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Chapter 9

Modeling and Simulation of Shape Memory Alloys using Microplane Model

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Abstract

In this chapter, a three-dimensional phenomenological constitutive model for the simulation of shape memory alloys is introduced. The proposed macromechanical model is based on microplane theory. Microplane approach is chosen to have limited material parameters in that all of those are measurable by simple tests. User material subroutine is developed to implement the proposed model in a commercial finite element package. NiTi hollow tube specimens are under various loading conditions in order to experimentally study the superelastic response of shape memory alloys. Comparing experimental data with numerical results in simple tension and pure torsion as well as proportional and nonproportional tension-torsion loadings demonstrates the capability of proposed model in constitutive modeling of shape memory alloys.

Keywords: Shape memory alloy, phenomenological model, microplane, proportional, nonproportional, experiment

1. Introduction

Shape memory alloys (SMAs) can recover their original shape when subjected to thermomechanical loading. If the original shape is remembered under external load, it is in superelastic form, and when the original shape is remembered under thermal load, it is in shape memory effect form. Commercial applications of these materials get more attention in recent years. Some of these unique properties are including biocompatibility, good mechanical properties

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(very similar to the different parts of human body), hysteresis damping, excellent fatigue properties in cyclic loads, and strain hardening. These characteristics make them attractive for diverse fields of application such as biomedical tools (blood clot filters, vascular stents, orthodontic arches), aerospace applications (space shuttle, morphing aircraft, hydraulic fittings and couplings for airplanes), automotive (engines and actuators for smart systems, thermostats), robotic (human robots, artificial muscle), eyeglass frames, cellular phone antennae, coffee maker, and so on [1-9].

In order to design new application of shape memory alloys, basic understanding behavior of these materials under different conditions is essential. Different aspects of SMAs are identified with constitutive modeling. Most models are based on thermodynamics using free energy formulation. However, some models are based on micromechanics concepts or macromechanics model [10]. Micromechanic models deal with crystallographic texture in microscale response of SMAs [11-17]. These models are used to model the phase transformation and grains propagation and consequently are appropriate for modeling the response of SMAs at the microscale [18]. In order to study SMAs polycrystalline, crystallographic texture is a key property. A micromechanic model for single crystals is used to study polycrystal structures [19]. In the micromechanics models, a volume fraction coefficient is defined for variants, and transformation strain is obtained from martensite variants by averaging procedure.

Even though micromechanical models reflect microscopic physical nature of SMAs, they are not suitable for finite element implementation and structural analysis. Therefore, macromechanical models based on phenomenological findings are proposed. These models are efficient in modeling the thermomechanical behavior of SMAs in different engineering applications. In a macromechanic model, macro-scale response of SMAs is considered [20-24]. Phenomenological models belong to a class of macromechanic models that are defined by macroscopic energy functions. These models are calibrated from material characterization and experimental data that depend on the internal variables.

Macrophenomenological models are categorized to one- and three-dimensional models. One-dimensional models are used for the simulation of wire and bar samples under uniaxial loads, while 3-D models can be used for complicated devices under complex loadings. Since most SMA devises are used in multidimensional or under complex loadings, one-dimensional models should extend to three-dimensional models. Three-dimensional constitutive modeling is an important step in analysis and design of SMAs in different industries. Some of the existing macro phenomenological models with specifications and limitations are summarized in Table 1.

Group	Formulation	Characteristics	Limitation
Tanaka [25]	Helmholtz free energy	(1) 1-D model (2) Exponential phase transformation equation	3-D, shape memory
Liang and Rogers [26]	Helmholtz free energy	(1) 1-D model, extension of the Tanaka model (2) Cosine phase transformation equation	Shape memory

