MICROMECHANICAL MODELING OF POROUS SHAPE MEMORY ALLOYS

A Dissertation

by

PAVLIN BORISSOV ENTCHEV

Submitted to the Office of Graduate Studies of Texas A&M University in partial fulfillment of the requirements for the degree of DOCTOR OF PHILOSOPHY

May 2002

Major Subject: Aerospace Engineering
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Major Subject: Aerospace Engineering
ABSTRACT

Micromechanical Modeling of
Porous Shape Memory Alloys. (May 2002)

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A thermomechanical constitutive model for fully dense shape memory alloys (SMAs) is developed in this work. The model accounts for development of transformation and plastic strains during martensitic phase transformation, as well as for the evolution of the transformation cycle. The developed model is used in a micromechanical averaging scheme to establish a micromechanics-based model for the macroscopic mechanical behavior of porous shape memory alloys. The derivation of the micromechanical model is presented for the general case of a composite with phases undergoing rate-independent inelastic deformations. Micromechanical averaging techniques are used to establish the effective elastic and inelastic behavior based on information about the mechanical response of the individual phases and shape and volume fraction of the inhomogeneities. An explicit expression for the effective tangent stiffness and an evolution equation for the effective inelastic strain are derived. A detailed study on the choice of the pore shape is performed for a random distribution of pores. The material parameters used by the model are estimated for the case of porous NiTi SMA processed from elemental powders and the results of the model simulations are compared with the experimental data. The numerical implementation of the model is also presented in this work. Various loading cases for porous SMA bars have been simulated using the implementation of the model.
To My Wife,

Natasha

My Son,

Bogdan

and My Parents,

Stoyanka and Boris
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CHAPTER I

INTRODUCTION
This chapter will cover some general aspects of Shape Memory Alloys (SMAs), including a brief description of the martensitic phase transformation, some commonly used SMAs, their thermomechanical characteristics and commercial applications. An overview of the latest developments in the area of porous SMAs will be given. The available constitutive models for fully dense SMAs as well as for porous SMAs will also be reviewed. Finally, the objectives of the current research effort will be outlined.

1.1. General Aspects of Shape Memory Alloys

SMAs are metallic alloys which can recover permanent strains when they are heated above a certain temperature. The key characteristic of all SMAs is the occurrence of a martensitic phase transformation. The martensitic transformation is a shear-dominant diffusionless solid-state phase transformation occurring by nucleation and growth of the martensitic phase from a parent austenitic phase (Olson and Cohen, 1982). When an SMA undergoes a martensitic phase transformation, it transforms from its high-symmetry, usually cubic, austenitic phase to a low-symmetry martensitic phase, such as the monoclinic variants of the martensitic phase in a NiTi SMA.

The martensitic transformation possesses well-defined characteristics that distinguish it among other solid state transformations:

1. It is associated with an inelastic deformation of the crystal lattice with no diffusive process involved. The phase transformation results from a cooperative and collective motion of atoms on distances smaller than the lattice parameters.

The journal model is Mechanics of Materials.
The absence of diffusion makes the martensitic phase transformation almost instantaneous (Nishiyama, 1978).

2. Parent and product phases coexist during the phase transformation, since it is a first order transition, and as a result there exists an invariant plane, which separates the parent and product phases. The lattice vectors of the two phases possess well defined mutual orientation relationships (the Bain correspondences, see Bowles and Wayman, 1972), which depend on the nature of the alloy.

3. Transformation of a unit cell element produces a volumetric and a shear strain along well-defined planes. The shear strain can be many times larger than the elastic distortion of the unit cell. This transformation is crystallographically reversible (Kaufman and Cohen, 1958).

4. Since the crystal lattice of the martensitic phase has lower symmetry than that of the parent austenitic phase, several variants of martensite can be formed from the same parent phase crystal (De Vos et al., 1978).

5. Stress and temperature have a large influence on the martensitic transformation. Transformation takes place when the free energy difference between the two phases reaches a critical value (Delaey, 1990).

Due to their unique properties, SMAs have attracted great interest in various fields of applications ranging from aerospace (Jardine et al., 1996; Liang et al., 1996) and naval (Garner et al., 2000) to surgical instruments (Ilyin et al., 1995) and medical implants and fixtures (Brailovski and Trochu, 1996; Gyunter et al., 1995). The SMAs have been used in coupling devices (Melton, 1999), as actuators in a wide range of applications (Ohkata and Suzuki, 1999) as well as in medicine and dentistry (Miyazaki, 1999).
These applications have mostly benefited from the ability of the inherent shape recovery characteristics of SMAs. In addition to the shape memory and pseudoelasticity effects that SMAs possess, there is also the promise of using SMAs in making high-efficiency damping devices that are superior to those made of conventional materials, partially due to their hysteretic response.

A relatively new area of applications utilizing the properties of SMAs is the area of active composites (Lagoudas et al., 1994). The design of these composites involves embedding SMA elements in the form of wires, short fibers, strips or particles into a matrix material. Controlling the phase transformation of the SMA inclusions through heating or cooling allows to control the overall behavior of the composite and change its macroscopic properties (Birman, 1997).

1.2. Characteristics of the Martensitic Transformation in Polycrystalline Shape Memory Alloys

The martensitic transformation (austenite-to-martensite) occurs when the free energy of martensite becomes less than the free energy of austenite at a temperature below a critical temperature $T_0$ at which the free energies of the two phases are equal. However, the transformation does not begin exactly at $T_0$ but, in the absence of stress, at a temperature $M_0^{s}$ (martensite start), which is less than $T_0$. The free energy necessary for nucleation and growth is responsible for this shift (Delaey, 1990). The transformation continues to evolve as the temperature is lowered until a temperature denoted $M_0^{f}$ is reached. For SMAs, the temperature difference $M_0^{s} - M_0^{f}$ is small compared to that for the martensitic transformation in ferrous alloys ($\sim 40^\circ C$ for SMAs versus $\sim 200^\circ C$ for ferrous alloys). This temperature difference $M_0^{s} - M_0^{f}$ is an important factor in characterizing shape memory behavior.
When the SMA is heated from the martensitic phase in the absence of stress, the reverse transformation (martensite-to-austenite) begins at the temperature $A^{0s}$ (austenite start), and at the temperature $A^{0f}$ (austenite finish) the material is fully austenite. The equilibrium temperature $T_0$ is in the neighborhood of $(M^{0s} + A^{0f})/2$. The spreading of the cycle $(A^{0f} - A^{0s})$ is due to stored elastic energy, whereas the hysteresis $(A^{0s} - M^{0f})$ is associated with the energy dissipated during the transformation.

Due to the displacive character of the martensitic transformation, applied stress plays a very important role. During cooling of the SMA material below temperature $M^{0s}$ in absence of applied stresses, the variants of the martensitic phase arrange themselves in a self-accommodating manner through twinning, resulting in no observable macroscopic shape change (see the stress-temperature diagram shown in Figure 1). By applying mechanical loading to force martensitic variants to reorient (detwin) into a single variant, large macroscopic inelastic strain is obtained. After heating to a higher temperature, the low-symmetry martensitic phase returns to its high-symmetry austenitic phase, and the inelastic strain is thus recovered. The martensitic phase transformation can also be induced by pure mechanical loading while the material is in the austenitic phase, in which case detwinned martensite is directly produced from austenite by the applied stress (Stress Induced Martensite, SIM) at temperatures above $M^{0s}$ (Wayman, 1983).

As a result of the martensitic phase transformation, the stress-strain response of SMAs is strongly non-linear, hysteretic, and a very large reversible strain is exhibited. This behavior is strongly temperature-dependent and very sensitive to the number and sequence of thermomechanical loading cycles. In addition, microstructural aspects have considerable influence on the stress-strain curve and on the strain-temperature curves. In polycrystals, the differences in crystallographical orientation
among grains produce different transformation conditions in each grain. The polycrystalline structure also requires the satisfaction of geometric compatibility conditions at grain boundaries, in addition to compatibility between austenite and the different martensitic variants. Thus, the martensitic transformation is progressively induced in the different grains and, as opposed to the single crystal case, no well-defined onset of the transformation is observed. In addition, the hysteresis size increases, and the macroscopic transformation strain decreases.

The austenite-to-martensite transformation is accompanied by the release of heat corresponding to the transformation enthalpy (exothermic phase transformation). The martensite-to-austenite (reverse) transformation is an endothermic phase trans-
formation accompanied by absorption of thermal energy. For a given temperature, the amount of heat is proportional to the volume fraction of the transformed material. This heat release (heat absorption) is utilized by the Differential Scanning Calorimetry (DSC) method to measure the transformation temperatures. Other methods, as the measurement of the electrical resistivity, internal friction, thermoelectric power and the velocity of sound are also used in establishing the values of the transformation temperatures (Jackson et al., 1972).

The key effects of SMAs associated with the martensitic transformation, which are observed according to the loading path and the thermomechanical history of the material are: pseudoelasticity, one-way shape memory effect and two-way shape memory effect. In this section, the characteristics associated with these classes of behavior are presented, and the various strain mechanisms behind these effects are described.

1.2.1. Shape Memory Effect

An SMA exhibits the *Shape Memory Effect* (SME) when it is deformed while in the martensitic phase and then unloaded while still at a temperature below $M_f^0$. If it is subsequently heated above $A_f^0$ it will regain its original shape by transforming back into the parent austenitic phase. The nature of the SME can be better understood by following the process described above in a stress-temperature phase diagram schematically shown in Figure 2. The parent austenitic phase (indicated by A in Figure 2) in the absence of applied stress will transform upon cooling to multiple martensitic variants (up to 24 variants for the cubic-to-monoclinic transformation) in a random orientation and in a twinned configuration (indicated by B). As the multivariant martensitic phase is deformed, a detwinning process takes place, as well as growth of certain favorably oriented martensitic variants at the expense of other variants. At
the end of the deformation (indicated by C) and after unloading it is possible that only one martensitic variant remains (indicated by D). Upon heating, when temperature reaches \( A_{\text{gs}} \), the reverse transformation begins to take place, and it is completed at temperature \( A_{\text{of}} \). The highly symmetric parent austenitic phase (usually with a cubic symmetry) forms only one variant, and thus the original shape (before deformation) is regained (indicated by E). Note that subsequent cooling will result in multiple martensitic variants with no substantial shape change (self-accommodated martensite). Also, note in Figure 2 that, in going from A to B many variants will start nucleating from the parent phase, while in going from D to E there is only one variant of the parent phase that nucleates from the single remaining martensitic variant indicated by D.

