^2 + 6(\bar{\varepsilon}_{12}^2 + \bar{\varepsilon}_{23}^2 + \bar{\varepsilon}_{31}^2)]^{1/2} \tag{12}$$

and

$$\bar{\sigma}_{eq} = \sqrt{\frac{1}{2}}\,[(\bar{\sigma}_{11} - \bar{\sigma}_{22})^2 + (\bar{\sigma}_{22} - \bar{\sigma}_{33})^2 + (\bar{\sigma}_{33} - \bar{\sigma}_{11})^2 + 6(\bar{\sigma}_{12}^2 + \bar{\sigma}_{23}^2 + \bar{\sigma}_{31}^2)]^{1/2}\,. \tag{13}$$

The Clausius–Duhem inequality in the original configuration can be derived from Eqs (6), (9) and (11) as

$$\mathrm{tr}\left[\left(\frac{1}{\rho_0}\,\bar{\boldsymbol{\sigma}} - \frac{\partial\Phi}{\partial\bar{\varepsilon}_{eq}}\,\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\boldsymbol{\varepsilon}}}\right)\dot{\bar{\boldsymbol{\varepsilon}}}\right] - \left(S + \frac{\partial\Phi}{\partial T}\right)\dot{T} - \frac{\partial\Phi}{\partial\xi}\,\dot{\xi} - \frac{1}{\rho_0 T}\,\mathbf{Q}\,\mathrm{Grad}\,T \geqslant 0\,. \tag{14}$$

The general stress–strain relation based on continuum mechanics is given by

$$\bar{\boldsymbol{\sigma}} = \rho_0\,\frac{\partial\Phi}{\partial\bar{\varepsilon}_{eq}}\,\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\boldsymbol{\varepsilon}}}\,. \tag{15}$$

From this step, the matrix form will be used for further derivation of the constitutive relations. The stress and strain vectors are

$$\{\bar{\sigma}\} = \{\bar{\sigma}_{11}\ \bar{\sigma}_{22}\ \bar{\sigma}_{33}\ \bar{\sigma}_{12}\ \bar{\sigma}_{23}\ \bar{\sigma}_{31}\}^T \tag{16}$$

and

$$\{\bar{\varepsilon}\} = \{\bar{\varepsilon}_{11}\ \bar{\varepsilon}_{22}\ \bar{\varepsilon}_{33}\ \bar{\varepsilon}_{12}\ \bar{\varepsilon}_{23}\ \bar{\varepsilon}_{31}\}^T\,. \tag{17}$$

The time derivative of the P–K stress from Eq. (15) may be written as

$$\{\dot{\bar{\sigma}}\} = D\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}^T\{\dot{\bar{\varepsilon}}\} + \Omega\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}\dot{\xi} + \Theta\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}\dot{T}\,, \tag{18}$$

where $\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\}$ is a 6×1 matrix, given by $\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}_{11}}\ \frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}_{22}}\ \frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}_{33}}\ \frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}_{12}}\ \frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}_{23}}\ \frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}_{31}}\}^T$. D, Ω, and Θ are the Young's modulus, transformation tensor, and thermoelastic tensor of the materials as defined in the one-dimensional model [1]. They are given by

$$\begin{cases} D = \rho_0\,\dfrac{\partial^2\Phi}{\partial\bar{\varepsilon}_{eq}^2} \\[2ex] \Omega = \rho_0\,\dfrac{\partial^2\Phi}{\partial\bar{\varepsilon}_{eq}\,\partial\xi} \\[2ex] \Theta = \rho_0\,\dfrac{\partial^2\Phi}{\partial\bar{\varepsilon}_{eq}\,\partial T}\,. \end{cases} \tag{19}$$

Equation (18) may be written in incremental form:

$$\{\mathrm{d}\bar{\sigma}\} = D\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}^T\{\mathrm{d}\bar{\varepsilon}\} + \Omega\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}\mathrm{d}\xi + \Theta\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}\mathrm{d}T\,. \tag{20}$$