Group	Formulation	Characteristics	Limitation
Brinson [27]	Helmholtz free energy	(1) 1-D model, martensite volume fraction separate into two parts induced by stress and temperature (2) Cosine phase transformation equation (3) Different elastic moduli for austenite and martensite	3-D
Auricchio et al. [22, 28]	Based on phase diagram	(1) 1-D and 3-D model (2) Finite-strain regime, rate-dependent behavior (3) Asymmetry behavior and numerical implementation	Shape memory
Lagoudas et al. [2, 20, 29-31]	Gibbs free energy	(1) 3-D model, exponential phase transformation equation (2) Tension-compression asymmetry behavior (3) Nonassociated flow rule during reverse transformation	Depend on the specific alloy
Panico and Brinson [32]	Helmholtz free energy	(1) 3-D model, extension of the Lexcellent model [33, 34] (2) Variant reorientation modeling under nonproportional loadings (3) Computational modeling of porous SMAs	Depend on the specific alloy
Helm and Haupt [35]	Free energy	(1) 3-D model based on continuum thermodynamics framework (2) Simulation of nonproportional loading (3) Finite strain regime	Depend on the specific alloy
Oliveira et al. [36]	Helmholtz free energy	(1) 3-D model (2) Based on Fremond's method (3) Asymmetric behavior and based on plasticity	Unmeasurable material parameter
Brocca et al. [37]	Microplane theory	(1) 3-D model (2) Constant module for different phases (3) Simulation of nonproportional loading	Fundamental concept need to be revised
Arghavani et al. [21, 38]	Helmholtz free energy	(1) 3-D model (2) Finite deformations (3) Martensite volume fraction is a scalar parameter and variant orientation is a tensor	Unmeasurable material parameter
Saleeb et al. [23, 39]	Gibbs free energy	(1) 3-D model (2) Deviation from normality and reorientation under nonproportional loading (3) Cyclic behavior	Unmeasurable material parameter
Mehrabi et al. [40, 41]	Gibbs free energy	(1) 3-D model, microplane formulation	Under investigation

Group	Formulation	Characteristics	Limitation
		(2) Anisotropic behavior under nonproportional loadings (3) Tension-compression asymmetry and numerical implementation	
Patoor et al. [15, 39, 42]	Gibbs free energy	(1) 3-D model (2) Tension-compression asymmetry (3) Cyclic behavior and nonproportional loading	Unmeasurable material parameter
Zaki et al. [43-46]	Helmholtz free energy	(1) 3-D model (2) cyclic and asymmetry behavior (3) Capture plastic deformations	Unmeasurable material parameter

Table 1. Macromechanical models

One-dimensional constitutive model was proposed by Tanaka [47] based on exponential phase transformation equation. Liang and Rogers [26] proposed a one-dimensional phase transformation based on cosine type. Martensite volume fraction suggested by Liang and Rogers is modified by Brinson [27] into two different parts. These two fractions included martensite volume fraction induced by stress and temperature. This assumption was done to distinct superelastic behavior from shape memory effect. Boyd and Lagoudas [30] had developed 1-D model to 3-D constitutive model. For this development, they used effective stress and strain in phase transformation equations. A three-dimensional constitutive model includes twinned martensite and detwinned martensite. In addition, multidimensional models could predict behavior of shape memory effect as well as superelastic behavior. A 3-D model based on the phase transformation equation of exponential type was proposed by Peng et al. [48]. They used classical plastic theory and defined equivalent stress and strain for modeling SMA response. Reali et al. [22] proposed a 3-D constitutive model, which is capable of simulating superelastic and shape memory behavior. Proposed model is developed within the framework of thermodynamics by defining a scalar and a tensorial internal variable [21]. The 3-D phenomenological model demonstrates the ability of developed model in proportional and nonproportional loadings. In most existing 3-D phenomenological constitutive models, some internal variables are necessary to be calibrated. In calibration process, most models estimate various material parameters in which some of those are not simply measurable by experimental tests. Among various phenomenological models, the microplane model is utilized due to its simplicity and the limited material parameters needed for calibration.

The behavior of some quasi-brittle materials, such as concrete, soil, and stiff foams, is studied using the microplane method [49-52]. A one-dimensional phase transformation model using microsphere formulation was proposed by Ostwald et al. [53] to simulate the polycrystalline materials. The three-dimensional model based on the microplane model was proposed by Brocca et al. [37]. In the microplane model, all material parameters can be determined from uniaxial tension tests at different temperatures. The microplane model considers 1-D equations for some directions on arbitrary plane and is extended to 3-D model using homogenization process [54]. Mehrabi et al. [40, 41, 55] developed this idea within the framework of thermodynamics and proved the capability of the proposed model under multiaxial loadings. Some unique characteristics of SMAs such as deviation from normality in nonproportional loading, anisotropic behavior, and tension-compression asymmetry behavior of SMAs were studied by Mehrabi et al. [56, 57] using the microplane approach.