The stress-free cooling of austenite produces a complex arrangement of several variants of martensite. Self-accommodating growth is obtained such that the average macroscopic transformation strain equals zero (Otsuka and Wayman, 1999b; Saburi, 1999; Saburi et al., 1980), but the multiple interfaces present in the material (boundaries between the martensite variants and twinning interfaces) are very mobile. This great mobility is at the heart of the SME. Movement of these interfaces accompanied by detwinning is obtained at stress levels far lower than the plastic yield limit of martensite. This mode of deformation, called reorientation of variants, dominates at temperatures lower than \( M_{\text{of}} \).

The above described phenomenon is called one-way shape memory effect (or simply, shape memory effect) because the shape recovery is achieved only during heating. The first step in the loading sequence induces the development of the self-accommodated martensitic structure, and no macroscopic shape change is observed. During the second stage, the mechanical loading in the martensitic phase induces reorientation of the variants and results in a large inelastic strain, which is not recov-
Fig. 2. Schematic representation of the thermomechanical loading path demonstrating the shape memory effect in an SMA.

The pseudoelastic behavior of SMAs is associated with recovery of the transformation strain upon unloading and encompasses both superelastic and rubberlike behavior (Otsuka et al., 1976; Otsuka and Wayman, 1999a). The superelastic behavior is observed
Fig. 3. Schematic of a stress-strain-temperature curve showing the shape memory effect.

during loading and unloading above $A_{0s}$ and is associated with stress-induced martensite and reversal to austenite upon unloading. When the loading and unloading of the SMA occurs at a temperature above $A_{0s}$, partial transformation strain recovery takes place. When the loading and unloading occurs above $A_{0f}$, full recovery upon unloading takes place. Such loading path in the stress-temperature space is schematically shown in Figure 4. Initially, the material is in the austenitic phase (point A). The simultaneous transformation and detwinning of the martensitic variants starts at point B and results in fully transformed and detwinned martensite (point C). Upon
unloading, the reverse transformation starts when point D is reached. Finally, at the end of the loading path (point E) the material is again in the austenitic phase.

Fig. 4. Schematic of a thermomechanical loading path demonstrating pseudoelastic behavior of SMAs.

If the material is in the martensitic state and detwinning and twinning of the martensitic variants occur upon loading and unloading, respectively, by reversible movement of twin boundaries, this phenomenon is called rubberlike effect (Otsuka and Wayman, 1999a). The rubberlike effect is less common, while the superelastic effect is very common in almost all SMAs.

Three distinct stages are observed on the uniaxial stress-strain curve representing the superelastic behavior of an SMA, schematically shown in Figure 5. For stresses
below $\sigma^{Ms}$, the material behaves in a purely elastic way. As soon as the critical stress is reached, forward transformation (austenite-to-martensite) initiates and stress-induced martensite starts forming. During the formation of SIM large transformation strains are generated (upper plateau of stress-strain curve in Figure 5). When the applied stress reaches the value $\sigma^{Mf}$ the forward transformation is completed and the SMA is in the martensitic phase. For further loading above $\sigma^{Mf}$ the elastic behavior of martensite is observed. Upon unloading, the reverse transformation initiates at a stress $\sigma^{As}$ and completes at a stress $\sigma^{Af}$. Due to the difference between $\sigma^{Mf}$ and $\sigma^{As}$ and between $\sigma^{Ms}$ and $\sigma^{Af}$ a hysteretic loop is obtained in the loading/unloading stress-strain diagram. Increasing the test temperature results in an increase of the values of critical transformation stresses, while the general shape of the hysteresis loop remains the same.

Fig. 5. Schematic of the superelastic behavior of SMAs.
Upon cooling under a constant applied stress from a fully austenitic state, it is observed that the transformation is characterized by a martensite start temperature \( M^{\sigma_s} \) and a martensite finish temperature \( M^{\sigma_f} \), which are functions of the applied stress. Macroscopic transformation strain obtained in that way (Figure 6) is a result of martensite formation and detwinning of the martensitic variants due to the applied load. The transformation strain is several orders of magnitude greater than the thermal strain corresponding to the same temperature difference required for the phase transformation. A hysteresis loop is observed for the cooling/heating cycle as shown in Figure 6 due to the fact that the reverse transformation begins and ends at different temperatures than the forward transformation does.

1.2.3. Behavior of SMAs Undergoing Cyclic Loading

The superelastic behavior described in Section 1.2.2 constitutes an approximation to the actual behavior of SMAs under applied stress. In fact, only a partial recovery of the transformation strain induced by the applied stress is observed. A small residual strain remains after each unloading. Further cooling of the material, in the absence of applied stress, is now related to the occurrence of a macroscopic transformation strain contrary to what is observed in the SMA material before cycling. Experimental results on the behavior of SMAs undergoing cyclic loading have been presented by Bo and Lagoudas (1999a); Kato et al. (1999); Lim and McDowell (1999, 1994); McCormick and Liu (1994); Strnadel et al. (1995a,b) and Sehitoglu et al. (2001), among others. The thermomechanical cycling of the SMA material results in training process as first observed by Perkins (1974). Different training sequences can be used (Contardo and Guénin, 1990; Miller and Lagoudas, 2001), i.e., by inducing a non-homogeneous plastic strain (torsion, flexion) at a martensitic or austenitic phase; by aging under applied stress, in the austenitic phase, in order to stabilize the parent phase, or
in the martensitic phase, in order to create a precipitant phase (Ni-Ti alloys); by thermomechanical, either superelastic or thermal cycles.

The main result of the training process is the development of Two-Way Shape Memory Effect (TWSME). In the case of TWSME, a shape change is obtained both during heating and cooling. The solid exhibits two stable shapes: a high-temperature shape in austenite and a low-temperature shape in martensite. Transition from the high-temperature shape to the low-temperature shape (and reverse) is obtained without any applied stress assistance.
In contrast with the previously discussed properties of SMAs (superelasticity, one-way shape memory) that are intrinsic, the TWSME is an acquired characteristic. In the heart of the TWSME is the generation of internal stresses and creation of permanent defects during training. The process of training leads to the preferential formation and reversal of a particular martensitic variant under the applied load. Generation of permanent defects eventually creates a permanent internal stress state, which allows for the formation of the preferred martensitic variant in the absence of the external load.

Another effect of the training cycle is the development of macroscopically observable plastic strain. The magnitude of this strain is comparable to the magnitude of the recoverable transformation strain. The training also leads to secondary effects, like change in the transformation temperatures, change in the hysteresis size and decrease in the macroscopic transformation strain. These effects are similar to those observed during thermomechanical fatigue tests (Rong et al., 2001). It is important to define optimal conditions of training, because an insufficient number of training cycles produces a non-stabilized two-way memory effect and over-training generates unwanted effects that reduce the efficiency of training (Stalmans et al., 1992).

1.3. Porous Shape Memory Alloys — Characteristics and Applications

Driven by biomedical applications, recent emphasis has been given to porous SMAs. The possibility of producing SMAs in porous form opens new fields of application, including reduced weight and increased biocompatibility. Perhaps the most successful application of porous SMAs to this date is their use as bone implants (Ayers et al., 1999; Shabalovskaya et al., 1994; Simske et al., 1997). One of the main reasons for such a success is the biocompatibility of the NiTi alloys used in the above cited works.
In addition, the porous structure of the alloys allows ingrowth of the tissue into the implant.

In the last several years since the fabrication techniques for porous SMAs have been established, additional applications have also been considered. The potential applications of porous SMAs utilize their ability to carry significant loads. Beyond the energy absorption capability of dense SMA materials, porous SMAs offer the possibility of higher specific damping capacity under dynamic loading conditions. One of the applications, which utilizes the energy absorption capabilities of the porous SMAs, is the development of effective dampers and shock absorbing devices. It has been demonstrated that a significant part of the impact energy is absorbed (Lagoudas et al., 2000a). The reason for such high energy absorption is the sequence of forward and reverse phase transformations in the SMA matrix. In addition to the inherent energy dissipation capabilities of the SMA matrix, it is envisioned that the pores will facilitate additional absorption of the impact energy due to wave scattering. This phenomenon has been studied in great detail by Sabina et al. (1993); Sabina and Willis (1988) and Smyshlyaev et al. (1993a,b). However, the effect of wave scattering in porous SMAs has not been investigated yet.

Another advantage of the porous SMAs over their fully dense counterparts is the possibility to fabricate them with gradient porosity. This porosity gradient offers enormous advantage in applications involving impedance matching at connecting joints and across interfaces between materials with dissimilar mechanical properties. The use of such porous SMA connecting elements will prevent failure due to wave reflections at the interfaces, while at the same time providing the connecting joint with energy absorption capabilities. Also currently of great interest is the use of porous SMAs in various vibration isolation devices. It is envisioned that such devices will find applications in various fields ranging from isolation of machines and equip-
ment to isolation of payloads during launch of space vehicles. To increase the energy absorption capabilities a second phase, which would fill the pores can be added. It should be noted that these latest developments are still being actively researched and have not yet been used in commercial applications.

Different fabrication techniques for producing porous SMAs have been established. While some of the works focus on fabrication of porous SMAs by injecting a gas into a melt (Hey and Jardine, 1994), most of the research work on fabrication of porous SMAs has focused on using powder metallurgy techniques (Goncharuk et al., 1992; Itin et al., 1994; Li et al., 1998; Martynova et al., 1991; Shevchenko et al., 1997; Tangaraj et al., 2000; Vandygriff et al., 2000; Yi and Moore, 1990). Different fabrication techniques for producing porous SMAs from elemental powders have been used. Some of the difficulties that may be encountered with the use of elemental powders include contamination from oxides and the formation of other intermetallic phases. On the other hand, producing pre-alloyed NiTi powder requires processing techniques which are both difficult and expensive due to the hardness of the alloy.