The strain increment may be decomposed into two components, the elastic strain and the

transformation strain, as follows, if the deformation does not reach plastic range and the temperature is constant:

$$\{d\bar{\varepsilon}\} = \{d\bar{\varepsilon}^e\} + \{d\bar{\varepsilon}^t\}\,, \tag{21}$$

where the elastic strain component is defined by

$$\{d\bar{\varepsilon}^e\} = \{\mathscr{E}\}^{-1}\{d\bar{\sigma}\}\,, \tag{22}$$

where $\{\mathscr{E}\}$ is the elastic material property matrix. After substituting Eqs (21) and (22) into Eq. (20), Eq. (20) becomes:

$$\left(\{I\} - D\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}^T\{\mathscr{E}\}^{-1}\right)\{d\bar{\sigma}\} = D\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}^T\{d\bar{\varepsilon}^t\} + \Omega\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}d\xi\,. \tag{23}$$

Note, if the SMA material is in the elastic range, the right side of Eq. (23) vanishes. This gives the elastic material property matrix as

$$\{\mathscr{E}\} = D\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}\left\{\frac{\partial\bar{\varepsilon}_{eq}}{\partial\bar{\varepsilon}}\right\}^T. \tag{24}$$

The martensite fraction, ξ, may be derived based on transformation kinetics. Liang [3] has proposed two empirical relations to describe the phase transformation processes. The cosine model is used here. In a martensitic transformation, the martensite fraction is given by

$$\xi = \tfrac{1}{2}\{\cos[a_M(T - M_f) + b_M\bar{\sigma}] + 1\}\,. \tag{25}$$

For a reverse transformation (martensite to austenite), the martensite fraction according to the cosine model is

$$\xi = \tfrac{1}{2}\{\cos[a_A(T - A_s) + b_A\bar{\sigma}] + 1\}\,, \tag{26}$$

where A_s and M_f are the austenite start temperature and martensite finish temperature, a_M and a_A can be derived from the transition temperatures, and b_M and b_A may be obtained by assuming the linear relations of transition temperatures and stress. Detailed discussion can be found in previous work [1, 3].

The martensite fraction given in Eq. (25) or (26) is function of stress and temperature. It is assumed that the martensite fraction can be expressed as follows for multi-dimensional problems according to the discussion of equivalent P–K stress and G–L strain:

$$\xi = \Xi(\bar{\sigma}_{eq}, T)\,, \tag{27}$$

where $\bar{\sigma}_{eq}$ is the equivalent P–K stress given by Eq. (13). The increment of martensite fraction, $d\xi$, therefore, can be written as

$$d\xi = \frac{\partial\Xi}{\partial\bar{\sigma}_{eq}}d\bar{\sigma}_{eq} + \frac{\partial\Xi}{\partial T}dT\,, \tag{28}$$

where $d\bar{\sigma}_{eq}$ can be expressed as

$$\mathrm{d}\bar{\sigma}_{\mathrm{eq}} = \left\{\frac{\partial \bar{\sigma}_{\mathrm{eq}}}{\partial \bar{\sigma}}\right\}^T \{\mathrm{d}\bar{\sigma}\} . \tag{29}$$

Substituting Eqs (28) and (29) into Eq. (23) and rearranging yields:

$$\{\mathrm{d}\bar{\sigma}\} = \frac{D\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\}\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\}^T}{\{I\} - D\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\}\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\}^T \{\mathscr{E}\}^{-1} - \Omega \frac{\partial \Xi}{\partial \bar{\sigma}_{\mathrm{eq}}}\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\}\left\{\frac{\partial \bar{\sigma}_{\mathrm{eq}}}{\partial \bar{\sigma}}\right\}^T} \{\mathrm{d}\bar{\varepsilon}^t\}$$

$$+ \frac{\Theta\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\} + \Omega \frac{\partial \Xi}{\partial T}\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\}}{\{I\} - D\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\}\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\}^T \{\mathscr{E}\}^{-1} - \Omega \frac{\partial \Xi}{\partial \bar{\sigma}_{\mathrm{eq}}}\left\{\frac{\partial \bar{\varepsilon}_{\mathrm{eq}}}{\partial \bar{\varepsilon}}\right\}\left\{\frac{\partial \bar{\sigma}_{\mathrm{eq}}}{\partial \bar{\sigma}}\right\}^T} \mathrm{d}T . \tag{30}$$