The proposed microplane model is implemented in a standard commercial finite element package. Some experimental studies under tension, torsion, proportional, and nonproportional loadings have been performed on SMA hollow tubes to assess the proposed model [58]. The numerical results extracted from the microplane model compared with experimental data demonstrate the ability of the microplane approach.

2. Phenomenological constitutive modeling

In this section, phenomenological model based on microplane theory is used to describe SMAs material behavior in a simple way. The general definition of the microplane approach is that the 1-D constitutive law is defined for associated normal and tangential stress/strain components on any microplane at each material point. The generalization of 1-D equation to 3-D model is done by homogenization process. In microplane formulation, strain tensor is in closed form of stress tensor. Mehrabi and co-workers have done a thorough research on 3-D phenomenological model based on microplane theory to demonstrate their model features [40, 41, 55, 57, 59, 60]. The three main steps of the microplane model are summarized in Figure 1.

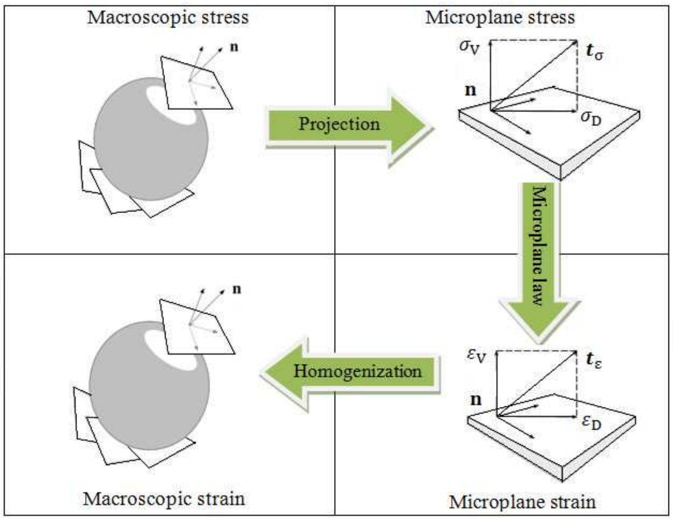

Figure 1. General schematic of the microplane model based on the volumetric-deviatoric split.

For any plane on the shape memory alloys, microscopic Gibbs free energy (G^{mic}) is defined as

$$G^{mic} = \hat{G}^{mic}\left(\sigma_V, \boldsymbol{\sigma}_D, T, \xi\right) \tag{1}$$

Here, σ_{V} and $\boldsymbol{\sigma}_{\mathrm{D}}$are stress components on each microplane, T is temperature, and ξ is martensite volume fraction, which is defined as internal variable [27, 61].

Macroscopic strain tensor is defined as [41]

$$\begin{aligned}\boldsymbol{\varepsilon} &= -\rho\frac{\partial G}{\partial \boldsymbol{\sigma}} = -\rho\frac{3}{2\pi}\int_{\Omega}\frac{\partial G^{\mathrm{mic}}}{\partial \boldsymbol{\sigma}}\mathrm{d}\Omega = \\ &= \frac{3}{2\pi}\int_{\Omega}\left[-\rho\frac{\partial G^{\mathrm{mic}}}{\partial \sigma_{\mathrm{V}}}\frac{\partial \sigma_{V}}{\partial \boldsymbol{\sigma}} - \rho\frac{\partial G^{\mathrm{mic}}}{\partial \boldsymbol{\sigma}_{\mathrm{D}}}\frac{\partial \boldsymbol{\sigma}_{D}}{\partial \boldsymbol{\sigma}}\right]\mathrm{d}\Omega = \\ &= \frac{3}{2\pi}\int_{\Omega}\left(\varepsilon_{\mathrm{V}}\mathbf{V} + \mathbf{Dev}^{\mathrm{T}}.\boldsymbol{\varepsilon}_{\mathrm{D}}\right)d\Omega\end{aligned} \tag{2}$$

