A thermodynamically-consistent microplane model for shape memory alloys

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Abstract

In microplane theory, it is assumed that a macroscopic stress tensor is projected to the microplane stresses. It is also assumed that 1D constitutive laws are defined for associated stress and strain components on all microplanes passing through a material point. The macroscopic strain tensor is obtained by strain integration on microplanes of all orientations at a point by using a homogenization process. Traditionally, microplane formulation has been based on the Volumetric–Deviatoric–Tangential split and macroscopic strain tensor was derived using the principle of complementary virtual work. It has been shown that this formulation could violate the second law of thermodynamics in some loading conditions. The present paper focuses on modeling of shape memory alloys using microplane formulation in a thermodynamically-consistent framework. To this end, a free energy potential is defined at the microplane level. Integrating this potential over all orientations provides the macroscopic free energy. Based on this free energy, a new formulation based on Volumetric–Deviatoric split is proposed. This formulation in a thermodynamic-consistent framework captures the behavior of shape memory alloys. Using experimental results for various loading conditions, the validity of the model has been verified.

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1. Introduction

Shape memory alloys (SMAs) are finding increasing number of engineering applications due to their unique properties. In general, there are two main approaches for modeling the complex behavior of SMAs, micromechanical and macromechanical. In general, a micro-scale viewpoint can result in a more accurate understanding of the material behavior. In micromechanical models, the micro-scale response of SMAs is investigated by considering the grain level of the two phases and the crystallographic texture of the material. These models use thermodynamics laws and micromechanics methods to describe the transformation and macro-scale equations (Gao et al., 2000; Auricchio et al., 2003; Thamburaja, 2005; Guthikonda et al., 2007; Sadjadpour and Bhattacharya, 2007; Peng et al., 2008; Yu et al., 2013). In macromechanical models, on the other hand, macro-scale behavior is captured by considering macroscopic energy functions that depend on internal state variables. Most of these macromechanical models are categorized as phenomenological models. The main differences among various phenomenological models are in the choice of internal state variables as well as in the evolution equations defining the thermomechanical driving forces (Brinson, 1993; Panico and Brinson, 2007; Arghavani et al., 2010; Saleeb et al., 2011; Chemisky et al., 2011; Zaki, 2012; Lagoudas et al., 2012; Andani et al., 2013). Some of these small-strain constitutive models are extended to large-scale and finite-strain models (Christ and Reese, 2009; Arghavani et al., 2011; Saleeb et al., 2013).

Asymmetry behavior in tension and compression is a well-known feature of shape memory alloys. In compression, the martensitic transformation from the austenitic phase is higher than in tension; maximum recoverable strain in compression is smaller than in tension; the hysteresis loop measured along the stress axis in compression is wider than in tension (Thamburaja and Nikabdollah, 2009). The difference of the hysteresis loops in tension and compression of the stress–strain response is due to different interaction energies and morphologies of the transformed phases for these loadings (Lim and McDowell, 1999). SMA models have been modified to capture these differences in tension and compression (Orgéas and Favier, 1998; Poorasadion et al., 2013).

Microplane theory is an efficient formulation in phenomenological models that describe complex material behaviors in a simple...
way. The rising interest in microplane modeling has led to its application to various materials such as quasi-brittle materials including concrete, soil, fiber composites, and stiff foams. Microplane formulation provides closed form relations for calculating the strain components in terms of the stress components. The other advantage of the approach is in the limited number of the required material parameters. These material parameters can be calculated in simple tension and torsion tests. The main feature of this modeling is in describing the behavior of a complex material with simple constitutive laws on each microplane. To this end, the approach finds the material behavior in any direction on each microplane and then uses the micro–macro homogenization process to obtain the overall macroscopic properties.

Various implementation methodologies exist (Bažant, 1984; Bažant and Prat, 1988a,b; Carol and Bažant, 1997). Carol and Prat (1990) used static constraint while Bažant and Caner (2005) used mixed static-kinematic constraint to implement microplane theory. In static constraint, the macroscopic stresses on a specific microplane are equal to the projections of the macroscopic stress while in kinematic constraint the macroscopic strain tensor is projected on each microplane. The Normal–Tangential (N–T) split, by Bažant and Oh (1985), produces acceptable results in tensile loadings and has limitations in predicting the compression and shear loadings. To address this limitation, Carol et al. (1992, 2001, 2004), Bažant et al. (2000), and Kuhl et al. (2001) adopted a Volumetric–Deviatoric–Tangential (V–D–T) split, where the microplane normal stress and strain are divided into the volumetric and deviatoric components. Carol et al. (2001) showed that using the principle of complementary virtual work (PCVW) in a homogenization process for obtaining the overall macroscopic properties might violate the second principle of thermodynamics in certain loading conditions. In addition, they showed that some of the strain components that are used in the microplane level model might not be conjugate with their stress counterparts. Leukart and Ramm (2002, 2003) and Leukart (2005) proposed a microplane model in thermodynamically-consistent framework with Volumetric–Deviatoric (V–D) split which can be viewed as a special case of the general V–D–T split. In this new split, the macroscopic strain tensor is projected into the normal and shear components and was shown that the new formulation in the strain components is an effective approach to remedy these deficiencies.