Techniques that are currently being used to produce porous NiTi from elemental powders include self-propagating high-temperature synthesis, conventional sintering, and sintering at elevated pressures via a Hot Isostatic Press (HIP). Some advantages of sintering at elevated pressure include shorter heating times than conventional sintering and the ability to produce near net shape objects that require less time to machine. The current work uses porous NiTi fabricated using the HIPping technique. The process is presented in detail by Vandygriff et al. (2000) and is not discussed here. Two different porous NiTi alloys were obtained: at lower fabrication temperature ($\approx 940^\circ$C) a porous material with smaller pore sizes is obtained, while for higher temperature ($\approx 1000^\circ$C) the sizes of the pores are significantly larger. Micrographs of both large and small pore specimens are shown in Figure 7.
1.4. Review of the Models for Dense and Porous SMAs

During the last two decades significant advancements in the area of constitutive modeling of SMAs have been reported. In addition to the models developed for fully dense SMAs, models for porous SMAs have started to appear during recent years. Achievements in both of these areas are summarized in the following subsections.

1.4.1. Modeling of Fully Dense SMAs

The area of constitutive modeling of fully dense SMAs has been a topic of many research publications in recent years. The majority of the constitutive models re-
ported in the literature can be formally classified to belong to one of the two groups: micromechanics-based models and phenomenological models. Representative works from both of these groups are reviewed in a sequel.

The essence of the micromechanics-based models is in the crystallographic modeling of a single crystal or grain and further averaging of the results over a representative volume element (RVE) to obtain a polycrystalline response of the SMA. Such models have been presented in the literature by different researchers. As an example, the micromechanics-based model based on the analysis of phase transformation in single crystals of copper-based SMAs has been presented by Patoor et al. (1988, 1994, 1996). The behavior of a polycrystalline SMA is modeled by utilizing the model for single crystals and using the self-consistent averaging method to account for the interactions between the grains. A micromechanical model for SMAs which is able to capture different effects of SMA behavior such as superelasticity, shape memory effect and rubber-like effect has been presented by Sun and Hwang (1993a,b). In their work, the evolution of the martensitic volume fraction is obtained by balancing the internal dissipation during the phase transformation with the external energy output. One of the recent micromechanical models for SMA has been presented by Gao et al. (2000a,b). The advantage of the crystallographical models is their ability to predict the material response using only the crystallographical parameters (e.g., crystal lattice parameters). Thus, their use provides valuable insight on the phase transformation process on the crystal level. Their disadvantage, however, is in the large number of numerical computations required to be performed. Thus the use of such models for modeling structural response is not feasible.

Contrary to the crystallographical models, in the case of the phenomenological models a macroscopic energy function is proposed and used in conjunction with the second law of thermodynamics to derive constraints on the constitutive behavior of
the material. Thus the resulting model does not directly predict the behavior of the material on microscopic level, but the effective behavior of the polycrystalline SMA. These models have the advantage of being easily integrated into an existing structural modeling system, e.g., using the finite element method.

Some of the early three-dimensional models from this group were derived by generalizing the one-dimensional results, such as the models by Boyd and Lagoudas (1994); Liang and Rogers (1992) and Tanaka et al. (1995). In a publication by Lagoudas et al. (1996) it has been shown that various phenomenological models can be unified under common thermodynamical formulation. The differences between the models arise due to the specific choice of transformation hardening function. More recent phenomenological models have also been presented by Auricchio et al. (1997); Leclercq and Lexcellent (1996); Levitas (1998); Reisner et al. (1998); Rengarajan et al. (1998) and Rajagopal and Srinivasa (1999). In a recent work Qidwai and Lagoudas (2000b) presented a general thermodynamic framework for phenomenological SMA constitutive models, which for different choice of the transformation function can be tuned to capture different effects of the martensitic phase transformation, such as pressure dependance and volumetric transformation strain.

In addition to modeling of the development of transformation strain during martensitic phase transformation, several other modeling issues have also been topics of intensive research. One of the most important problems recently addressed by the researchers is the behavior of SMAs under cycling loading. During cycling phase transformation a substantial amount of plastic strains is accumulated. In addition, the transformation loop evolves with the number of cycles and TWSME is developed. Based on the experimental observations researchers have attempted to create models able to capture the effects of cycling loading. One-dimensional models for the behavior of SMA wires under cycling loading have been presented by Lexcellent and
Bourbon (1996); Lexcellent et al. (2000); Tanaka et al. (1995) and Abeyaratne and Kim (1997), among others. A three-dimensional formulation is given by Fischer et al. (1998). Their model defines a transformation function to account for the development of the martensitic phase transformation and a separate yield function to account for the development of plasticity. However, neither the identification of the material parameters nor implementation of the model is presented in that work. One of the most recent works on the cyclic behavior of SMA wires has been presented in a series of papers by Bo and Lagoudas (1999a,b,c) and Lagoudas and Bo (1999). In that work most of the issues regarding behavior of SMA wires under cycling loading, including the development of TWSME, have been addressed and the results compared with the experimental data.

While most of the constitutive models for dense SMAs assume that the material exhibits rate-independent behavior, a notable exception from this is the model developed by Abeyaratne and Knowles (1993) and Abeyaratne et al. (1993, 1994). Abeyaratne and Knowles (1994a,b, 1997) have applied their model to model the propagation of phase boundaries in an SMA rod.

1.4.2. Modeling of Porous SMAs

In this subsection the models potentially applicable to modeling of porous SMAs are reviewed. Since the porous SMA can be viewed as a composite with an SMA matrix and the pores as the second phase, the models presented for active SMA-based composites are also reviewed.

A great number of research papers have appeared in the literature devoted to modeling of porous materials. While some of them deal with the elastic response of the materials, the inelastic and more specifically, plastic behavior has also been a topic of research investigations. Different aspects of modeling of porous and cellular solids
are presented by Green (1972); Gurson (1977); Jeong and Pan (1995) and Gibson and Ashby (1997), among others. The idea behind the works of Green (1972) and Gurson (1977) is to derive a macroscopic constitutive model with an effective yield function for the onset of plasticity. In addition, the work of Gurson (1977) deals with the nucleation and evolution of porosity during loading. A comprehensive study on porous and cellular materials is presented in the book by Gibson and Ashby (1997). However, most of the modeling in that work is presented in the context of a single cell modeling for high-porosity materials. The cells are modeled using the beam theory to account for the ligaments between the pores. In addition, the walls of the pores in the case of closed cell porosity are modeled as membranes. Both the elastic properties as well as the initiation of plasticity are modeled.

Since the emerging of the SMA-based active composites their modeling has been the subject of a number of research papers. One approach to modeling of these composites is to extend the theories for linear composites, which is well developed (e.g., see the review papers by Willis, 1883, 1981 and the monograph by Christensen, 1991).

Some of the modeling work on SMA composites has been performed using the approximation of an existence of a periodic unit cell (Achenbach and Zhu, 1990; Lagoudas et al., 1996; Nemat-Nasser and Hori, 1993). One of the recent works on porous SMAs also used the unit cell approximation to evaluate the properties of porous SMAs (Qidwai et al., 2001). Even though the existence of periodic arrangement of pores in a real porous SMA material is an approximation, this assumption provides insight into global material behavior in the form of useful limiting values for the overall properties. Additionally, an approximate local variation of different field variables like stress and strain indicating areas of concentration due to porosity can be obtained. These results may provide design limitations in order to minimize or even
avoid micro-buckling, plastic yielding and consequently loss of phase transformation capacity over number of loading cycles. The assumption of periodicity and symmetry boundary conditions reduce the analysis of the porous SMA material to the analysis of a unit cell. In addition, appropriate loading conditions need to be applied, which do not violate the symmetry of the problem (Qidwai et al., 2001). In a recent work DeGiorgi and Qidwai (2001) have investigated the behavior of porous SMA using a mesoscale representation of the porous structure. In addition, DeGiorgi and Qidwai (2001) have studied the effect of filling the pores with a second polymeric phase.

The variational techniques have initially been used to establish bounds on the properties of linear composites. Various bounds have been presented in the literature, ranging from the simplest Reuss and Voigt bounds (Christensen, 1991; Paul, 1960) to Hashin–Shtrikman bounds (Hashin and Shtrikman, 1963; Walpole, 1966). The variational techniques have also been extended to obtain estimates for the behavior of non-linear composites. Most notably, in the works of Talbot and Willis (1985) and Ponte Castañeda (1996) bounds for the properties of non-linear composites have been reported.

Micromechanical averaging techniques have also been used to determine the averaged macroscopic composite response. Among the micromechanics averaging methods, the two most widely used are the self-consistent method and the Mori–Tanaka method. Both approaches are based on the presumption that the effective response of the composite can be obtained by considering a single inhomogeneity embedded in an infinite matrix. According to the self-consistent method (Budiansky, 1965; Hershey, 1954; Hill, 1965; Kröner, 1958) the interactions between the inhomogeneities are taken into account by associating the properties of the matrix with the effective properties of the composite, i.e., embedding the inhomogeneity in an effective medium. Some self-consistent results for spherical pores in an incompressible material are presented.
by Budiansky (1965). Contrary to this approach, the Mori–Tanaka method initially suggested by Mori and Tanaka (1973) and further developed by Weng (1984) and Benveniste (1987) takes into account the interactions between the inhomogeneities by appropriately modifying the average stress in the matrix from the applied stress, while the properties of the matrix are associated with the real matrix phase. These averaging techniques can also be used to determine the averaged macroscopic response of the porous material with random distribution of pores. In this case the material is treated as a composite with two phases: dense matrix and pores.