Equation (30) is a general expression of the constitutive relation for SMAs. It can describe both the stress–strain–temperature relations of SMA and the shape memory effect. Although it is derived based on thermomechanics, it is very much similar in form to the constitutive relations of thermo-plasticity [11]. An internal state variable, ξ, is introduced in this thermomechanical model to represent the history dependence of the stress–strain behavior of SMAs instead of the plastic strain for the constitutive model of plasticity. In fact, the internal state variable, ξ, has a direct relation with the transformation strain, $\bar{\varepsilon}^t$, which is defined similarly to the plastic strain [3]. To use this thermomechanical constitutive relation, the empirical relation of transformation kinetics must be used. Equation (30) can be used to predict and describe the multi-dimensional stress–strain field without relying on the input of stress–strain data. The simplified Eq. (30) is

$$\{\mathrm{d}\bar{\sigma}\} = \{\mathscr{D}\}\{\mathrm{d}\bar{\varepsilon}^t\} + \{\kappa\}\,\mathrm{d}T , \tag{31}$$

where $\{\mathscr{D}\}$ and $\{\kappa\}$ can be found by comparing Eq. (31) with (30). Solving for the transformation strain yields:

$$\{\mathrm{d}\bar{\varepsilon}^t\} = \{\mathscr{D}\}^{-1}\{\mathrm{d}\bar{\sigma}\} - \{\mathscr{D}\}^{-1}\{\kappa\}\,\mathrm{d}T . \tag{32}$$

The elastic strain, plastic strain, and thermal expansion strain can be added to the above equation to generate a complete thermomechanical elasto-plastic constitutive relation for shape memory alloys. The Lévy–von Mises model provides a plastic strain increment:

$$\{\mathrm{d}\bar{\varepsilon}^p\} = \frac{3}{2}\frac{\mathrm{d}\varepsilon^p_{\mathrm{eq}}}{\bar{\sigma}_{\mathrm{eq}}}\{\bar{s}\} , \tag{33}$$

where $\varepsilon^p_{\mathrm{eq}}$ is the equivalent plastic strain and $\{s\}$ the deviatoric stress vector [12].

The thermal expansion strain is given by

$$\{\mathrm{d}\varepsilon_T\} = \{\alpha\}\,\mathrm{d}T = \{\alpha\ \alpha\ \alpha\ 0\ 0\ 0\}^T\,\mathrm{d}T , \tag{34}$$

where α is the thermal expansion coefficient.

The total deformation of SMAs may be decomposed into elastic, transformation related, plastic, and thermal strain because the four types of deformation are different in nature. Elastic deformation is thermodynamically reversible. The deformation associated with phase transformation is not thermodynamically reversible but differs essentially from the plastic deformation which is caused by dislocation, a permanent damage to the crystal structures. However, the transformation deformation of SMAs resulting from the de-twining or twining deformation of martensitic or reverse phase transformation is recoverable when thermal energy is input to the SMAs. A complete constitutive equation can thus be described by

$$\begin{aligned}\{\mathrm{d}\bar{\varepsilon}\} &= \{\mathrm{d}\bar{\varepsilon}^{e}\} + \{\mathrm{d}\bar{\varepsilon}^{t}\} + \{\mathrm{d}\bar{\varepsilon}^{p}\} + \{\mathrm{d}\bar{\varepsilon}_{T}\} \\ &= \{\mathscr{E}\}^{-1}\{\mathrm{d}\bar{\sigma}\} + \{\mathscr{D}\}^{-1}\{\mathrm{d}\bar{\sigma}\} - \{\mathscr{D}\}^{-1}\{\kappa\}\,\mathrm{d}T + \frac{3}{2}\frac{\mathrm{d}\varepsilon^{p}_{\mathrm{eq}}}{\bar{\sigma}_{\mathrm{eq}}}\{\bar{s}\} + \{\alpha\}\,\mathrm{d}T\,. \end{aligned} \tag{35}$$