The first microplane modeling for SMAs was performed by Brocca et al. (2002). They divided shear stress on each microplane into two perpendicular components within the plane and used a 1D constitutive law for stress and strain components in normal and two shear directions on any arbitrary plane. They showed that some features such as stress–strain minor loops and tension–compression asymmetry could be predicted by the microplane model. Kadkhodaei et al. (2007, 2008) showed that microplane formulations with two shear directions on each plane have a directional bias nature and may result in prediction of unrealistic behaviors. Therefore, they utilized one resultant shear direction within each plane and proposed to use the Volumetric–Deviatoric split for normal direction. Mehrabi et al. (2012) and Mehrabi and Kadkhodaei (2013a) proposed a 3D phenomenological model based on the microplane theory in V–D–T split. They showed the capability of this approach in predicting martensite reorientation in multiaxial loadings. Due to thermodynamic inconsistencies of the V–D–T split, there is a need for a more effective microplane formulation for SMAs. Therefore, in this work a microplane formulation based on V–D split in a thermodynamically-consistent framework is proposed. Within the context of these relations, Volumetric–Deviatoric components of the stresses in each microplane based on static constraint are presented. The new formulation based on the V–D split is compared numerically with the V–D–T split in uniaxial and pure torsion. The proposed model is also validated with experimental data.

This paper is organized as follows: in the second section, a standard thermodynamical procedure to obtain the microplane constitutive relations is summarized. Special focus of this section is on the microplane formulation extraction in a thermodynamic framework and motivation of this concept. The result of the new formulation in microplane model (V–D split) is compared with microplane formulation based on V–D–T split in Section 3. Finally, simulation results are compared with experimental results to assess the validity of the proposed model.

2. Microplane formulation based on thermodynamic approach

2.1. Thermodynamic derivation

Kadkhodaei et al. (2007, 2008), Mehrabi and Kadkhodaei (2013a) proposed a microplane model based on a static constraint in which a macroscopic stress tensor is projected on each plane. This leads to a decomposition of the stress vector into volumetric, deviatoric and tangential components, illustrated in Fig. 1. Macroscopic strain tensor based on microplane model (V–D–T split) derivative from principle of complementary virtual work (PCVW) is:

\[ \epsilon = \epsilon_V : \mathbf{I} + \frac{3}{2\pi} \int_\Omega (\epsilon_\alpha \mathbf{N}) d\Omega + \frac{3}{2\pi} \int_\Omega (\epsilon_T \mathbf{T}) d\Omega \]  \( \text{(1)} \)

where

\[ \epsilon_V : \mathbf{V} = \mathbf{D} : \mathbf{D} , \quad \epsilon_T : \mathbf{T} , \quad \text{and} \quad \epsilon_N = \mathbf{N} : \epsilon \]  \( \text{(2)} \)

and

\[ \mathbf{V} = \frac{\delta_y}{3} \mathbf{N} + \mathbf{D} = n_i n_j \mathbf{n}_i \mathbf{n}_j - \frac{\delta_y}{3} \mathbf{I} , \quad \text{and} \quad \mathbf{T} = T_{jk} - \frac{1}{2} (n_i \delta_{jk} + n_j \delta_{ik} - 2 n_i n_j n_k) \]  \( \text{(3)} \)

Carol et al. (2001) showed that microplane formulation based on principle of complementary virtual work (PCVW) might violate the thermodynamic consistency in some loadings conditions. Therefore, Kuhl et al. (2001) as well as Leukart and Ramm (2002) proposed microplane formulations based on V–D split in a thermodynamically-consistent framework. The proposed formulation was based on a kinematic constraint in order to relate the macroscopic strain tensor to their microplane counterparts. Here, the procedure proposed by Carol et al. (2001), Kuhl et al. (2001) and Leukart and Ramm (2002) is revised based on a static constraint for shape memory alloys.

For the first step in a thermodynamically-consistent framework, a free energy \( G^{\text{mic}}(\sigma, k) \) is defined, where \( k \) is a set of internal variables. The macroscopic Gibbs free energy might be written as the integral of all microscopic free energies defined at the microplane level:

![Fig. 1. The Volumetric–Deviatoric–Tangential microplane components of stress and strain.](image-url)
The microplane formulation based on (V–D–T) microplane model derivative from the internal energy, and temperature at the reference state, respectively. The function $f(\zeta)$ is a transformation kinetic represents the martensite fraction as a function of stress and temperature.

According to the standard procedure (Coleman and Gurtin, 1967), the strain's conjugate of $\sigma$ is the derivative of the free energy per unit volume (Zhou et al., 2009):

$$
\varepsilon = -\frac{1}{\rho} \frac{\partial G^\text{mic}}{\partial \sigma}
$$

Substituting Eq. (4) into (6) and using the chain rule of differentiation results in:

$$
\varepsilon = \frac{3}{2\pi} \int_\Omega \frac{\partial}{\partial \sigma} \left[ \frac{1}{2\rho} \sigma \cdot \sigma \right] d\Omega = \frac{3}{2\pi} \int_\Omega \frac{\partial}{\partial \sigma} \left[ \frac{1}{2\rho} G^\text{mic} \right] d\Omega
$$

It is assumed that the stress components on any microplane are $\sigma_N$ and $\sigma_T$, according to the stress vector: $\tau = \sigma_N + \sigma_T = \sigma_T - \sigma_N$. Therefore, Eq. (7) can be expanded to:

$$
\varepsilon = \frac{3}{2\pi} \int_\Omega \left[ \frac{\partial}{\partial \sigma_N} \right] N d\Omega + \frac{3}{2\pi} \int_\Omega \left[ \frac{\partial}{\partial \sigma_T} \right] T d\Omega
$$

Consistent definitions of the microplane strains $\varepsilon_N$ and $\varepsilon_T$ as the work-conjugate quantities of the microplane stresses $\sigma_N$ and $\sigma_T$ are defined as:

$$
\varepsilon_N = -\frac{1}{\rho} \frac{\partial G^\text{mic}}{\partial \sigma_N}, \quad \varepsilon_T = -\frac{1}{\rho} \frac{\partial G^\text{mic}}{\partial \sigma_T}
$$