These integrals calculated on different orientations of hemisphere at a material point. Projection tensor ***Dev*** and the transpose of the deviatoric projection tensor $\boldsymbol{Dev}^{\mathrm{T}}$ are defined as [62]

$$\mathbf{Dev} := \boldsymbol{n}.\mathbf{I}^{\mathrm{dev}}, \mathbf{Dev}^{\mathrm{T}} := \mathbf{I}^{\mathrm{dev}}.\boldsymbol{n} \tag{3}$$

in which $\boldsymbol{n}$ represents the unit normal vector on the plane and $\boldsymbol{I}^{\mathrm{dev}}$ is deviatoric projection tensor (forth-order identity tensor) that is defined as follows

$$\mathbf{I}^{\mathrm{dev}} = \frac{3}{2\pi}\int_{\Omega}\mathbf{Dev}^{\mathrm{T}}.\mathbf{Dev}d\Omega \tag{4}$$

The local 1-D constitutive laws in the volumetric and deviatoric components of the strain for SMAs are defined as

$$\varepsilon_{\mathrm{V}} = \frac{\sigma_{\mathrm{V}}}{E_{\mathrm{V}}^{0}},\ \boldsymbol{\varepsilon}_{\mathrm{D}} = \frac{\boldsymbol{\sigma}_{\mathrm{D}}}{E_{\mathrm{D}}^{0}} + \mathbf{R}\varepsilon^{*}\xi \tag{5}$$

where ε^{*} is the axial maximum recoverable strain, $E_{\mathrm{V}}^{0}$and E_{D}^{0} are the local linear elastic modulus, which are a function of the global elastic constants. Transformation strain is only initiated in deviatoric direction of microplanes.

Here a standard procedure in the microplane model [57] is used to generalize the 1-D equations to 3-D formulation. Macroscopic strain tensor for shape memory alloys is calculated as

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{e} + \boldsymbol{\varepsilon}^{tr} = \frac{3}{2\pi}\int_{\Omega}\left(\frac{1-2\upsilon}{E(\xi)}\mathbf{V}\otimes\mathbf{V}:\boldsymbol{\sigma} + \frac{1+\upsilon}{E(\xi)}\mathbf{Dev}^{\mathrm{T}}.\mathbf{Dev}:\boldsymbol{\sigma}\right)d\Omega + \frac{3}{2\pi}\int_{\Omega}\varepsilon^{*}\xi\mathbf{Dev}^{\mathrm{T}}.\mathbf{R}\ d\Omega \tag{6}$$

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where R is a vector that is defined in reference [41]. In order to numerically calculate these integrals, an integration technique consisting of 21 Gaussian integration points is utilized [63].

3. Experimental study

In order to have a robust constitutive modeling, an experimental study of polycrystalline SMAs gets more attention in recent years. Since some SMA devices experience complex loading paths, investigation of material behavior under multiaxial loadings is essential. Some of the experimental findings are summarized in Table 2. In this table, some of the famous groups and loading schemes on the specific materials are introduced. As it is shown, most experimental studies are on the NiTi materials and copper based SMAs.

Group	Specification	Material
Sittner et al. [64, 65]	Tension-Torsion	CuAlZnMn
Jacobus et al. [66, 67]	Triaxial stress	CuZnAl, NiTi
Tokuda et al. [68, 69]	Tension-Torsion	CuAlZnMn
Lim and McDowell [70]	Tension-Torsion	NiTi
McNaney et al. [71]	Tension-Torsion	NiTi
Grabe and Bruhns [72, 73]	Tension-Torsion	NiTi
S. Arbab-Chirani and C. Lexcellent [74, 75]	Tension-Pressure-Torsion	CuAlBe, NiTi
Wang et al. [76, 77]	Tension-Torsion	NiTi
Reedlunn et al. [78]	Tension-Pressure-Bending	NiTi
Mehrabi et al. [55-58]	Tension-Torsion	NiTi

Table 2. Experimental study

A vast experimental study of the NiTi hollow tubes under uniaxial tension, pure torsion, and proportional and nonproportional tension-torsion were done by the author in the Dynamic and Smart Systems Laboratory at the University of Toledo, USA. The Johnson Matthey provided NiTi tube specimens, and the experimental tests were performed using BOSE ElectroForce machine. All mechanical tests were performed at room temperature, and in order to have an isothermal condition, the loading rate was below $10^{-3}s^{-1}$ [76]. The experimental results are compared with numerical findings to show the capability of the proposed approach in the next section.