Most applications of SMA are in the transformation region with very few applications utilizing the plastic deformation range. The thermomechanical constitutive relation for SMAs may be further simplified if the plastic strain is neglected. The stress–strain relation, thus, can be written as

$$\{\mathrm{d}\bar{\sigma}\} = \frac{\{I\}}{\{\mathscr{E}\}^{-1} + \{\mathscr{D}\}^{-1}}\{\mathrm{d}\bar{\varepsilon}\} + \frac{\{\mathscr{D}\}^{-1}\{\kappa\} - \{\alpha\}}{\{\mathscr{E}\}^{-1} + \{\mathscr{D}\}^{-1}}\,\mathrm{d}T\,, \tag{36}$$

where the $\{\mathscr{D}\}^{-1}$ is zero in the elastic range. Therefore, the above constitutive equation is of the same form as Hooke's law within the elastic region. In case of proportional loading at a constant temperature, Eq. (36) may be integrated on both sides, resulting in a total strain theory similar to Hencky's stress–strain relation of plastic materials [12] and given by

$$\{\bar{\sigma}\} = \frac{\{I\}}{\{\mathscr{E}\}^{-1} + \{\mathscr{D}\}^{-1}}\{\bar{\varepsilon}\}\,. \tag{37}$$

In a one-dimensional tensile test the martensitic transformation starts at an elastic stress limit, σ_e. It is assumed that the phase transformation in a multi-dimensional stress state occurs when the equivalent P–K stress, $\bar{\sigma}_{\mathrm{eq}}$, reaches the elastic stress limit, σ_e.

A case study

The constitutive relations developed in the previous section are material and geometrically nonlinear. Solving even a simple problem requires sophisticated finite element programs. Here, in order to demonstrate the utility of the multi-dimensional constitutive relation, a simple example of a circular SMA rod under torsion is presented.

As we know, it is very difficult to solve finite strain problems, even a simple problem such as the torsion of a circular rod. Since the purpose of this paper is to demonstrate the modeling of the material nonlinearity of SMAs, it is assumed here that the cross-section of the circular SMA rod remains planar and its radius does not change in order to simplify the analysis. This assumption is reasonable if the rod is thin and the shear strain (which is proportional to the radius of the rod) is relatively small.

Stress–strain analysis

Considering a point $(X\ Y\ Z)$ in the un-twisted rod (original configuration), its new position is at $(x\ y\ z)$ if the rod twists by θZ where θ is the angle of twist per unit length. The new position can be expressed as follows if the cross-section of the rod is assumed to remain planar:

$$\begin{cases} x = X\cos(\theta Z) - Y\sin(\theta Z) \\ y = X\sin(\theta Z) + Y\cos(\theta Z) \\ z = Z\,. \end{cases} \tag{38}$$

The Green–Lagrange strains solved from Eq. (3) are

$$\{\bar{\varepsilon}_{XX}\ \bar{\varepsilon}_{YY}\ \bar{\varepsilon}_{ZZ}\ \bar{\gamma}_{XY}\ \bar{\gamma}_{YZ}\ \bar{\gamma}_{ZX}\} = \{0\,0\,0\,0\ X\theta - Y\theta\}\,. \tag{39}$$

The $\bar{\varepsilon}_{ZZ}$ is assumed to be zero. Accordingly, the following geometrical relation can still be used for the finite rotation problem:

$$\bar{\gamma} = r\theta Z\,. \tag{40}$$

Since only $\bar{\gamma}_{YZ}$ and $\bar{\gamma}_{ZX}$ exist, the non-zero stress components are $\bar{\tau}_{YZ}$ and $\bar{\tau}_{ZX}$. The Cauchy shear stress τ_{yz} and τ_{zx} can be solved from Eq. (4) as follows:

$$\begin{cases} \tau_{zx} = \bar{\tau}_{ZX}\cos(\theta Z) - \bar{\tau}_{YZ}\sin(\theta Z) \\ \tau_{yz} = \bar{\tau}_{YZ}\cos(\theta Z) + \bar{\tau}_{ZX}\sin(\theta Z) \end{cases}. \tag{41}$$

The main boundary and equilibrium condition at the end of the rod where torque, $\mathcal{T}$, is applied can be expressed as

$$\int\int (\tau_{zy}x - \tau_{zy}y)\,\mathrm{d}x\,\mathrm{d}y = \mathcal{T}_{zz} = \bar{\mathcal{T}}_{ZZ} = \mathcal{T}\,, \tag{42}$$

where $\mathcal{T}_{zz}$ is the torque measured in the current reference and $\bar{\mathcal{T}}_{ZZ}$ is the torque in the original reference. Substituting Eqs (38) and (41) into Eq. (42) yields:

$$\int\int (\bar{\tau}_{ZX}X - \bar{\tau}_{ZY}Y)\,\mathrm{d}X\,\mathrm{d}Y = \mathcal{T}\,, \tag{43}$$

which indicates that the following equation can be still applied to this finite strain rotation problem. The rod is assumed to be a unit length long and only the stress and strain at the end of the rod are examined.