Recently, both averaging approaches have been applied to obtain effective properties of composites with inelastic phases. For example, a variant of the self-consistent method using incremental formulation (Hutchinson, 1970) has been used to model composites undergoing elastoplastic deformations. Lagoudas et al. (1991) have used an incremental formulation of the Mori–Tanaka method to obtain the effective properties of a composite with an elastoplastic matrix and elastic fibers. Boyd and Lagoudas (1994) have applied the Mori–Tanaka micromechanical method to model the effective behavior of a composite with elastomeric matrix and SMA fibers and have obtained the effective transformation temperatures for the composite. In a different work, Lagoudas et al. (1994) have applied the incremental Mori–Tanaka method to model the behavior of a composite with elastic matrix and SMA fibers. Another group of researchers (Cherkaoui et al., 2000) has applied the self-consistent technique to obtain the effective properties of a composite with elastoplastic matrix and SMA fibers. A two-level micromechanical method has been presented by Lu and Weng (2000), where the SMA constitutive behavior has been derived at the microscopic level and the overall composite behavior has been modeled at the mesoscale level using the Mori–Tanaka method.

In summary, it should be mentioned that all of the methods have their advantages
as well as disadvantages. The approach offered by Gibson and Ashby (1997) requires the existence of a very regular pore structure and is applicable only for high-porosity materials (porosity on the order of 90%). Similarly, the unit cell methods are accurate for regular pore structure. The advantage of these methods is that they can accurately model the stress distribution in the vicinity of the pore boundaries and are not limited by the shape of the pores. The difficulty associated with these methods is their computational intensity which makes them not feasible for structural calculations. On the other hand, the phenomenological approach, presented by Green (1972); Gurson (1977) and Jeong and Pan (1995) can easily be adapted to model large structural systems. Its disadvantage is the fact that the effect of pore shapes and orientations on the properties of the porous SMA cannot easily be taken into account.

The micromechanical averaging techniques combine some of the advantages of both of the approaches. While the pore shape choices are limited to ellipsoids, pores with any orientations can easily be taken into account. By varying the ratio of the axes of the ellipsoid, different shapes (e.g., cylinders, prolate and oblate spheroids, cracks) can be represented. The micromechanical averaging schemes can also easily be implemented numerically to model structural response of complex systems.

1.5. Outline of the Present Research

The research effort presented in this work is divided into two major parts. The first part is devoted to the constitutive modeling of fully dense SMAs using a phenomenological constitutive model. The second part describes the modeling of porous SMAs using micromechanical averaging techniques. Thus, the research objectives are summarized as follows:
1. Develop a three-dimensional constitutive model for fully dense SMAs which is able to account for non-linear transformation hardening, simultaneous development of transformation and plastic strains during phase transformation and evolution of the material behavior during cyclic loading. The experimental observations for the mechanical behavior of porous SMAs in the pseudoelastic regime have shown that a significant part of the developed strain is not recovered upon unloading. Even upon heating the specimen in a furnace with no load applied this unrecoverable strain remains unchanged. Thus, the development of this strain has been attributed to plasticity (Lagoudas and Vandygriff, 2002). As described in the literature review, similar observations are presented in the literature for fully dense SMAs. Therefore, to be able to successfully model the behavior of porous SMAs, a model for the dense SMA matrix which is able to capture the development of plastic strains is needed. However, the majority of such models found in the literature have one-dimensional formulation. Due to the three-dimensional effects existing in a porous SMA, its successful modeling requires a three-dimensional model. A three-dimensional model for sequential transformation and plasticity is presented by Fischer et al. (1998). However, the current work will focus on modeling of simultaneous phase transformation and plasticity, i.e., development of plastic strains during the phase transformation. The three-dimensional model development will follow the methodology presented for the one-dimensional case by Bo and Lagoudas (1999a,b,c) and Lagoudas and Bo (1999). Since the above-mentioned works describe the behavior of SMAs undergoing temperature-induced transformation, the necessary modifications to adapt the formulation for the case of stress-induced martensitic transformation will be made.
2. **Develop a macroscopic thermomechanical constitutive model for the porous SMA material using micromechanical averaging techniques.**

The current work will extend micromechanical averaging techniques for inelastic composites to establish a macroscopic constitutive model for the porous SMA material. The micromechanical methods based on Eshelby’s solution will be used in incremental formulation. The response of the porous SMA will be deducted using the properties of the dense SMA and information about pore shape, orientation and volume fraction. Analytical expressions for the overall elastic and tangent stiffness of the porous SMA material will be derived and an evolution equation for the overall transformation strain will also be derived. The derivations will first be given for the more general case of a two-phase composite with rate-independent constituents. After the derivation of the general expressions, the properties of the porous SMA material will be obtained by using the constitutive model for dense SMA developed in this work to model the matrix, and treating the inhomogeneities as elastic phases with stiffness equal to zero.

3. **Provide a detailed procedure for the estimation of the material parameters for the model using experimental data and demonstrate the capabilities of the model by comparing the model simulations to the results from the available experiments.** The material parameters used by the model in characterizing the porous SMA material will be identified and their values will be estimated using the experimental results for porous NiTi SMA. Porous NiTi alloys fabricated from elemental powders will be used in this research effort. Two different porous SMAs will be tested under compressive loading. The complete set of material parameters for both alloys will be pre-
4. **Develop a numerical implementation of the thermodynamical constitutive model for both dense and porous SMAs.** The numerical implementation of the model for dense SMAs using return mapping algorithms will be presented. The numerical implementation of the model for porous SMAs will be accomplished using the implementation of the model for dense SMAs and the direct iteration method. The derivations of the numerical implementation will be given in a sufficiently general form suitable for any displacement-based numerical code. The approach presented by Qidwai and Lagoudas (2000a) for the fully dense SMA model with a polynomial hardening function will be followed. The model will be implemented as a user-material constitutive subroutine for the finite element package ABAQUS.

The content of each chapter of this work is as follows: in Chapter II the derivations of the fully dense SMA constitutive model are given. The chapter contains sections on the identification of the internal state variables, their evolution and on the estimation of the material parameters. The numerical implementation of the model is presented in Chapter III, which also contains a section on the comparison of the model simulations with the experimental results. Chapter IV proceeds with the derivation of the micromechanical averaging model for porous SMAs. Detailed derivations of the effective elastic stiffness, effective tangent stiffness and the evolution of the effective inelastic strain is presented. The numerical implementation of the model for porous SMAs is discussed in Chapter V. The estimation of the material parameters for the porous NiTi SMA and results for numerical simulation of various boundary value problems for porous SMA bars are also presented in Chapter V. A summary of the research effort presented in this work as well as recommendations for
future work on the subject are presented in Chapter VI.

The direct notation is adopted in this work. Capital bold Latin letters represent fourth-order tensors (effective stiffness \( \mathbf{L} \), compliance \( \mathbf{M} \), etc.) while bold Greek letters are used to denote second-order tensors — lower case for the local quantities (stress \( \sigma \), strain \( \varepsilon \)) and capital for the macroscopic quantities (effective stress \( \Sigma \), strain \( \mathbf{E} \)). Regular font is used to denote scalar quantities as well as the components of the tensors. Multiplication of two fourth-order tensors \( \mathbf{A} \) and \( \mathbf{B} \) is denoted by \( \mathbf{AB} = (AB)_{ijkl} \equiv A_{ijpq}B_{pqkl} \), while the operation “:” defines contraction of two indices when a fourth-order tensor acts on a second-order one, \( \mathbf{A} : \mathbf{E} \equiv A_{ijkl}E_{kl} \).
CHAPTER II

THERMOMECHANICAL CONSTITUTIVE MODELING
OF FULLY DENSE POLYCRYSTALLINE SHAPE MEMORY ALLOYS

In this chapter the derivation of a three-dimensional thermomechanical constitutive model for SMAs undergoing cyclic loading which results in simultaneous development of transformation and plastic strains will be presented. The model is an extension of the one-dimensional model presented by Bo and Lagoudas (1999a,b,c) and Lagoudas and Bo (1999) to three dimensions. Of most interest in this model is the evolution of plastic strains during stress-induced martensitic phase transformation as well as the non-linear transformation hardening.

While the basic ideas for the formulation of the current model have been presented by many authors in the literature and specifically by Lagoudas and Bo (1999) and Bo and Lagoudas (1999a,b,c) there are several important distinctions between the model presented here and the one reported by Bo and Lagoudas (1999b) which must be pointed out. The major difference between the two models is that the current model is capable of simulating three-dimensional behavior of SMAs while the model by Bo and Lagoudas (1999b) has only been implemented for the case of one-dimensional SMA wires. While some of the applications of SMAs can utilize the one-dimensional model, an increasing number of applications requires three-dimensional modeling. As an example, smart wing design, presented by Jardine et al. (1996) utilizes SMA torque tubes and their successful modeling requires three-dimensional formulation. The three-dimensional capabilities of the model are demonstrated in Section 3.4.1 where a model is used to simulate the behavior of an SMA torque tube. The three-dimensional formulation is essential for the further application of micromechanical averaging techniques for porous SMAs, which is the ultimate goal of the current
Another difference between the current model and the model by Bo and Lagoudas (1999b) is the way of calibrating the model parameters. While the previous publications (Bo and Lagoudas, 1999a,b,c; Lagoudas and Bo, 1999) have been devoted exclusively to characterizing the behavior of SMA wires undergoing temperature-induced phase transformation, the current work is aimed at characterizing the SMAs undergoing stress-induced phase transformation. Thus, the procedure for estimation of the material parameters, presented in Section 2.7 utilizes data for SMAs undergoing stress-induced phase transformation. While the present model can still be used to model temperature-induced phase transformation, to obtain accurate results some of the material parameters may need to be re-calibrated. The evolution equation for the plastic strain used here also differs from the expression presented by Bo and Lagoudas (1999a). The use of the current expression is motivated by the experimental observations for the evolution of plastic strains during stress-induced phase transformation.

Finally, the functional form of the back stress different from the one used by Bo and Lagoudas (1999b) is used in the current work. As explained earlier, the current functional form of the back stress simplifies the estimation of the material parameter and it is simpler to numerically implement, than the one used by Bo and Lagoudas (1999b). In addition, evolution equations for the back stress material parameters used here are also different from the ones presented by Bo and Lagoudas (1999a). While the evolution of these parameters in the work of Bo and Lagoudas (1999a) depends on the effective accumulated plastic strain, in this work it is connected to the accumulated detwinned martensitic volume fraction. Such a modification significantly simplifies the calibration of the model.
2.1. Experimental Observations for Polycrystalline SMAs Undergoing Cyclic Loading

As shown in the introduction, the behavior of SMAs under cyclic loading has been studied by a number of researchers. Experimental results have been reported for both thermally-induced transformation and for stress-induced transformation. Since the focus of the current work is on modeling the SMA constitutive behavior undergoing stress-induced phase transformation, the experimental observation for stress-induced transformation will be discussed here.