Here, V–D split is used ($N = V + D$) therefore, macroscopic stress tensor based on (V–D–T) microplane model derivative from thermodynamic is:

$$
\varepsilon = \frac{3}{2\pi} \int_\Omega \varepsilon_N V d\Omega + \frac{3}{2\pi} \int_\Omega \varepsilon_D D d\Omega + \frac{3}{2\pi} \int_\Omega \varepsilon_T T d\Omega
$$

with the consistent microplane strains $\varepsilon_N$ and $\varepsilon_T$ defined as:

$$
\varepsilon_N = -\frac{1}{\rho} \frac{\partial G^\text{mic}}{\partial \sigma_N}, \quad \varepsilon_T = -\frac{1}{\rho} \frac{\partial G^\text{mic}}{\partial \sigma_T}
$$

It should be noted that there are two differences between the strains of Eqs. (1) and (10); The first difference is that $\varepsilon_T$ in Eq. (10) is replaced by the integral involving the volumetric term in Eq. (10). This difference will vanish if $\varepsilon_T$ is assumed to be a function of $\sigma_T$ but not a function of $\sigma_N$ and $\sigma_D$. Therefore, $\varepsilon_T$ would be the same for all microplanes and could be taken out of the integral:

$$
\frac{3}{2\pi} \int_\Omega \varepsilon_N V d\Omega = \frac{1}{2\pi} \int_\Omega \tau d\Omega = \frac{1}{2\pi} \int \varepsilon_N I d\Omega = \varepsilon_N I
$$

Since we have defined $\varepsilon_N = -\frac{1}{\rho} \frac{\partial G^\text{mic}}{\partial \sigma_N}$ and $\varepsilon_T$ is independent of the $\sigma_D$ and $\sigma_T$, the mixed derivatives $\frac{\partial G^\text{mic}}{\partial \sigma_N \partial \sigma_T}$ and $\frac{\partial G^\text{mic}}{\partial \sigma_T \partial \sigma_N}$ vanish, and according to the definition $\varepsilon_D = -\rho \frac{\partial G^\text{mic}}{\partial \sigma_D}$ and $\varepsilon_T = -\rho \frac{\partial G^\text{mic}}{\partial \sigma_T}$, neither $\varepsilon_D$ nor $\varepsilon_T$ depend on $\sigma_D$. As a result, the microplane free energy must have the following decoupled form:

$$
G^\text{mic}(\sigma_N, \sigma_D, \sigma_T, k) = G^\text{mic}(\sigma_N, k) + G^\text{mic}(\sigma_D, \sigma_T, k)
$$

where a set of internal variables is collected in the vector $k$.

The second difference is that $D = N - V$ is used:

$$
\int_\Omega \varepsilon_0 N d\Omega = \int_\Omega \varepsilon_0 V d\Omega
$$

This second difference between Eqs. (1) and (10) will be eliminated if the second term on the right-hand side vanished. This term will only vanish if the average deviatoric strain is zero. This assumption is only satisfied for the isothermal elasticity models and very limited models. Therefore, the SMA model based on V–D–T split might not satisfy the second law of thermodynamics in some loading situations.

### 2.2 Microplane modeling based on Volumetric–Deviatoric split for shape memory alloys

In this section, a microplane formulation based on a continuum thermodynamic framework is proposed. A standard thermodynamic procedure is used to obtain the necessary constitutive relations. After satisfying the principles of conservation of mass, linear momentum, and angular momentum, the first law of thermodynamics is written at a local material point as:

$$
\rho \dot{U} = \sigma : \dot{\varepsilon} - \text{div}(q) + \rho r
$$

where $U$ is the mass-specific internal energy, $q$ is the heat flux vector, and $r$ is the rate of internal heat generation. Likewise, by satisfying the conservation laws, the second law of thermodynamics is written in the form of the Clausius–Planck inequality (Paglietti, 1977) as:

$$
\rho s + \frac{1}{\tau} \text{div}(q) - \rho \frac{\dot{r}}{\tau} \geq 0
$$

where $s$ is the mass-specific entropy. Multiplying Eq. (16) by $T$ and substituting in Eq. (15) to eliminate $\text{div}(q)$:

$$
\rho s T + \sigma : \dot{\varepsilon} - \rho \dot{U} \geq 0
$$

Various energy potentials (e.g., Gibbs, Helmholtz, etc.) at a material point are related by Legendre transformations. Here, only the relationship between the internal energy $U$, and Gibbs free energy $G$ are considered:

$$
G = U - \frac{1}{\rho} \sigma : \varepsilon - s T
$$

Thermodynamic constraint on the rate of the Gibbs free energy is derived by substituting the time rate of Eq. (18) into (17):

$$
-\frac{\partial G}{\partial \sigma} : \dot{\varepsilon} - \rho s T \geq 0
$$

For shape memory alloys, as is shown in Fig. 2, stress and strain vectors on each microplane are decomposed into volumetric and deviatoric parts:

$$
\varepsilon = \varepsilon_N + \varepsilon_D, \quad \sigma = \sigma_N + \sigma_D
$$

**Fig. 2.** The Volumetric–Deviatoric (V–D) microplane components of stress and strain.
Volumetric and deviatoric parts are defined as follows:

\[ \varepsilon_v = \frac{1}{3} \operatorname{Tr}(\varepsilon) = \varepsilon^\text{vol} : \varepsilon, \quad \varepsilon_0 = \varepsilon - \frac{1}{3} \operatorname{Tr}(\varepsilon) = \varepsilon^\text{dev} : \varepsilon, \]

\[ \sigma_v = \frac{1}{3} \operatorname{Tr}(\sigma), \quad \sigma_0 = \sigma - \frac{1}{3} \operatorname{Tr}(\sigma) \]

(21)

Here, \( \varepsilon^\text{vol} \) and \( \varepsilon^\text{dev} \) are the second-order identity tensor, volumetric and deviatoric projection tensors (forth-order identity tensor), respectively:

\[ \varepsilon^\text{vol} = \frac{1}{2} \int_\Omega \varepsilon \Omega \, d\Omega = \frac{1}{2} \mathbf{1} \quad \text{and} \quad \varepsilon^\text{dev} = \frac{3}{2\pi} \int_\Omega \mathbf{D} : \mathbf{D} \, d\Omega = \varepsilon^\text{vol} - \varepsilon^\text{dev} \]