$$\bar{\tau} = G\bar{\gamma} = Gr\theta = \frac{2\mathcal{T}r}{\pi a^4}\,. \tag{44}$$

The equivalent stress and strain from Eqs (12) and (13) are

$$\bar{\sigma}_{\text{eq}} = \sqrt{3}\bar{\tau} \tag{45}$$

and

$$\bar{\varepsilon}_{\text{eq}} = \frac{1}{\sqrt{3}}\,\bar{\gamma}\,. \tag{46}$$

Since the shear stress has its greatest value at $r = a$, the bar begins to have stress-induced phase transformation at the outer surface. When the equivalent stress , $\bar{\sigma}_{\text{eq}}$, at the radius, a, reaches σ_e, the corresponding critical torque and twist are

$$\mathcal{T}_e = \tfrac{1}{6}\sqrt{3}\pi\sigma_e a^3 \tag{47}$$

and

$$\theta_e = \frac{\sigma_e}{\sqrt{3}Ga}\,. \tag{48}$$

If the torque is increased further, a transformation annulus forms near the boundary, leaving a central zone of elastic material within a radius, c. The stress distribution in the elastic region is linear with the equivalent stress reaching σ_e at $r = c$. The shear stress in the central elastic region is given by

$$\bar{\tau} = \frac{\sigma_e}{\sqrt{3}}\,\frac{r}{c} \quad 0 \leqslant r \leqslant c\,. \tag{49}$$

The stress distribution in the transformation annulus obeys the constitutive relation given in Eq. (36). From Eqs (12) and (13), the terms $\{\frac{\partial\bar{\varepsilon}_{\text{eq}}}{\partial\bar{\gamma}}\}$ and $\{\frac{\partial\bar{\sigma}_{\text{eq}}}{\partial\bar{\tau}}\}$ may be determined to be

$$\left\{\frac{\partial\bar{\varepsilon}_{\text{eq}}}{\partial\bar{\gamma}}\right\} = \frac{1}{\sqrt{3}} \tag{50}$$

and

$$\left\{\frac{\partial\bar{\sigma}_{\text{eq}}}{\partial\bar{\tau}}\right\} = \sqrt{3}\,. \tag{51}$$

The inverse of the elastic material property matrix is simply $1/G$ in this case. The shear modulus, G, is $D/3$ for incompressible material. All material properties are assumed to be constant herein. Based on the above discussion, $\{\mathcal{D}\}^{-1}$ and $\{\kappa\}$ are given by

$$\{\mathcal{D}\}^{-1} = 3\varepsilon_L\,\frac{\partial\bar{\Xi}}{\partial\bar{\sigma}_{\text{eq}}} \tag{52}$$

and

$$\{\kappa\} = -\frac{\Theta + \Omega\,\dfrac{\partial\bar{\Xi}}{\partial T}}{\sqrt{3}\Omega\,\dfrac{\partial\bar{\Xi}}{\partial\bar{\sigma}_{\text{eq}}}}\,. \tag{53}$$

The stress–strain relation in the transformation annulus is given by

$$\left(1 - \Omega \frac{\partial \bar{\Xi}}{\partial \bar{\sigma}_{eq}}\right) d\bar{\tau} = G\, d\bar{\gamma} . \tag{54}$$

Integrating on both sides yields:

$$(\bar{\tau} - \bar{\tau}_0) = G(\bar{\gamma} - \bar{\gamma}_0) + \frac{\Omega}{\sqrt{3}} (\xi - \xi_0) , \tag{55}$$

where the variables with subscript '0' are the initial conditions. Assuming the initial phase of the bar is austenite and the ambient temperature is above M_s, the stress–strain relation can be simplified to:

$$\bar{\tau} = G\bar{\gamma} + \frac{\Omega}{\sqrt{3}} \xi . \tag{56}$$

The martensite fraction, ξ, from Eq. (25) is

$$\xi = \tfrac{1}{2}\{\cos[a_M(T - M_f) + b_M\sqrt{3}\bar{\tau}] + 1\} . \tag{57}$$