4. Numerical simulation

In order to use microplane approach to simulate real SMA devices, the proposed model is implemented and developed into the FE code. The computational algorithm is outlined in Table 3.

1. Import the strain increment and the stress evaluated from ABAQUS
2. Check for transformation according to the phase diagram and compute the transformation strain if necessary
3. Compute the elastic strain
4. Compute the total strain
5. Compute the Jacobian matrix
6. Compute the incremental stress tensor
7. Update stress
8. End the program

Table 3. Algorithm for implementation of constitutive modeling of SMA

Tensile and torsional tests are conducted on the NiTi tubes to investigate the capability of the microplane approach in capturing the behavior of SMAs. The material parameters calibrated for the microplane model are listed in Table 4 [55].

Symbols	Values	Units
E_A	20,000	MPa
E_M	13,300	MPa
$\upsilon_A = \upsilon_M$	0.33	
T_f^M	-32	$^\circ C$
T_s^M	-15	$^\circ C$
T_s^A	-5	$^\circ C$
T_f^A	15	$^\circ C$
σ_s^{cr}	20	MPa
σ_f^{cr}	100	MPa
C_M	6	MPa / $^\circ C$
C_A	8.2	MPa / $^\circ C$
ε^*	0.038	

Table 4. Material properties

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Figures 2 and 3 represent comparison between the axial stress-strain responses of the microplane model and the experimental results as well as shear stress-strain response at room temperature. These comparisons confirm the fact that material parameter calibration process is done as well. Calibrated material parameters are constant during numerical study of proportional and nonproportional loadings.

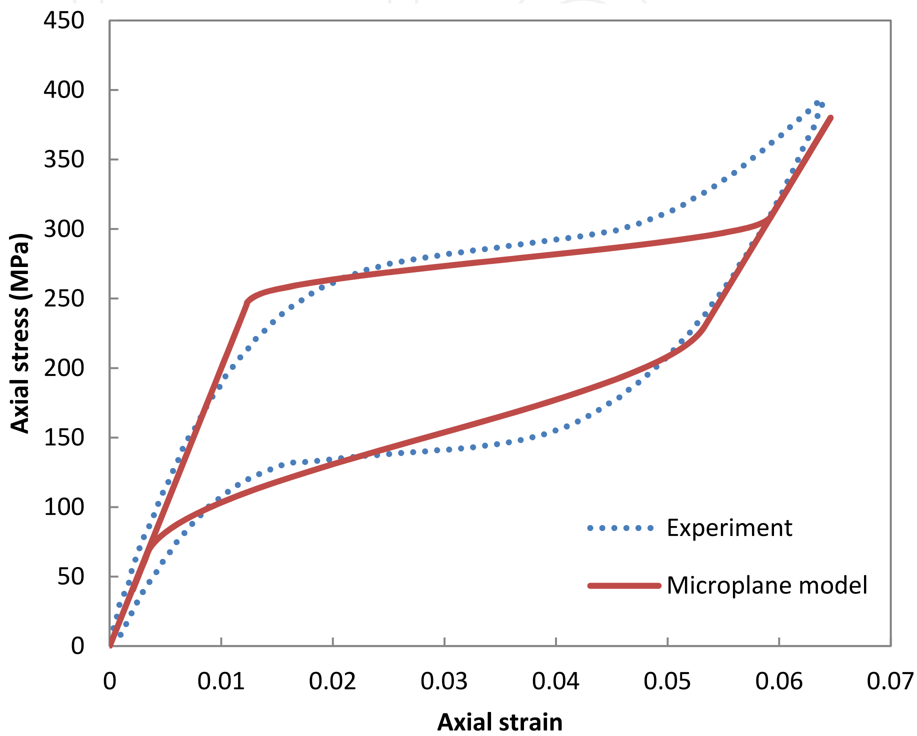

Figure 2. Comparison of the microplane model with experimental result [55].