(22)

For calculation of \( \sigma : \varepsilon \) in Eq. (19), one can write:

\[ \sigma : \varepsilon = (\sigma_v + \sigma_0) : (\varepsilon_v + \varepsilon_0) = \sigma_v : \varepsilon_v + \sigma_0 : \varepsilon_0 \]

(23)

The terms \( \sigma_v : \varepsilon_v \) and \( \sigma_0 : \varepsilon_0 \) of Eq. (23) are zero and substituting Eq. (23) into (19) results in:

\[-\rho \ddot{G} - \sigma_v : \varepsilon_v - \sigma_0 : \varepsilon_0 - \rho \dot{s} \dot{T} \geq 0 \]

(24)

After applying the chain rule, the SMA Gibbs free energy is written as:

\[ G(\sigma_v, \sigma_0, T, \xi) = \dot{G} = \frac{\partial G}{\partial \sigma_v} : \dot{\sigma}_v + \frac{\partial G}{\partial \sigma_0} : \dot{\sigma}_0 + \frac{\partial G}{\partial \zeta} : \dot{\xi} \]

(25)

Substituting Eq. (25) into (24):

\[-(\varepsilon_v + \rho \frac{\partial G}{\partial \sigma_v}) : \dot{\sigma}_v - (\varepsilon_0 + \rho \frac{\partial G}{\partial \sigma_0}) : \dot{\sigma}_0 - \rho G T \frac{\partial G}{\partial \xi} : \dot{\xi} \geq 0 \]

(26)

Using the method described by Coleman and Noll (1964), the volumetric and deviatoric infinitesimal strains and entropy are obtained:

\[ \varepsilon_v = -\rho \frac{\partial G}{\partial \sigma_v}, \quad \varepsilon_0 = -\rho \frac{\partial G}{\partial \sigma_0}, \quad s = -\frac{\partial G}{\partial T} \]

(27)

The Clausius–Planck inequality (26) is reduced to:

\[-\rho \frac{\partial G}{\partial \xi} : \dot{\xi} \geq 0 \]

(28)

In shape memory alloys, phase transformation is an energy dissipation process and transformation dissipation is defined as:

\[ D^\text{trans} = -\rho \frac{\partial G}{\partial \xi} : \dot{\xi} \geq 0 \]

(29)

The term \( \rho \frac{\partial G}{\partial \xi} : \dot{\xi} \) represents the rate of latent heat, where the thermodynamic forces associated with the internal variables can be defined as \( \rho \frac{\partial G}{\partial \xi} \). The two terms \( \rho \frac{\partial G}{\partial \xi} \) and \( \dot{\xi} \) have opposite signs, while \( \dot{\xi} \) is positive, the process is exothermic and \( \rho \frac{\partial G}{\partial \xi} \) is negative. The opposite happens when \( \dot{\xi} \) is negative and the process is endothermic.

Here, a constitutive assumption for the microscopic free energy \( G^\text{mic} \) of one plane on the shape memory alloys has to be made. In its general form, the microscopic free energy depends on the stress components \( \sigma_v, \sigma_0 \) as well as temperature \( T \), and one internal variable \( \xi \):

\[ G^\text{mic} = \tilde{G}^\text{mic}(\sigma_v, \sigma_0, T, \xi) \]

(30)

Stress traction vector in the microplane, illustrated in Fig. 2, is:

\[ \mathbf{t}_\sigma = \sigma \cdot \mathbf{n} = \sigma^\text{vol} + \sigma^\text{dev} \cdot \mathbf{n} = \frac{1}{3} \mathbf{1} : \sigma = \sigma^\text{vol} + \sigma^\text{dev} \cdot \mathbf{n} = \mathbf{V} : \sigma \cdot \mathbf{n} = \mathbf{V} \cdot \sigma \cdot \mathbf{n} = \sigma_v \mathbf{n} + \sigma_0 \]

(31)

Note that the macroscopic stresses are denoted by \( \sigma^\text{vol, dev} \) and their counterparts on each microplane are \( \sigma_v, \sigma_0 \). Also the volumetric and deviatoric microplane stress components are defined as:

\[ \sigma_v = \mathbf{V} : \sigma, \quad \sigma_0 = s - \sigma_v \cdot \mathbf{n} = \mathbf{D} : \sigma \]

(32)

where projection tensors \( \mathbf{D} \) is defined as (Leukart and Ramm, 2003):

\[ \mathbf{D} = \mathbf{n} : \varepsilon^\text{dev} \Rightarrow \mathbf{D}_{ik} = n_i \varepsilon_{jk} = n_i \left[ \frac{1}{2} (\delta_{ik} \varepsilon_{jk} + \delta_{ik} \varepsilon_{jk}) - \frac{1}{3} \delta_{ik} \varepsilon_{jk} \right] \]

(33)

The transpose of the deviatoric projection tensor \( \mathbf{D}^\text{T} \), is defined as:

\[ \mathbf{D}^\text{T} \Rightarrow \mathbf{D}^\text{T} = \mathbf{n} \Rightarrow \mathbf{D}^\text{T}_{ik} = n_i \varepsilon_{jk} = n_i \left( \frac{1}{2} (\delta_{ik} \varepsilon_{jk} + \delta_{ik} \varepsilon_{jk}) - \frac{1}{3} \delta_{ik} \varepsilon_{jk} \right) \]

(34)

Microplane strain components using work conjugate of the microplane stresses are defined as:

\[ \varepsilon_v = -\rho \frac{\partial G^\text{mic}}{\partial \sigma_v}, \quad \varepsilon_0 = -\rho \frac{\partial G^\text{mic}}{\partial \sigma_0} \]