The shear stress distribution in the transformation annulus $\bar{\tau}(r)$ is given by

$$\bar{\tau} = G\theta_r + \frac{\Omega}{2\sqrt{3}} \{\cos[a_M(T - M_f) + b_M\sqrt{3}\bar{\tau}] + 1\} \quad c \leqslant r \leqslant a . \tag{58}$$

A numerical iteration scheme is required to determine the shear stress. The equivalent stress at the elastic interface is the elastic stress limit, σ_e. The radius of the central elastic zone, c, can be determined from the following equation:

$$c = \frac{\sigma_e}{\sqrt{3}G\theta} . \tag{59}$$

The resultant moment from the distributed shear stress is expressed as

$$\mathcal{T} = \int_0^c \frac{\sigma_e r^3}{\sqrt{3}c} 2\pi\, dr + \int_c^a \bar{\tau}(r) r^2 2\pi\, dr . \tag{60}$$

A closed-form integration of Eq. (60) may be obtained by integrating by part of its second integration term, yielding:

$$\mathcal{T} = \frac{\sigma_e \pi c^3}{2\sqrt{3}} + \frac{1}{3}\left(\bar{\tau}_{out} a^3 - \frac{\sigma_e}{\sqrt{3}} c^3\right) - \frac{1}{3}\int_{\sigma_e\sqrt{3}}^{\bar{\tau}_{out}} r^3\, d\bar{\tau} , \tag{61}$$

where $\bar{\tau}_{out}$ is the shear stress at $r = a$, and r can be solved from Eq. (58) in terms of $\bar{\tau}$.

With increasing torque, the equivalent stress at $r = a$ reaches the yield strength, σ_y, which corresponds to a critical torque, $\mathcal{T}_y$. A torque higher than $\mathcal{T}_y$ will result in plastic deformation requiring plastic constitutive relations. The applied torque is restricted to be below $\mathcal{T}_y$ in this study. This critical twisting angle, θ_y, can thus be determined from Eq. (58) as

$$\theta_y = \frac{1}{\sqrt{3}Ga} (\sigma_y - \Omega) . \tag{62}$$

The critical torque, $\mathscr{T}_y$, can then be determined from Eq. (61). The martensite fraction distribution, $\xi(r)$, can be determined by substituting $\bar{\tau}(r)$ into Eq. (57).

The residual stress–strain distribution may be obtained by superimposing an elastic stress distribution caused by a torque of $-\mathscr{T}$. It is assumed that the maximum equivalent stress of the residual stress field is less than σ_e, so the martensite fraction distribution may not be altered. The residual stress distribution may then be given by

$$\bar{\tau}_{\text{res}} = \bar{\tau}(r) - \frac{2\mathscr{T} r}{\pi a^4} . \tag{63}$$

The residual twist, θ_{res}, is determined by the same superposition approach,

$$\theta_{\text{res}} = \theta(T) - \frac{2\mathscr{T}}{\pi G a^4} , \tag{64}$$

and the residual strain is obtained from the expression:

$$\bar{\gamma}_{\text{res}} = r\theta_{\text{res}} . \tag{65}$$

Analysis of the shape memory effect

Some of the residual twist of the SMA bar will be recovered upon heating due to the shape memory effect. If the boundary condition of the SMA bar is free, heating of the SMA bar results in a controlled recovery. This is different from the uniaxial free recovery in which the residual transformation strain is fully recovered and the stress is zero. In the case of the 'free recovery' of an SMA bar, the central elastic zone may generate an internal reactionary force to the recovery of the outside transformation annulus. Heating the bar results in a certain amount of twist recovery while storing energy to the central elastic zone. The stored energy will be released upon cooling the SMA bar, resulting in a reverse deformation of the outside transformation annulus (generating new martensite). It is similar to a bias spring SMA actuator or an SMA bar with a two-way effect.

This unique characteristic of an SMA bar (or other similar geometries) may be very useful. This 3-D SME characteristic is actually a two-way effect by structure rather than a two-way effect by material. An SMA bar itself functions as an actuator without bias springs. Proper design of the size of the central elastic region may achieve an overall two-way effect. A 'smart' blade of turbine compressors which can adjust its attacking angle according to in-coming flux may be designed based on this concept.