A set of experimental results presented by Strnadel et al. (1995b) showing the SMA response undergoing cycling stress-induced transformation is shown in Figure 8. The results shown on the figure are for three different NiTi alloys and the tests have been performed above the austenitic finish temperature. Two different tests were performed: cyclic loading with a constant maximum value of strain and cyclic loading with a constant maximum value of stress. Both sets of the results are shown in the figure.

Several observations can be made from Figure 8. First, it can be seen that during the cycling loading a substantial amount of unrecoverable plastic strain accumulates. The rate of accumulation of plastic strain is high during the initial cycles and asymptotically decreases with the increase of the number of cycles, as the plastic strain reaches a saturation value. The second observation is that the value of critical stress for onset of the transformation lowers with the number of cycles. The third observation is the substantial increase of the transformation hardening. In addition, in some cases it is also observed that the value of the maximum transformation strain decreases with the number of cycles. Finally, it can also be seen that the width of the transformation loop decreases.
Fig. 8. Cyclic stress-elongation diagrams for NiTi SMA: (a) cycling up to a constant maximum value of strain; (b) cycling up to a constant maximum value of stress. The elongation of 0.2 mm corresponds to a uniaxial strain of 0.008.

Similar observations have also been reported by other researchers (see, for example, the works of Kato et al., 1999; Lim and McDowell, 1994; McCormick and Liu, 1994; Sehitoglu et al., 2001; Strnadel et al., 1995a). Thus, the constitutive model presented in this work will address the effects described above.

2.2. Gibbs Free Energy of a Polycrystalline SMA

The formulation of the model starts with the definition of Gibbs free energy. The total Gibbs free energy of a polycrystalline SMA (Bo and Lagoudas, 1999b) is given by

\[
G(\sigma, T, \xi, \varepsilon_t, \varepsilon_p, \alpha, \eta) = -\frac{1}{2\rho} \sigma : S : \sigma - \frac{1}{\rho} \sigma : [\bar{\alpha}(T - T_0) + \varepsilon_t + \varepsilon_p]
\]

\[
- \frac{1}{\rho} \int_0^\xi \left( \alpha : \frac{\partial \varepsilon_t}{\partial \tau} + \eta \right) d\tau + c \left[ T - T_0 - T \ln \left( \frac{T}{T_0} \right) \right]
\]

\[
-s_0(T - T_0) + G_{ch} + G_p.
\]

(2.1)

In the above equation \( \sigma, \varepsilon_t, \varepsilon_p, \xi, T \) and \( T_0 \) are the Cauchy stress tensor, transformation strain tensor, plastic strain tensor, martensitic volume fraction, temperature and reference temperature, respectively. \( S, \bar{\alpha}, \rho, c \) and \( s_0 \) are the compliance tensor, thermal expansion coefficient tensor, density, specific heat and specific entropy at the reference state, respectively. The above effective material properties are calculated in terms of the martensitic volume fraction \( \xi \) using the rule of mixtures\(^1\) as

\(^1\)Different expressions for the elastic properties of the SMA based on the properties of the martensitic and austenitic phases have appeared in the literature. Boyd and Lagoudas (1994) have used the rule of mixtures for the elastic stiffness tensor, while in a later publication Lagoudas et al. (1996) have used the rule of mixtures for the elastic compliance tensor. Yet another method could be used based on the Mori–Tanaka averaging scheme for random orientation of martensitic inclusions in austenitic matrix for the forward transformation and random orientation of austenitic inclusions in martensitic matrix for the reverse transformation as presented by Auricchio and Sacco (1997) and Entchev and Lagoudas (2002).
\[ S = S^A + \xi (S^M - S^A) = S^A + \xi \Delta S, \quad (2.2a) \]
\[ \bar{\alpha} = \bar{\alpha}^A + \xi (\bar{\alpha}^M - \bar{\alpha}^A) = \bar{\alpha}^A + \xi \Delta \bar{\alpha}, \quad (2.2b) \]
\[ c = c^A + \xi (c^M - c^A) = c^A + \xi \Delta c, \quad (2.2c) \]
\[ s_0 = s_0^A + \xi (s_0^M - s_0^A) = s_0^A + \xi \Delta s_0. \quad (2.2d) \]

\(G_0^{ch}\) and \(G^p\) are the specific Gibbs chemical free energy at the reference state and the interaction energy induced by plastic strains in the austenitic phase, respectively. Finally, \(\alpha\) and \(\eta\) are the back and drag stresses, which are introduced to describe the influence of local stresses induced by the transformation and plastic strains on the phase transformation.

The Gibbs free energy \(G\) and the internal energy \(U\) are related by the following Legendre transformation:
\[ G = U - sT - \frac{1}{\rho} \sigma : \varepsilon. \quad (2.3) \]

In the equation above \(\varepsilon\) is the total strain tensor. Next, the laws of thermodynamics are used to obtain constraints on the material response. The procedure used in this work is outlined by Coleman and Noll (1963). The first law of thermodynamics is formulated as
\[ \rho \dot{U} = \sigma : \dot{\varepsilon} + \rho r - \text{div} \ q, \quad (2.4) \]
where \(q\) is the heat flux and \(r\) is the heat source density. Next, the Clausius-Duhem inequality is formulated in the following form (Malvern, 1969):
\[ \gamma \equiv \dot{s} - \frac{r}{T} + \frac{1}{\rho T} \text{div} \ q - \frac{q}{\rho T^2} \cdot \text{grad} \ T \geq 0, \quad (2.5) \]
where \(\gamma\) is the internal entropy production rate per unit mass. A stronger assumption
is proposed by Truesdell and Noll (1965) requiring separately

\[
\gamma_{\text{loc}} = \dot{s} - \frac{r}{T} + \frac{1}{\rho T} \text{div} \mathbf{q} \geq 0, \tag{2.6}
\]

\[
\gamma_{\text{con}} = -\frac{\mathbf{q}}{\rho T^2} \cdot \text{grad} \ T \geq 0, \tag{2.7}
\]

where \(\gamma_{\text{loc}}\) is the local entropy production rate and \(\gamma_{\text{con}}\) is the rate of entropy production by heat conduction. Using equations (2.3), (2.4) and (2.6) the local entropy production rate \(\gamma_{\text{loc}}\) is expressed as

\[
\gamma_{\text{loc}} = -\left(\mathbf{e} + \rho \frac{\partial G}{\partial \mathbf{\sigma}}\right) : \dot{\mathbf{\sigma}} - \rho \left(s + \frac{\partial G}{\partial T}\right) \dot{T} - \rho \frac{\partial G}{\partial \xi} \dot{\xi}. \tag{2.8}
\]

In the present formulation \(\xi\) is selected as an “intrinsic time” of the system, i.e., the change of the current state of the system is represented by the change of \(\xi\). The other internal state variables, i.e., \(\mathbf{\varepsilon}^t, \mathbf{\varepsilon}^p, \mathbf{\alpha}\) and \(\eta\) are assumed to evolve with \(\xi\) only. Therefore, in the above equation the derivative of \(G\) is taken only with respect to the independent variables \(\mathbf{\sigma}, T\) and the martensitic volume fraction \(\xi\). Thus the following constitutive equations are obtained from equation (2.8):

\[
\mathbf{\varepsilon} = -\rho \frac{\partial G}{\partial \mathbf{\sigma}} = \mathbf{S} : \mathbf{\sigma} + \bar{\mathbf{\alpha}}(T - T_0) + \mathbf{\varepsilon}^t + \mathbf{\varepsilon}^p, \tag{2.9}
\]

\[
s = -\frac{\partial G}{\partial T} = \frac{1}{\rho} \mathbf{\sigma} : \bar{\mathbf{\alpha}} + c \ln \left(\frac{T}{T_0}\right) + s_0. \tag{2.10}
\]

The local dissipation rate is given by

\[
-\rho \frac{\partial G}{\partial \xi} \dot{\xi} = \pi \dot{\xi} \geq 0. \tag{2.11}
\]

In the above equation \(\pi\) is the thermodynamic force conjugate to \(\xi\) and is given by

\[
\pi = \frac{1}{2} \mathbf{\sigma} : \Delta \mathbf{S} : \mathbf{\sigma} + \mathbf{\sigma} : \Delta \bar{\mathbf{\alpha}}(T - T_0) + \mathbf{\sigma} : \frac{\partial \mathbf{\varepsilon}^t}{\partial \xi} + \mathbf{\alpha} : \frac{\partial \mathbf{\varepsilon}^t}{\partial \xi} + \eta
\]

\[
- \rho \Delta c \left[T - T_0 - T \ln \left(\frac{T}{T_0}\right)\right] + \rho \Delta s_0(T - M^{0s}) + Y. \tag{2.12}
\]
The material parameter $M^{0s}$ is introduced in equation (2.12) as a combination of other parameters as

$$M^{0s} = T_0 + \frac{1}{\rho \Delta s_0} (Y + \rho \Delta G^{ch}),$$  

(2.13)

and $Y$ is a material constant representing a measure of the internal dissipation during phase transformation. The effective stress $\sigma^\text{eff}$ is defined as a sum of the applied stress $\sigma$ and the back stress $\alpha$ is the thermodynamic force conjugate to $\varepsilon^t$:

$$\sigma^\text{eff} = -\rho \frac{\partial G}{\partial \varepsilon^t} = \sigma + \alpha.$$  

(2.14)

2.3. Evolution of Internal State Variables

The evolution equations of internal state variables $\xi$, $\varepsilon^t$, $\varepsilon^p$, $\alpha$ and $\eta$ are presented here. As stated earlier, the transformation strain, plastic strain and back and drag stresses evolve with the martensitic volume fraction $\xi$. Therefore, the evolution of $\xi$ is discussed first.