(35)

These equations are extension of Eqs. (11) in the V–D split. Microplane dissipation in the microplane level is defined as Eq. (29):

\[ D^\text{mic} = -\rho \frac{\partial G^\text{mic}}{\partial \xi} : \dot{\xi} \]

(36)

Applying the chain rule to Eq. (30) with using Eqs. (31), (32), and (35):

\[ \varepsilon = -\rho \frac{\partial G}{\partial \sigma} = -\rho \frac{3}{2\pi} \int_\Omega \frac{\partial G^\text{mic}}{\partial \sigma} \, d\Omega \]

(37)

In order to satisfy the macroscopic dissipation inequality:

\[ D^\text{mic} = \frac{3}{2\pi} \int_\Omega \frac{\partial G^\text{mic}}{\partial \sigma} \, d\Omega \geq 0 \]

(38)

The total microplane energy dissipation on every microplane is required to be non-negative:

\[ D^\text{mic} \geq 0 \]

(39)

This equation is a stronger requirement than Eq. (38) and therefore represents a sufficient condition to fulfill the second law of thermodynamics.

To define the constitutive laws on the microplane level, 1D constitutive relations are used between the projected stresses and the corresponding strains. Since martensitic transformation induces shear deformation, shear is assumed to be the only source of inelastic behavior. Consequently, a 1-D SMA constitutive law is used for the shear direction and a linear elastic stress–strain relation is used for the normal direction. The local constitutive equations for the volumetric of the strain as well as the elastic part of the deviatoric strain are defined as follow:

\[ \varepsilon_v = \frac{\sigma_v}{E_v}, \quad \varepsilon_0 = \frac{\sigma_0}{E_0} \]

(40)
where $E^a$ and $E^g$ are local components of the linear elastic stiffness tensor. By substituting Eq. (40) into (37) and using Eq. (33) and following equation (Carol et al., 2004):

$$\frac{3}{2\pi} \int_{\Omega} \eta \eta \, d\Omega = \delta_{ij} \tag{41}$$

Macroscopic strain tensor after simplification is:

$$\varepsilon_{ij} = \frac{\sigma_{ij}}{E^a} + \frac{\sigma_{ij} \sigma_{kk}^a}{3} \left( \frac{1}{E^a} - \frac{1}{E^g} \right) \tag{42}$$

Eq. (42) can be compared with constitutive equation of a linear elasticity material:

$$\varepsilon_{ij} = \frac{1 + \nu}{E^a} \sigma_{ij} - \frac{\nu}{E^a} \sigma_{kk} \sigma_{ij} \tag{43}$$

The relations between local and global components of the modulus are derived as:

$$E^a_0 = \frac{E^a}{1 - 2\nu}, \quad E^g_0 = \frac{E^a_0}{1 + \nu} \tag{44}$$

where $\nu$ is Poisson’s ratio and $E$ is the Young’s modulus. It should be noted that Poisson’s ratio for austenite and martensite are assumed to be equal. Following Brinson and Huang (1996), Auricchio et al. (2007), we have adopted a Reuss scheme in this paper. The equivalent elastic modulus is:

$$\frac{1}{E^a_0} = \frac{1}{E^a} + \frac{1}{E^g_0} \tag{45}$$

Auricchio et al. (2007) have considered that SMA materials behave as austenite–martensite periodic composites. The total elongation of the composite in uniaxial loading is the sum of the elongation of the austenitic and the martensitic parts. From a mechanical point of view, austenitic and martensitic parts behave as two springs with different elastic properties acting in series. Therefore, Eq. (45) gives a lower bound for the overall equivalent elastic. It should be noted that, the realistic values would lie between Reuss and Voigt scheme, which provides an upper bound (Auricchio and Sacco, 1997). In addition, the elastic term, when compared with the inelastic term of the total strain, is significantly smaller. Therefore, predictions of both schemes are very close.

The local constitutive equations are obtained by substituting Eq. (44) into (40):

$$\varepsilon_{ij}^a = \frac{1 - 2\nu}{E^a} \sigma_{ij}^a, \quad \varepsilon_{ij}^g = \frac{1 + \nu}{E^a} \sigma_{ij}^g \tag{46}$$

The decomposition of the deviatoric microplane strain is defined as: $\varepsilon_{ij}^a = \varepsilon_{ij}^a + \varepsilon_{ij}^a$. Moreover, the inelastic tangential strain is considered to be in the form of:

$$\varepsilon_{ij}^a = \mathbf{R} \cdot \xi_{ij} \tag{47}$$

where $\mathbf{R}$ is a vector, $\varepsilon^r$ is the axial maximum recoverable strain, and $\xi_{ij}$ is the stress-induced martensite volume fraction that is (Brinson, 1993):

Conversion to Detwinned Martensite:

For $T > T_s^a$ and $\sigma_{ij}^a = C_M (T - T_s^a) < \sigma_{ij}^a = C_M (T - T_s^a)$:

$$\xi_{ij} = \frac{1 - \tilde{\xi}_{ij}}{2} \cos \left( \frac{\pi}{\sigma_{ij}^a - \sigma_{ij}^a} \times \left[ \sigma_{ij} - \sigma_{ij}^a = C_M (T - T_s^a) \right] \right) + \frac{1 + \tilde{\xi}_{ij}}{2} \tag{48}$$

For $T < T_s^a$ and $\sigma_{ij}^a < \sigma_{ij}^a$:

$$\xi_{ij} = \frac{1 - \tilde{\xi}_{ij}}{2} \cos \left( \frac{\pi}{\sigma_{ij}^a - \sigma_{ij}^a} \times \left[ \sigma_{ij} - \sigma_{ij}^a < C_M (T - T_s^a) \right] \right) + \frac{1 + \tilde{\xi}_{ij}}{2} \tag{49}$$

where $\tilde{\xi}_{ij}$ represents the detwinned martensite volume fraction prior to the current transformation, $T_s^a$, $T_g$, and $T_s^g$ are transformation temperatures, and $C_M$ and $C_A$ are the slope of martensite and austenite strips in the stress–temperature phase diagram shown in Fig. 3.