The theoretical analysis of this 'free recovery' of an SMA bar is very difficult. A numerical technique such as the finite element method must be used. On the contrary, it is relatively easy to analyze the behavior of restrained recovery in this case.

In the restrained recovery case, the residual deformation is restrained and no deformation is allowed during the heating and cooling process. It is assumed that heating starts from A_s (ignoring the thermoelastic effect) and the temperature is uniform throughout the SMA bar. Equation (36) becomes:

$$\{\mathrm{d}\bar{\sigma}^r\} = -\frac{\{\mathscr{D}\}^{-1}\{\kappa\}}{\{\mathscr{E}\}^{-1} + \{\mathscr{D}\}^{-1}} \mathrm{d}T , \tag{66}$$

where superscript 'r' denotes 'recovery'. In the case of restrained recovery of SMA bars, the above equation may be simplified to:

$$\left(1-\Omega\frac{\partial\bar{\Xi}}{\partial\bar{\sigma}_{eq}}\right)\mathrm{d}\bar{\tau}^{r}=\frac{\Theta+\Omega\dfrac{\partial\bar{\Xi}}{\partial T}}{\sqrt{3}}\,\mathrm{d}T\,. \tag{67}$$

Integrating on both sides yields:

$$\bar{\tau}-\bar{\tau}_0=\frac{\Theta}{\sqrt{3}}(T-T_0)+\frac{\Omega}{\sqrt{3}}(\xi-\xi_0)\,, \tag{68}$$

where $\bar{\tau}_0$ is the residual stress obtained from Eq. (63), T_0 is A_s, and ξ_0 is the martensite fraction obtained from the stress–strain analysis (Eq. (57)). ξ from Eq. (26) is given by

$$\xi=\frac{\xi_0}{2}\{\cos[a_A(T-A_s)+b_A\sqrt{3}\bar{\tau}^{r}]+1\}\,. \tag{69}$$

Substituting Eq. (69) into Eq. (68) yields the shear stress distribution in the transformation annulus. Note that the residual stress in the central elastic zone is not altered due to the restrained boundary condition. The resultant torque from the recovery shear stress thus may be calculated using Eq. (61).

Results and analysis

The numerical results of the torsion of a round SMA rod are given in this section. The diameter and length of the rod are 5 mm and 1 m, respectively. The rod is assumed to be made of a Nitinol SMA and its properties are listed in Table 1.

An average elastic modulus is used in this paper. ε_L is the maximum recoverable strain. The phase transformation tensor, Ω, is related to the elastic modulus by

$$\Omega=-\varepsilon_L D\,. \tag{70}$$

M_f, M_s, A_s, and A_f are the transition temperatures of SMAs. C_A and C_M are the stress influence coefficients of SMAs. The elastic stress limit, σ_e, and yield strength, σ_y, are given by

$$\begin{cases}\sigma_e=C_M(T-M_s)\\ \sigma_y=C_A(T-M_f)\,.\end{cases} \tag{71}$$

The four constants, a_M, a_A, b_M, and b_A appearing in Eqs (25) and (26), are defined by

Table 1. Material constants for a Nitinol alloy [3]

MPa	°C				MPa/°C			%
D	M_s	M_f	A_s	A_f	C_A	C_M	Θ	ε_L
46,650	9.0	18.4	34.5	49	10.3	10.3	0.55	6.7

$$\begin{cases} a_A = \pi/(A_f - A_s) \\ a_M = \pi/(M_s - M_f) \\ b_A = -a_A/C_A \\ b_M = -a_M/C_M \,. \end{cases} \tag{72}$$

Shown in Fig. 1 is the shear stress and martensite distribution at the end of the SMA rod for various angles, θ. The dashed line is the martensite fraction and the solid line is the shear stress distribution. If the twisting angle is less than θ_e, the shear stress has a linear distribution with respect to the radial distance and there is no stress-induced martensitic phase transformation. There will be some stress-induced martensite once the twisting angle exceeds θ_e. When $\theta = \theta_y/10$, only one-fifth of the rod (radial direction) remains elastic, as shown in Fig. 1, and the maximum martensite fraction (8%) is at $r = a$. When θ reaches θ_y, only a very small portion of the cylinder (in the radial direction at this cross section) is elastic.