To demonstrate other aspects of the microplane model, proportional tension-torsion loading is experimentally performed. Proportional loading path is shown in Figure 4(a). According to this loading path, axial stress and shear stress are increasing in step 1 and are decreasing to zero during step 2. The experimental findings are compared with the numerical results for axial stress-strain and shear stress-strain in Figures 4(b) and (c). The studied proportional loading demonstrates the capability of the proposed model.

In order to show the capability of the proposed approach in multiaxial loading, one complex loading path is considered here. In Figure 5, nonproportional tension-torsion loading path is shown. At first, shear stress increases while axial stress is zero. During step 2, shear stress is constant, and axial stress increases. Then, shear stress and axial stress are recovered to zero, respectively. Experimental results are compared with microplane numerical results in Figure 6. Comparison of results shows that the proposed model has good agreement with experimental results in both axial stress-strain and shear strain-axial strain. It is obvious that a discrepancy between experimental results and numerical results in the shear stress-strain curve is found. As the proposed model could predict general behavior of SMAs in different loadings, this negligible discrepancy is acceptable.

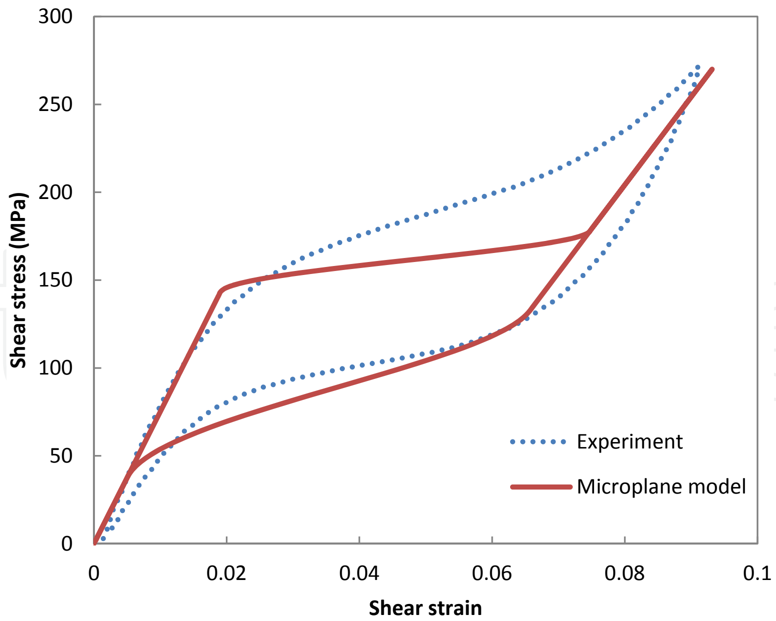

Figure 3. Comparison of the microplane model with experimental result [55].