As these material parameters are obtained from uniaxial tensile tests, they have to be properly adjusted for shear direction. Martensite volume fraction is an internal variable and is calculated with Eqs. (48)–(50). According to these equations, it is clear that martensite fraction is a volumetric parameter. Therefore, it is constant in any direction of the material point. In addition, Kadkhodaei et al. (2008) shown that, transformation switching of all planes occurs according to the macroscopic response of SMAs. Therefore, a modification factor is considered to be equal to the exact ratio between each shear stress and the macroscopic effective stress $\bar{\sigma}$ applied at the material point. For example, while the factor $\tilde{\xi}_{ij}$ in deviatoric direction is used in the start and final transformation region:

$$\xi_{ij}(\sigma_D, T) = \frac{1 - \tilde{\xi}_{ij}}{2} \cos \left[ \frac{\pi}{\sigma_{ij}^a} \left( \sigma_{ij}^a - \sigma_{ij}^a = C_M (T - T_s^a) \right) \right] + \frac{1 + \tilde{\xi}_{ij}}{2} = \xi_{ij}(\bar{\sigma}, T) \tag{51}$$

So, the martensite fraction is a function of effective stress and consequently in all directions within all microplanes at a point are the same.

Therefore, relations between microplane stress and strain based on Volumetric–Deviatoric split (V–D) are as follows:

$$\sigma_{ij}^a = \frac{1 - 2\nu}{E^a} \sigma_{ij}, \quad \sigma_{ij}^g = \frac{1 + \nu}{E^a} \sigma_{ij} + \mathbf{R} \cdot \xi_{ij}(\bar{\sigma}, T) \tag{52}$$

Substituting Eq. (52) into (37) and using Eq. (32):

$$\varepsilon = \frac{3}{2\pi} \int_{\Omega} \left[ \frac{1 - 2\nu}{E^a} \mathbf{V} \cdot \sigma_{ij} + \frac{1 + \nu}{E^a} \xi_{ij}(\mathbf{V} \cdot \sigma_{ij}) \right] d\Omega + \frac{3}{2\pi} \int_{\Omega} \varepsilon^r \mathbf{Dev}^T \mathbf{R} \, d\Omega = \varepsilon^r + \varepsilon^p \tag{53}$$

Fig. 3. Critical stress–temperature phase diagram.
The elastic strain term is:
\[
\varepsilon^e = \frac{1 - 2\nu}{E(\zeta)} \mathbf{I}^{\text{vol}} \cdot \sigma + \frac{1 + \nu}{E(\zeta)} \mathbf{I}^{\text{dev}} \cdot \sigma \tag{54}
\]
and transformation strain term is:
\[
\varepsilon^T = \varepsilon^e \varsigma_s \frac{3}{2\pi} \int \mathbf{Dev}_v^T \cdot \mathbf{R} \, d\Omega \tag{55}
\]

Calculation of vector \( \mathbf{R} \) is one of the main points in this formulation. We assume that \( \varepsilon^0 \) (Superscript \( O \) refers to the traditional formulation introduced in relations (1)) in the V–D–T split formulations is equal to the \( \varepsilon^0 \) (Superscript \( N \) refers to the new formulation introduced in relations (52)), in V–D split and the \( \varepsilon^0 \) and \( \varepsilon^T \) in the V–D–T split are equal to the new \( \varepsilon^0 \), in V–D split formulation (Leukart, 2005; Mehrabi et al., 2013b):
\[
\varepsilon^0 = \varepsilon^N \tag{56a}
\]
\[
\varepsilon^0 + \varepsilon^T = \varepsilon^0 \tag{56b}
\]

It is clear that Eq. (56a) is satisfied and for Eq. (56b):
\[
\varepsilon^0 \mathbf{n} + \varepsilon^T \mathbf{t} = \varepsilon^0 \tag{57}
\]

Relationships between stress and strain from the V–D–T split (Mehrabi and Kadkhodaei, 2013a) are substituted into the left-hand side of Eq. (57):
\[
\frac{1 + \nu}{E(\zeta)} \mathbf{\sigma}_q \mathbf{n}_n + \frac{1 + \nu}{E(\zeta)} \mathbf{\sigma}^T_0 \mathbf{t}_n + \varepsilon^T \varsigma_n = \varepsilon^N \tag{58}
\]

substituting projected tensors into the left-hand side and Eq. (52) into the right-hand side of Eq. (58):
\[
\frac{1 + \nu}{E(\zeta)} \mathbf{\sigma}_q \left( \mathbf{n}_n \mathbf{n}_n - \frac{\varsigma_n}{3} \mathbf{I} \right) \mathbf{n}_n + \frac{1}{2} \mathbf{t}_n + \frac{1 + \nu}{E(\zeta)} \mathbf{\sigma}^T_0 \left( 2 \mathbf{n}_n \mathbf{n}_n - \frac{\varsigma_n}{3} \mathbf{I} \right) \mathbf{t}_n = \varepsilon^N \tag{59}
\]

Vector \( \mathbf{R}_n \) is simplified with using definition (33):
\[
\mathbf{R}_n = \mathbf{t}_n + \frac{1 + \nu}{E(\zeta)} \mathbf{\sigma}_q \left( \frac{1}{3} (\mathbf{n}_n \mathbf{n}_n - \frac{\varsigma_n}{3} \mathbf{I}) \mathbf{n}_n + \frac{1}{2} \mathbf{t}_n \right) + \frac{1 + \nu}{E(\zeta)} \mathbf{\sigma}^T_0 \left( \frac{1}{2} (\mathbf{n}_n \mathbf{n}_n - \frac{\varsigma_n}{3} \mathbf{I}) \mathbf{t}_n \right) \tag{60}
\]