Shown in Fig. 2 is the applied torque vs. the twisting angle of the rod. The torque and twisting angle are normalized by maximum elastic torque and twisting angle. It can be seen that the rotation can be enormous before reaching plastic for this long, thin rod (10 mm in diameter and 1 m in length).

We have demonstrated the capability of the multi-dimensional constitutive equations in solving the torsion problem of SMA rod. The results illustrated in both Figs 1 and 2 show that the torsion of SMAs is a very complicated problem. Detailed analysis, including the shape memory effect in torsion, will be given in another paper in order to reduce the length of this paper.

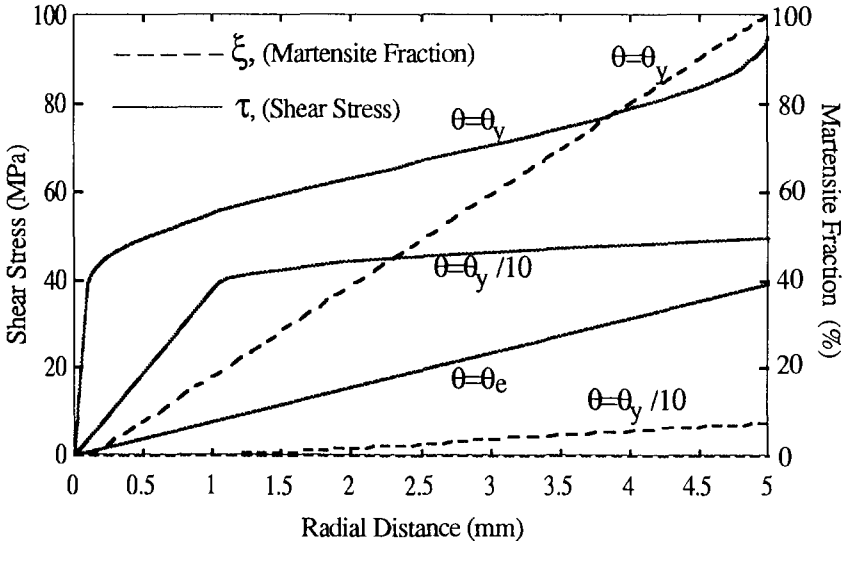

Fig. 1. Shear stress and martensite distribution at the end of an SMA rod for various twisting angles.

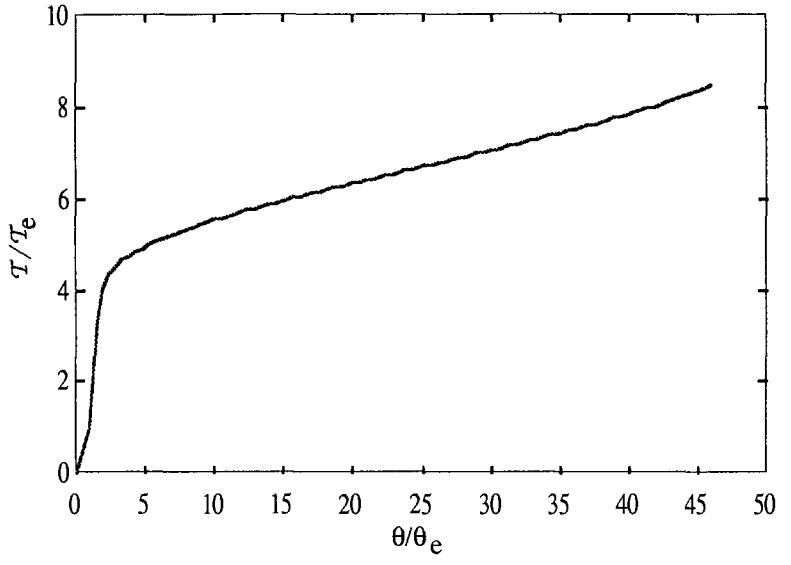

Fig. 2. Normalized torque and twisting angle relation for an SMA rod.

Concluding remarks

A multi-dimensional thermomechanical constitutive model of SMAs is developed in this paper. The multi-dimensional constitutive model is based on the thermomechanical aspects of shape memory alloys and can be used to study the mechanical behavior of complex structures made of shape memory alloys. A numerical analysis of the torsion of a shape memory alloy rod was presented to show how the constitutive relations could be used.

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