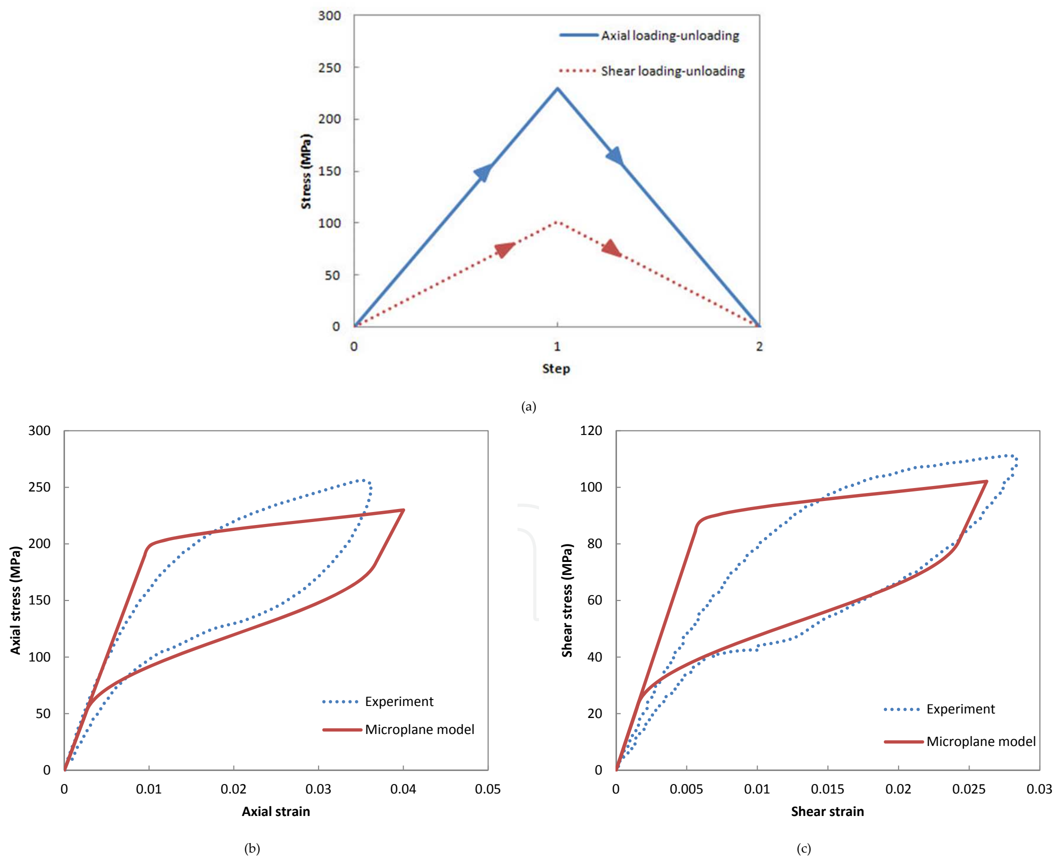

Figure 4. Comparison of the microplane model with experimental result in proportional loading: (a) proportional loading path, (b) axial stress-strain, (c) shear stress-strain [55].

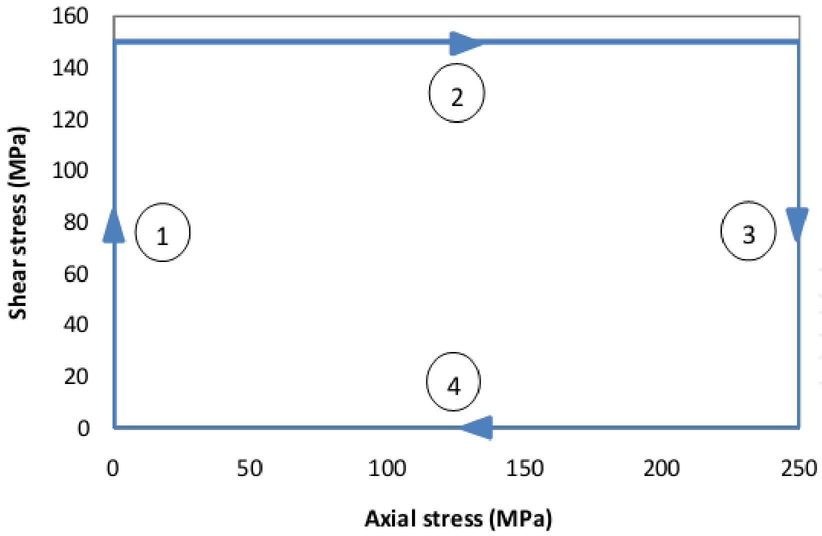

Figure 5. Nonproportional loading path.