Using Eqs. (33) and (34) into (53), elastic and transformation strain are:
\[
\varepsilon^e_{ij} = \frac{1 - 2\nu}{3E(\zeta)} \mathbf{\sigma}_{mn} \mathbf{\delta}_{ij} + \frac{1 + \nu}{E(\zeta)} \frac{3}{2\pi} \int_{\Omega} \left[ \frac{1}{2} \left( \mathbf{\sigma}_{mn} \mathbf{\sigma}^T_{mn} - \frac{3}{2} \mathbf{\sigma}_{mn} \mathbf{\sigma}^T_{mn} \right) \right] \, d\Omega \tag{61}
\]
and
\[
\varepsilon^T_{ij} = \varepsilon^e \varsigma_s \frac{3}{2\pi} \int \mathbf{Dev}^v_{ij} \mathbf{R}_n \, d\Omega \tag{62}
\]

It should be noted that in the microplane formulation described in this section, the homogenization procedure is based on integration over the surface of a unit sphere (\( \Omega \)). This integration is evaluated by follow discrete method:
\[
\int_{\Omega} f(x) \, d\Omega \approx \sum_{i=1}^{n} f(x_i) w_i \tag{63}
\]

3. Results and discussion

The objective of this section is to compare prediction of microplane models in both formulations of V–D–T split and V–D split with experimental results in uniaxial tension, pure torsion and proportional loading on a NiTi thin-walled tube.

It should be mentioned that the present simulations are based on the modified von Mises definition of the equivalent stress and strain for the macroscopic SMAs model. Numerical simulations use the same material parameters that are extracted in uniaxial loading and pure torsion.

The proposed model is implemented with a user subroutine (UMAT) in the commercially available finite element program ABAQUS. In simulation with ABAQUS, 1240 three dimensional eight-node continuous solid brick (C3D8R) elements are used to model an SMA thin-walled tube (Fig. 4). In numerical simulations produced by the UMAT, the time step is fixed at 0.01, and each step is divided into 100 increments. Material Jacobian and strain are calculated by Eqs. (61) and (62) in each increment. In the last step, stresses incremental are updated. All the reported results are for the outer diameter of the thin-walled tube. More details of the numerical implementation and computational algorithm in UMAT can be found in Mehrabi et al. (2014).

3.1. Experimental setup

All experiments are performed on NiTi thin-walled tubes with the length of 33 mm, outer diameter of 1.5 mm and thickness of 0.08 mm (Johnson Mathey). A BOST ElectroForce machine is used for mechanical tests. For the experimental work, uniaxial tension, pure torsion and proportional tension–torsion test are considered. For this purpose, a NiTi tube is under uniaxial tension and pure torsion on one end and the other end is fixed. In order to have a stable stress–strain behavior of the SMA tube, a series of 30 axial loading–

Fig. 4. Finite element model and boundary condition for a thin-walled tube under tension and torsion loadings.
unloading cycles are conducted. This training procedure was conducted at 323 K to obtain a stable response and remove residual strains possibly generated through the manufacturing processes. All of the mechanical tests were performed in strain control mode. The strain rate was 0.001/sec to simulate an isothermal loading condition and it is slow enough to prevent self-heating of the specimen and thus guarantees the isothermal condition. An infrared camera is used to record surface temperature of the specimen during the tests. Since the recorded temperature rise was less than 1 °C, experiments were deemed to be isothermal. Axial displacement and rotation were chosen as the control parameters in strain control tests. Force and torque were measured using an axial–torsional load cell (with the capacity of 4400 N tensile and 25 Nm torsion).

In order to calibrate material parameters, phase diagram (Fig. 3. Critical stress–temperature phase diagram) based on tangent intersection method is used (Lagoudas, 2008). Isothermal loading is applied to the trained thin-walled tube specimens at three different constant temperatures (296 K, 313 K and 323 K) to calibrate the material parameters. By measuring where transformations begin and end, a detailed phase diagram can be constructed. The material parameters calibrated from these uniaxial experiments are listed in Table 1. All of the tests are carried out at the room temperature of 296 K.

3.2. Uniaxial tension test

Fig. 5 shows the resulting axial stress–strain curves for uniaxial tension. Axial stress and axial strain on the outer surface of the tube is calculated by

$$\sigma = \frac{4F}{\pi (d_e^2 - d_i^2)}, \quad \epsilon = \frac{L}{L_0}$$

(64)

where $d_e$ and $d_i$ are the outer and inner diameter of the tube, respectively. The solid line corresponds to the microplane formulation with V–D split, and the dashed lines represent the results of the microplane formulation with V–D–T split. Both of these results are compared with experimental results. As this Figure shows, both formulations predict very close results. According to the Eq. (56), this result is expected.

3.3. Pure torsion test

It has been reported that the simple concept of von-Mises equivalence for describing the macroscopic material behavior is not sufficient to capture the complicated interaction of the microstructure with respect to the tension–compression asymmetry as well as the tension–torsion asymmetry (McNaney et al., 2003; Grabe and Bruhns, 2009; Andani et al., 2013). According to these findings, the modified effective stress is defined as:

$$\sigma = \sqrt{\sigma^2 + C_l^2 \tau^2}$$

(65)

where $\sigma$ and $\tau$ are macroscopic tensile and shear stresses, respectively. In addition, transformation strain of uniaxial and shear direction in Eq. (62) is:

$$\varepsilon_{11}^{\text{tr}} = \varepsilon_{11}^\epsilon \frac{3}{2\pi} \int_\Omega \left( R_{11} n_1 - \frac{1}{3} n_i n_i \right) d\Omega$$

(66)

$$\varepsilon_{22}^{\text{tr}} = \frac{\varepsilon_{12}^\epsilon}{C_e} \frac{3}{2\pi} \int_\Omega \frac{1}{2} \left( R_{12} n_2 + R_{21} n_1 \right) d\Omega$$

(67)

It should be noted that only shear direction of transformation strain is divided to an empirical coefficient.