2.3.1. Martensitic Volume Fraction

To obtain an evolution equation for $\xi$, Edelen’s formalism of thermodynamic dissipation potentials (Edelen, 1974) is utilized. Introducing a dissipation potential $\phi(\pi; \sigma, T, \xi)$ the evolution equation for the internal state variable $\xi$ is given by

$$\dot{\xi} = \lambda \frac{\partial \phi(\pi; \sigma, T, \xi)}{\partial \pi},$$  

(2.15)

and $\lambda$ satisfies the following Kuhn-Tucker conditions:

$$\lambda \geq 0, \quad \phi \leq Y^*, \quad \lambda(\phi - Y^*) = 0.$$  

(2.16)

The quantity $Y^*$ related to the dissipation rate of the system is assumed to be constant during phase transformation. Assuming a convex quadratic functional representation
of the dissipation potential

\[ \phi = \frac{1}{2} \pi^2, \]  

(2.17)

and using the Kuhn–Tucker conditions (2.16) for the case of \( \lambda > 0 \) the phase transformation condition is given by

\[ \pi = \pm \sqrt{2Y^*} \equiv \pm Y. \]  

(2.18)

The application of the thermodynamical constraint (2.11) leads to the following choice of the transformation function \( \Phi \):

\[ \Phi = \begin{cases} 
\pi - Y, & \dot{\xi} > 0, \\
-\pi - Y, & \dot{\xi} < 0.
\end{cases} \]  

(2.19)

Constraints on the evolution of \( \xi \) are expressed in terms of the Kuhn-Tucker conditions as

\[ \dot{\xi} \geq 0, \quad \Phi \leq 0, \quad \Phi \dot{\xi} = 0, \]  

\[ \dot{\xi} \leq 0, \quad \Phi \leq 0, \quad \Phi \dot{\xi} = 0. \]  

(2.20)

The role of the transformation function \( \Phi \) defined by equation (2.19) is similar to the role of the yield function in theory of rate-independent plasticity. It defines the elastic domain where no phase transformation occurs. The inequality conditions on \( \Phi \) are usually called the consistency conditions and act as a constraint on the admissibility of the state variables. Conditions expressed by equation (2.20) should be satisfied along any loading path. When \( \Phi < 0 \) equation (2.20) enforces the condition \( \dot{\xi} = 0 \) and the material response is elastic. When \( \Phi = 0 \) the material transforms: forward phase transformation is obtained for \( \dot{\xi} > 0 \) and reverse for \( \dot{\xi} < 0 \).
2.3.2. Transformation Strain

During the martensitic phase transformation the high-symmetry austenitic parent phase transforms into lower-symmetry martensitic phase. Thus, during forward transformation the parent phase can deform into many possible variants. It has been generally assumed that the direction of transformation is determined by the effective stress at each material point. During reverse phase transformation the high-symmetry austenitic phase, consisting of only one variant is recovered. Thus the final configuration is unique, but the sequence of reverse transformation can still be biased by the applied stress. In addition to the direction of the transformation a second factor, representing the magnitude must be taken into account. Differences exist between stress- and temperature-induced phase transformation, which have an effect on the magnitude of the transformation strain.

During the stress-induced phase transformation, simultaneous transformation and reorientation (detwinning) occur in the material. Due to the constraints between different grains in a polycrystalline SMA, different grains transform in a different way. As a result not all martensitic variants are created equally and the maximum transformation strain observed for single-crystal SMA can not be fully achieved. It can be approximately assumed, however, that the martensitic variants are equally detwinned through the stress-induced phase transformation. Therefore, the magnitude of the transformation strain can be characterized by a single material parameter, the maximum transformation strain.

During temperature-induced phase transformation at a constant applied load the achieved transformation strain strongly depends on the value of the load. In addition, the transformation strain depends on the conditioning of the material. It has been experimentally observed that the training achieved by cycling of the SMA material
has a very strong effect on the relationship between the value of the transformation strain and the applied load. For a trained SMA it is possible to achieve non-zero transformation strain even when the applied load is zero. In fact, to fully suppress the transformation strain a load in the direction opposite to the training load must be applied, as shown by Stalmans et al. (1992). Therefore, the magnitude of the transformation strain for the case of temperature-induced phase transformation depends on the applied load as well as on the previous thermomechanical loading.

During the reverse phase transformation it is assumed that the transformation strain will decrease with the decrease of $\xi$ from its maximum value to zero. Based on the above discussion the following evolution equation for the transformation strain $\varepsilon^t$ is adopted in this work:

$$\dot{\varepsilon}^t = \Lambda \dot{\xi},$$

(2.21)

where $\Lambda$ is the transformation direction tensor and is given by

$$\Lambda = \begin{cases} \frac{3}{2} H_{\text{cur}} \frac{\sigma_{\text{eff}}'}{\sigma_{\text{eff}}}, & \dot{\xi} > 0, \\ \frac{\varepsilon_{\text{max}}^t}{\xi_{\text{max}}}, & \dot{\xi} < 0. \end{cases}$$

(2.22)

The quantity $H_{\text{cur}}$ appearing in the above equation is defined to be the maximum current transformation strain and is a function of the applied stress. It is a measure of the degree of “detwinning” of the martensitic variants. $\varepsilon_{\text{max}}^t$ and $\xi_{\text{max}}$ are defined to be the transformation strain and the martensitic volume fraction at the beginning of the reverse phase transformation, respectively. The deviatoric part of the effective stress $\sigma_{\text{eff}}'$ and the effective von Mises stress $\bar{\sigma}_{\text{eff}}$ are defined as

$$\sigma_{\text{eff}}' = \sigma_{\text{eff}} - \frac{1}{3} (\text{tr} \sigma_{\text{eff}}) \mathbf{1}, \quad \bar{\sigma}_{\text{eff}} = \sqrt{\frac{3}{2} \| \sigma_{\text{eff}}' \|},$$

(2.23)

where $\mathbf{1}$ is the rank two identity tensor. Its components in indicial notation are given by $\delta_{ij}$. The condition for evaluation of $H_{\text{cur}}$ used here is the one suggested by
Lagoudas and Bo (1999), i.e., $H_{\text{cur}}$ is evaluated from the condition that the effective applied stress $\bar{\sigma}$ is equal to the effective back stress $\bar{\alpha}$ at the value of the martensitic volume fraction $\xi = 1$:

$$\bar{\sigma} = \bar{\alpha}|_{\xi=1}.$$  \hfill (2.24)

As shown in Section 2.3.4, the back stress $\alpha$ is a function of both $\xi$ and $H_{\text{cur}}$. Thus, for $\xi = 1$ (2.24) becomes an equation of one variable only, $H_{\text{cur}}$ and it can be solved to determine its value. This also implies that when the value of stress changes, a new value of the current maximum transformation strain should be calculated. The latter case arises not only during stress-induced phase transformation, but also during temperature-induced phase transformation when the material is constrained, e.g., in applications where SMA acts as an actuator.

It should be mentioned here that the current three-dimensional formulation of the model will not properly take into account the development of two-way shape memory effect. The one-dimensional reduced model, however, will be able to account for the TWSME. This limitation of the model is caused by the fact that the current choice for calculating $H_{\text{cur}}$ cannot take into account the direction of the developed TWSME. To be able to properly model the training and development of TWSME a tensorial quantity must be introduced which will replace $H_{\text{cur}}$. Note, however, that for the case of stress-induced martensitic phase transformation the current formulation is still suitable. This is due to the fact that the transformation strain during stress-induced phase transformation will develop in the direction of the applied stress.

2.3.3. Plastic Strain

The plastic strain considered here is different from conventional plasticity in metals. The observable macroscopic plastic strain is developed simultaneously with the trans-
formation strain during martensitic phase transformation. It is a collective result of
the accommodation of different martensitic variants during the phase transformation.
Due to the misfit between the austenite-martensite interfaces significant distortion is
created. In addition, in a polycrystalline SMA different grains transform in a differ-
ent manner. This causes additional distortion and movement of the grain boundaries.
These two phenomena act in concert and the final result is an observable macroscopic
plastic strain.

Similar to the evolution of transformation strain, the direction of plastic strain
is determined by the direction of the applied stress. In addition to the applied stress
another factor must be taken into account. Lim and McDowell (1994) have suggested
that the plastic strain rate depends on the magnitude of $\dot{\xi}$. However, in this work
the assumption by Bo and Lagoudas (1999a) that the evolution of the plastic strain
depends on the magnitude of detwinned martensitic volume fraction rate, $\xi^d \equiv \frac{H^{cur}}{H} \xi$, 
where $H$ is the maximum value of $H^{cur}$ for large values of the applied stress, is used.
This assumption implies that self-accommodating martensitic phase transformation
does not result in a change in the plastic strain. Thus, following the latter assumption,
the evolution equation for $\varepsilon^p$ is proposed as

$$\dot{\varepsilon}^p = \Lambda^p \dot{\xi}^d, \quad (2.25)$$

where $\dot{\xi}^d$ is defined as

$$\dot{\xi}^d = \int_0^t |\dot{\xi}^d(\tau)| \, d\tau. \quad (2.26)$$

It is seen from its definition that $\dot{\xi}^d$ may be viewed as the accumulated detwinned
martensitic volume fraction and that $\dot{\xi}^d = |\dot{\xi}|$. The quantity $\Lambda^p$ is the plastic direc-
tion tensor and its functional form is discussed next.