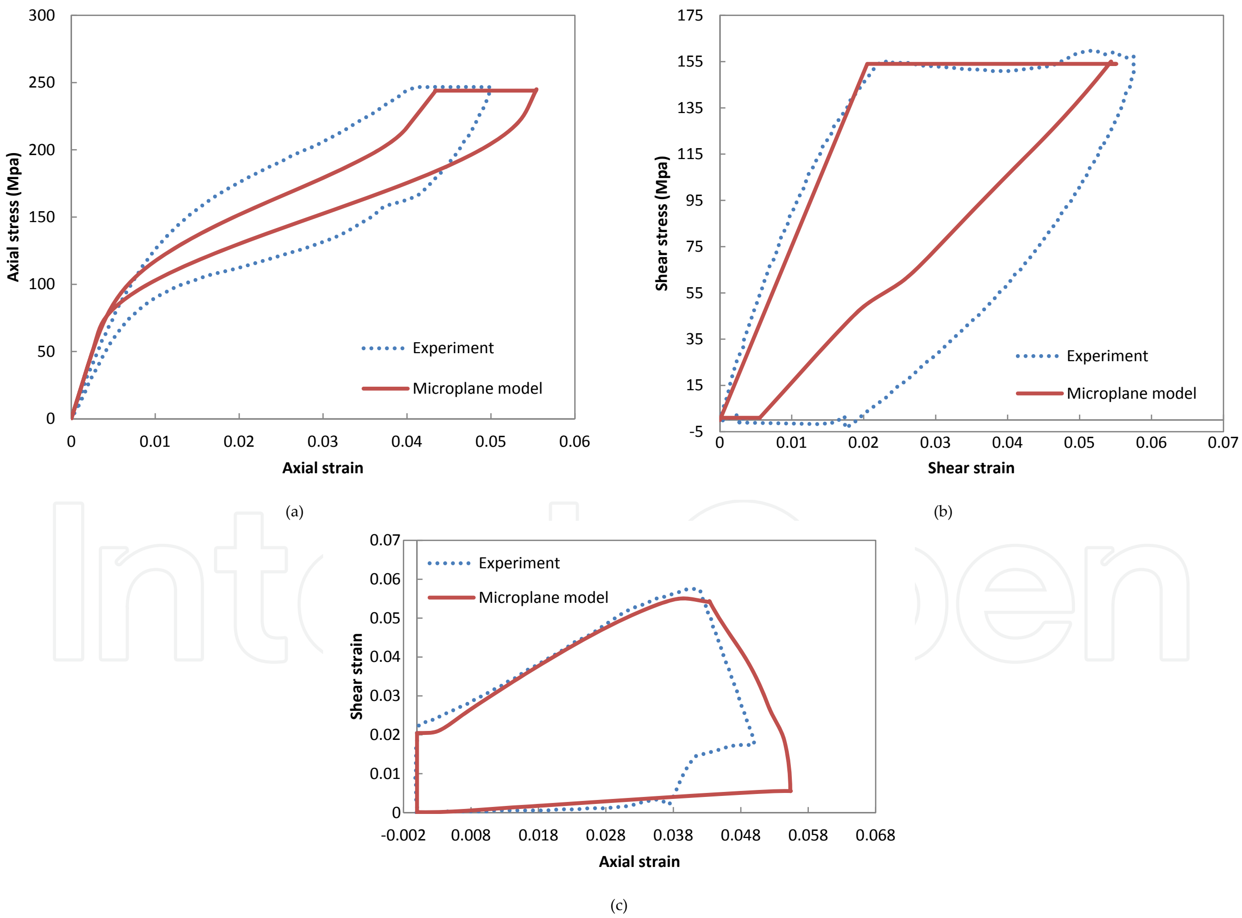

Figure 6. Comparison of the microplane model with experimental result in nonproportional loading: (a) axial stress-strain, (b) shear stress-strain, (c) axial strain-shear strain [57].

In recent years, some biomedical applications [5] such as stent [79], catheters [80], muscle [81], artificial muscles [82], and shape memory implants [83] are produced by SMAs. Therefore, the simulation of biomedical devices using 3-D finite element method [84] is an interesting topic that leads to future works.

5. Conclusion

Constitutive modeling of shape memory alloys (SMAs) is a key property that leads researchers to find new engineering applications. Phenomenological modeling in macroscopic frame is an appropriate way for modeling the thermomechanical response of SMAs. One of the unique constitutive models based on the microplane model is utilized to investigate behavior of SMAs. Material parameters defined in the proposed model are limited and are calibrated with simple experimental tests. The proposed model is developed to implement and analyze in a finite element package. Some multiaxial loadings as proportional and nonproportional loadings are investigated with constitutive model. Numerical results in comparison of experimental findings show the microplane approach ability in simulation of SMAs behavior.

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