Empirical coefficients $C_e$ and $C_s$ are defined by Eq. (68). These two parameters are calculated experimentally for every specimen and are equal to 1.1 and 2.5 for the NiTi thin-walled tube, respectively.

$$C_i = \frac{\sigma_m}{\varepsilon_m} = \frac{224}{204} = 1.1, \quad C_e = \frac{\gamma_m}{\varepsilon_m} = \frac{0.0134}{0.0053} = 2.5$$

(68)

Here $\sigma_m$ and $\varepsilon_m$ are shown in Fig. 5 and $\tau_m$ and $\gamma_m$ are shown in Fig. 6.

Fig. 6 shows the resulting shear stress–shear strain curves for pure torsion. Shear stress and shear strain on the outer surface of the tube are calculated through

$$\tau = \frac{16Td_o}{\pi (d_o^2 - d_i^2)} , \quad \gamma = \frac{d_i \theta}{2L}$$

(69)

where $T$ and $\theta$ are torque and angle of rotation, respectively. The solid line corresponds to the microplane formulation with V–D split and the dashed lines represent the results of the microplane formulation with V–D–T split. These results are compared with experimental data and show a good agreement with experiment results.

It should be noted that a reason for the discrepancy between model predictions and experimental data could be due to the effect of material texture on the yield transformation and the transformation strain. As the present microplane model does not take into account the effect of the material texture, some discrepancy can occur with experimental data.

These results show that the new formulation based on the V–D split can predict as well as V–D–T split in uniaxial and pure shear, while the new formulation also guarantees thermodynamic consistency. It should be emphasized that our modification is on the thermodynamic consistency not only improving the numerical results. Also it should be noticed that these two formulations yield the same numerical results since adjustment is done to obtain the present formulation.

3.4. Proportional loading test

As both formulations predict the same results in different loadings, only a microplane model based on V–D split is considered in this section. In order to demonstrate aspects of the proposed new formulation, proportional loading is experimentally performed, and the findings are compared with the obtained numerical results using the same material parameters extracted in uniaxial loading. The studied proportional loading path is shown in Fig. 7. Thereby, maximum displacement reached to 1.5 mm and maximum rotations is reached to 1.57 radian simultaneously and both of them remove to zero in the second step. Two repetitions are carried out for each loading path.

The proposed model predictions are reasonably similar to the experimental results as shown in Fig. 8. Uniaxial stress–uniaxial strain and shear stress–shear strain responses are shown in Fig. 8(a) and (b). Fig. 8(c) shows effective stress versus effective
strain using Eq. (65) for the effective stress and following equation for the effective strain:

\[ \varepsilon = \sqrt{\varepsilon^2 + \gamma^2 C_e} \]  

(70)

where \( \varepsilon \) and \( \gamma \) are macroscopic uniaxial strain and macroscopic shear strain, respectively.

According to Fig. 8(c), there is a reasonable agreement between microplane predictions and experimental results.

The effective stress–strain corresponding to the proportional loading and uniaxial tension are shown in Fig. 9. This shows that the effective stress–strain curve corresponding to the proportional loading is similar to axial stress–strain curve corresponding to the uniaxial tension. This implies that the behavior of the SMA polycrystal under nonproportional loading can be characterized by the effective stress–strain obtained from uniaxial or proportional experiment (Sittner et al. (1995)). Sittner et al. (1995) showed that the effective stress–strain corresponding to different nonproportional loadings were consistent with the uniaxial loading.

It should be noted that polycrystalline tube samples show very strong tension–compression asymmetry (Orgéas and Favier, 1998; Lim and McDowell, 1999). Asymmetry behavior in tension–compression is believed to be due to the texture-induced anisotropy in the macroscopic model. Therefore, modeling of this behavior is an interesting topic in the literature (Poorasadion et al., 2013). In our initial attempts, because the grips were design for tension and torsion test, under compression, the thin-walled tube buckled.

Fig. 5. Comparison of microplane formulation based on V–D–T split and V–D split with experiment results in uniaxial loading.

Fig. 6. Comparison of microplane formulation based on V–D–T split and V–D split with experiment results in pure torsion.

Fig. 7. Proportional loading path.
microplane modeling based on Volumetric–Deviatoric–Tangential (V–D–T) split: (1) microplane strains might not be conjugate with their microplane stress counterparts, and (2) the second principle of thermodynamics might be violated in certain loading conditions. The proposed Volumetric–Deviatoric (V–D) split addresses these issues. Theory predictions verify that macroscopic dissipation might expressed as the integral of dissipation on each microplane, so the energy dissipation on each plane is guaranteed to be nonnegative. Therefore, the second law of thermodynamics is satisfied for the macroscopic equations.

New formulations are compared numerically with V–D–T split model and shows that both formulations predict the same results. Predicted results of two formulations are compared with experiment results and good agreement between results verify constitutive modeling of shape memory alloys in a thermodynamically-consistent approach. In the future, the asymmetric and anisotropic behavior need to be more thoroughly investigated.

Fig. 8. Comparison of the microplane formulation based on V–D split with experimental data in proportional loading: (a) axial stress–strain, (b) shear stress–strain, (c) effective stress–strain.

Fig. 9. Effective stress–strain at different loading paths.

4. Conclusion

In this work, a constitutive model for shape memory alloys within the concept of the microplane theory with a thermodynamically-consistent approach was proposed and implemented. This model resolve the following shortcomings of the former constitutive

References