One form of $\Lambda^p$ is suggested by Bo and Lagoudas (1999a) for the one-dimensional
case. It depends on the the value of the applied stress, the accumulated detwinned martensitic volume fraction and on the value of the plastic strain itself. As explained by Bo and Lagoudas (1999a) the plastic strain predicted by their model never reaches a saturation value. While this is observed during temperature-induced phase transformation, for the case of stress-induced transformation the experimental results reported by Strnadela et al. (1995b) indicate that the plastic strain reaches a saturation value. Thus, to be able to accurately model stress-induced phase transformation the following form of $\Lambda^p$ is used:

$$
\Lambda^p = \begin{cases} 
\frac{3}{2} C^p_1 \exp \left[ - \frac{C^d}{C^p_2} \frac{\sigma_{\text{eff}}}{\sigma_{\text{ref}}} \right], & \dot{\xi} > 0, \\
C^p_1 \exp \left[ - \frac{C^d}{C^p_2} \frac{\epsilon_{\text{t},\text{max}}}{\bar{\epsilon}_{\text{t},\text{max}}} \right], & \dot{\xi} < 0.
\end{cases}
$$

Equation (2.27) suggests that the rates of the transformation strain and the plastic strain during phase transformation are proportional. An evolution equation for the plastic strain during stress-induced phase transformation, similar to equation (2.27) has also been proposed by Lim and McDowell (1994). However, in their equation the governing parameter is the accumulated martensitic volume fraction, while in the equation proposed in this work the governing parameters is the accumulated detwinned martensitic volume fraction. In addition, the equation proposed here is valid for three-dimensional case, while the equation presented by Lim and McDowell (1994) is given only for the one-dimensional case. This form of the plastic direction tensor enables a saturation of the plastic strain after a certain number of cycles. The material parameters $C^p_1$ and $C^p_2$ govern the saturation value as well as the number of cycles necessary for the plastic strain to saturate. The quantity $\bar{\epsilon}_{\text{t},\text{max}}$ is the effective transformation strain and is defined as

$$
\bar{\epsilon}_{\text{t},\text{max}} = \sqrt{\frac{2}{3}} \| \epsilon_{\text{t},\text{max}} \|. 
$$
2.3.4. Back and Drag Stress

The back stress $\alpha$ and the drag stress $\eta$ control the transformation hardening during the martensitic phase transformation. They are physically related to the local residual stresses which are developed in the material due to material heterogeneity. As explained by Bo and Lagoudas (1999a) $\alpha$ and $\eta$ take into account the effects of both the initial material imperfections and heterogeneities, e.g., grain boundaries, crystal lattice imperfections, precipitates, as well as the transformation-induced heterogeneities, e.g., transformation eigenstrains and misfit between martensite-austenite interfaces.

In this work the back stress is assumed to have the following polynomial functional representation:

$$\alpha = -\frac{\varepsilon_t}{\bar{\varepsilon}_t} \sum_{i=1}^{N^b} D^b_i(H^{\text{cur}}\xi)^{(i)},$$

(2.29)

where $N^b$ is the degree of the polynomial and $D^b_i$ are the coefficients associated with the back stress. Note that the form of the back stress used here differs from the expression used by Bo and Lagoudas (1999a), where a logarithmic function has been used. The use of a polynomial expression significantly simplifies the estimation of the material parameters and the calibration of the model. Using equation (2.29) the back stress parameters can be calibrated using a least square fit of the experimental data, while the logarithmic expression used by Bo and Lagoudas (1999a) would result in a non-linear optimization problem.

The expression for $\eta$ used in this work is similar to the one used by Bo and Lagoudas (1999a):

$$\eta = -D^d_1[-\ln(1 - \xi)]^{\frac{1}{m_1}} + D^d_2 \xi,$$

(2.30)

where $D^d_1$, $D^d_2$ and $m_1$ are parameters governing the evolution of the drag stress.
2.4. Continuum Tangent Moduli Tensors

Due to the non-linear nature and history dependance of the model its implementation requires an incremental formulation, where the increment of stress is updated for given increments of strain and temperature. Such an implementation utilizes the tangent stiffness tensor $\mathbf{L}$ and the tangent thermal moduli tensor $\Theta$, which appear in the following incremental form of the SMA constitutive model Qidwai and Lagoudas (2000a):

$$d\sigma = \mathbf{L} : d\varepsilon + \Theta dT.$$ (2.31)

In this section expressions for $\mathbf{L}$ and $\Theta$ for the SMA constitutive model are derived.

First, the stress-strain relation (2.9) is differentiated to give

$$d\sigma = S^{-1} \left[ d\varepsilon - \bar{\alpha} dT - \left[ \Delta \bar{\alpha} (T - T_0) + \Delta S : \sigma + \Lambda + \text{sign} \left( \dot{\xi} \right) \frac{H \text{cur}}{H} \Lambda_p \right] d\xi \right].$$

where $\chi$ is introduced as

$$\chi \equiv \Delta \bar{\alpha} (T - T_0) + \Delta S : \sigma + \Lambda + \text{sign} \left( \dot{\xi} \right) \frac{H \text{cur}}{H} \Lambda_p.$$ (2.33)

Taking the differential of the transformation condition (2.19) gives the following expression

$$d\Phi = \partial_\sigma \Phi : d\sigma + \partial_\xi \Phi dT + \partial_\xi \Phi d\xi = 0,$$ (2.34)

which combined with equation (2.32) results in

$$d\xi = \frac{\partial_\sigma \Phi : S^{-1} : d\varepsilon + \left[ \partial_\tau \Phi - \partial_\sigma \Phi : S^{-1} : \bar{\alpha} \right] dT}{\partial_\sigma \Phi : S^{-1} : \chi - \partial_\xi \Phi}.$$ (2.35)

Finally, substituting the above expression for $d\xi$ into equation (2.32) the following expressions for the tangent stiffness tensor $\mathbf{L}$ and the tangent thermal moduli tensor
\( \Theta \) are obtained:

\[
\begin{align*}
\mathcal{L} &= S^{-1} - \frac{S^{-1} : \chi \otimes \partial_\sigma \Phi : S^{-1}}{\partial_\sigma \Phi : S^{-1} : \chi - \partial_\xi \Phi}, \\
\Theta &= S^{-1} : \left[ \chi \frac{\partial_\sigma \Phi : S^{-1} : \bar{\alpha} - \partial_\tau \Phi}{\partial_\sigma \Phi : S^{-1} : \chi - \partial_\xi \Phi - \bar{\alpha}} \right].
\end{align*}
\]  

(2.36)

(2.37)

2.5. SMA Material Response under Cycling Loading

During cycling loading there are several characteristic changes of the thermomechanical response of SMAs. Along with the accumulation of non-recoverable plastic strain the change of the hysteresis loop has also been experimentally observed (Lim and McDowell, 1994; Strnadel et al., 1995b). The hysteresis loop progressively evolves with the number of cycles, until a stabilization point is reached. Some of the characteristic changes of the hysteresis loop are: (i) decrease of the stress level necessary for the onset of the transformation; (ii) increase of the transformation hardening; (iii) decrease of the width of the hysteresis loop; (iv) decrease of the maximum transformation strain. In addition, as noted in the literature (Bo and Lagoudas, 1999a; McCormick and Liu, 1994) the martensitic start temperature \( M^{0s} \) can also change during the transformation cycling.

The accumulation of the plastic strain has been addressed in the previous section, where an evolution equation for \( \varepsilon^p \) has been proposed. This section addresses the evolution of the hysteresis loop. The approach taken here is to identify two sets of parameters — the first set for annealed material which has not undergone any thermodynamic loading and the second set for the material which has undergone transformation cycling and the hysteresis loop has stabilized. Then, having identified these two sets of material parameters, evolution equations are proposed such that during the cycling the material parameters evolve from the first set to the second set. The procedure is described in detail in the following paragraphs.
First, the evolution of the back stress parameters $D^b_i$ is investigated. The initial and final values of the back stress parameters are denoted by $(D^b_i)^{\text{init}}$ and $(D^b_i)^{\text{fin}}$. Following the work of Bo and Lagoudas (1999a) it is assumed that the evolution of the parameters $D^b_i$ is governed by the same equation, which is selected to be

$$\dot{D}^b_i = \lambda_1 \left( (D^b_i)^{\text{fin}} - D^b_i \right) \dot{\zeta}^d. \quad (2.38)$$

As seen from equation (2.38) it is assumed that the back stress parameters change with the evolution of the accumulated detwinned martensitic volume fraction $\zeta^d$. In their work Bo and Lagoudas (1999a) have assumed that the evolution of $D^b_i$ is governed by the change in plastic strain. However, as indicated by equations (2.25) and (2.27) the plastic strain $\varepsilon^p$ and $\zeta^d$ are connected. Choosing $\zeta^d$ to be the governing parameter for the change of $D^b_i$ simplifies the model calibration, since for stress-induced transformation where full detwinning takes place $\zeta^d$ is proportional to the number of cycles, i.e., $\zeta^d = 2N$, where $N$ is the number of cycles. The parameter $\lambda_1$ in equation (2.38) is a positive material constant which governs the increasing rate of $D^b_i$.

Equation (2.38) is integrated explicitly with the initial condition of $D^b_i(\zeta^d = 0) = (D^b_i)^{\text{init}}$ to obtain the following expressions for $D^b_i$ in terms of $\zeta^d$:

$$D^b_i = (D^b_i)^{\text{fin}} + \exp \left[ -\lambda_1 \zeta^d \right] \left( (D^b_i)^{\text{fin}} - (D^b_i)^{\text{init}} \right). \quad (2.39)$$

As explained in Section 2.3.2 the current maximum transformation strain $H^{\text{cur}}$ is calculated using the effective back stress $\bar{\alpha}$. Since the maximum transformation strain $H$ is a limit value of $H^{\text{cur}}$ then it is assumed that the change of $H$ obeys the same governing equation as the change of $D^b_i$. Therefore, $H$ is given by

$$H = H^{\text{fin}} + \exp \left[ -\lambda_1 \zeta^d \right] \left( H^{\text{init}} - H^{\text{fin}} \right). \quad (2.40)$$
Similar evolution equations are proposed for the drag stress parameters $D_i^d$. The evolution of $D_i^d$ is described by

$$D_i^d = (D_i^d)^{\text{fin}} + \exp \left[ -\lambda_2 \zeta \right] ( (D_i^d)^{\text{init}} - (D_i^d)^{\text{fin}} ) .$$ \hspace{1cm} (2.41)

where $\lambda_2$ is a material parameter governing the evolution of $D_i^d$. As seen from equation (2.41) the evolution of the drag stress parameters is governed by the total accumulated martensitic volume fraction $\zeta$ and not it’s detwinned portion $\zeta^d$. This is related to the fact that microstructural changes can be induced by cyclic self-accommodating phase transformation (Bo and Lagoudas, 1999a). It should be noted that for stress-induced phase transformation with large values of the applied stress equations (2.38) and (2.41) are identical (if, of course, $\lambda_1 = \lambda_2$), since in this case $\zeta = \zeta^d$.

Finally, the evolution of the material parameters $Y$, $M^{0s}$ and $\rho \Delta s_0$ is considered. The equations governing the change of these parameters are similar to equation (2.41):

$$Y = Y^{\text{fin}} + \exp \left[ -\lambda_3 \zeta \right] ( Y^{\text{init}} - Y^{\text{fin}} ) ,$$ \hspace{1cm} (2.42)

$$M^{0s} = (M^{0s})^{\text{fin}} + \exp \left[ -\lambda_4 \zeta \right] ( (M^{0s})^{\text{init}} - (M^{0s})^{\text{fin}} ) ,$$ \hspace{1cm} (2.43)

$$\rho \Delta s_0 = (\rho \Delta s_0)^{\text{fin}} + \exp \left[ -\lambda_5 \zeta \right] ( (\rho \Delta s_0)^{\text{init}} - (\rho \Delta s_0)^{\text{fin}} ) ,$$ \hspace{1cm} (2.44)

where $\lambda_3$, $\lambda_4$ and $\lambda_5$ are material parameters.

It should be noted that it may be very difficult to determine unique values for the parameters $\lambda_1$–$\lambda_5$, because it is difficult to determine different values for the number of cycles for each of the parameters to reach its final value. A reasonable argument can be made that two unique values of the parameters $\lambda_1$–$\lambda_5$ can be determined. The first value is for the parameter $\lambda_1$ and it can be obtained by performing cyclic loading during which the material undergoes stress-induced transformation. The second value


can be determined for the parameters $\lambda_2-\lambda_5$ by performing thermal cycling with no applied stress. This separation of the parameters is explained by the different forms of the evolution equations, in which $\lambda_1-\lambda_5$ enter. While the evolution equation for the back stress parameters involves the accumulated detwinned martensitic volume fraction $\zeta^d$, the other evolution equations involve the accumulated total martensitic volume fraction $\zeta$. Therefore, in the case of self-accommodated thermally induced transformation cycling the value of $\zeta^d$ is zero. Then, any change of the parameters will be caused by the change in $\zeta$, which will allow to determine the value of $\lambda_2-\lambda_5$.

Note, however, that in the case that only stress-induced transformation cycling results are available, the above described approach is not applicable. One possible approach in this case is to assume that the values of $\lambda_1-\lambda_5$ are all equal.

As discussed above, two sets of the material parameters need to be identified — the initial set, characterizing the initial response of the annealed material and the final set, characterizing the stable material response. Then, having identified these two sets, the material parameters continuously change according to the evolution equations. However, this situation poses a problem in identifying the initial and final values of the parameters. Indeed, if the material parameters change continuously during the identification of the first set, it is impossible to take into account the change during the first cycle due to the nonlinearity introduced by that change.

This problem is addressed by keeping the value of the material parameters constant during forward or reverse phase transformation. The parameters will be recalculated according to the evolution equations when a reversal of the phase transformation occurs. Thus, the change in sign of the martensitic volume fraction rate $\dot{\xi}$ triggers the change of the material parameters. Note, however, that the above procedure is valid only for the material parameters. The plastic strain during cyclic loading is continuously calculated during both forward and reverse phase transformation, according to
the evolution equation (2.25).

2.6. Modeling of Minor Hysteresis Loops

An important part of the thermomechanical constitutive modeling of SMAs is the accounting for the minor hysteresis loops. In the context of the presented model a major loop is characterized by a full transformation cycle with the martensitic volume fraction $\xi$ monotonically increasing from 0 to 1 and then monotonically decreasing from 1 to 0. On the other hand, during a minor loop the martensitic volume fraction $\xi$ initial value is strictly greater than 0 and less than 1. To express the above conditions in term of measurable physical quantities, consider a stress-induced phase transformation. A major hysteresis loop occurs when the applied stress cycle has a range greater than $(\sigma^{Af} - \sigma^{Mf})$. For a stress path strictly inside $(\sigma^{Af} - \sigma^{Mf})$ a minor loop occurs.\(^2\)

The above described model in its current form indicates that the transformation criterion is identical for both major and minor loops. This assumption has also been made in the derivation of the majority of the models presented in the literature (Bo and Lagoudas, 1999b; Boyd and Lagoudas, 1996; Tanaka, 1986). The ramification of the above assumption is the prediction that a minor hysteresis loop is a part of a major loop and, therefore, the incorrect prediction of the SMA response during minor hysteresis loops. To illustrate the above discussion, minor hysteresis loops predicted by the model are schematically shown inside a major loop in Figure 9. As seen from Figure 9 during the minor loop the stress initially increases leading to partial forward phase transformation. When unloading occurs the reverse phase transformation does not start until the major hysteresis loop is reached. However, experimental results

\(^2\)The definition of $\sigma^{Af}$ and $\sigma^{Mf}$ is given in Section 1.2.2
Fig. 9. Schematic of minor hysteresis loops predicted by the current model and experimentally observed.

(see, for example, the works of Lim and McDowell, 1994; Strnadel et al., 1995b) indicate that the area enclosed by a minor hysteresis loop is much smaller than the area enclosed by the corresponding part of the major loop, i.e., the minor hysteresis loops exhibit much smaller hysteresis than the model predictions, as schematically shown in Figure 9. Similar results have also been observed for temperature-induced phase transformation (Bo and Lagoudas, 1999a).

The solution to the above described problem presented in this work, closely follows the one presented by Bo and Lagoudas (1999c) for the case of thermally-induced phase transformation, which is also credible for the case of stress-induced transformation. The results given here is generalized for three dimensions, while the details of the derivations can be found in the above-cited original publication and are omitted for brevity. The main idea behind the modeling of minor loops is the
modification of the transformation function, depending on whether the loading path follows a major or a minor loop.

First, an order of each branch of the hysteresis curve is defined as follows: the two branches of the major hysteresis loop are defined to be of order 0. The order of a minor loop branch is defined to be the number of times the hysteresis curve has reversed from a branch of the major loop (see Figure 10). For example, all first-order branches are attached to the major loop, all second order are attached to a first-order branch, etc.

Next, the thermodynamic driving force $\pi$ conjugate to $\xi$ for the $n$th order branch of the hysteresis curve is introduced as $\pi_n$. The transformation condition [cf. equa-
tion (2.18)] is modified as

\[
\Phi = \begin{cases} 
\pi_n - Y_n = 0, & \dot{\xi} > 0, \\
-\pi_n - Y_n = 0, & \dot{\xi} < 0, 
\end{cases}
\]

(2.45)

where \( Y_n(\xi) \) is now the local energy dissipation per unit volume for the \( n \)th order branch and is a function of \( \xi \). \( \pi_n \) is given by

\[
\pi_n = \frac{1}{2} \sigma : \Delta S : \sigma + \sigma : \Delta \alpha(T - T_0) + (\sigma + \alpha_n) : \Lambda + \eta_n
\]

\[
- \rho \Delta c \left[ T - T_0 - T \ln \left( \frac{T}{T_0} \right) \right] + \rho \Delta s_0 (T - M^{0s}),
\]

(2.46)

where \( \alpha_n \) and \( \eta_n \) are the back and drag stresses for the \( n \)th order branch of the hysteresis loop. The effect of the difference between \( \alpha_n \) and \( \eta_n \) and the corresponding quantities for the major hysteresis loop is taken into account by introducing the following function \( \Delta \psi_n(\xi) \):

\[
\Delta \psi_n(\xi) = [\alpha_n(\xi) - \alpha_0(\xi)] : \Lambda + \eta_n(\xi) - \eta_0(\xi).
\]

(2.47)

Using equations (2.46) and (2.47) the following expression relating the thermodynamic force for the \( n \)th branch \( \pi_n \) and the corresponding one for the major hysteresis curve \( \pi_0 \) is derived:

\[
\pi_n = \pi_0 + \Delta \psi_n.
\]

(2.48)

Note that for a major loop \( Y_0 \) is constant and \( \Delta \psi_0 = 0 \).

The evolution of the local energy dissipation \( Y_n \) during a minor loop is proposed as

\[
Y_n(\xi) = A_n \left( 1 - \exp \left( -\frac{\gamma}{C_n} |\xi - \xi^n_r| \right) \right).
\]

(2.49)

In the above equation \( \gamma \) is a material constant, \( \xi^n_r \) is the value of the martensitic
volume fraction at the reversal point and the parameter $C_n$ is defined as

$$C_n = \min \{\xi^n_r, 1 - \xi^n_r\}.$$  

(2.50)

The choice of $C_n$ as introduced by the above equation (2.50) is made to account for the different rate of $\xi$ at different transformation stages. The parameter $A_n$ is calculated from the following equation:

$$A_n = \frac{Y_{n-1}(\xi^n_r)}{1 - \exp \left[ -\frac{\gamma C_n}{\xi^n_r - \xi^n_r} \right]}.$$  

(2.51)

Finally, it is assumed that the evolution of $\Delta \psi_n$ is similar to the evolution of $Y_n$:

$$\Delta \psi_n(\xi) = \begin{cases} 
\Delta \psi_n(\xi^n_r) - Y_n(\xi), & \dot{\xi} > 0, \\
\Delta \psi_n(\xi^n_r) + Y_n(\xi), & \dot{\xi} < 0.
\end{cases}$$  

(2.52)

The initial condition for $\Delta \psi_n$ at $\xi = \xi^n_r$ is derived assuming that the phase transformation starts immediately at the point of reversal. It is given by

$$\Delta \psi_n(\xi^n_r) = \begin{cases} 
\Delta \psi_{n-1}(\xi^n_r) - Y_{n-1}(\xi^n_r), & \dot{\xi} > 0, \\
\Delta \psi_{n-1}(\xi^n_r) + Y_{n-1}(\xi^n_r), & \dot{\xi} < 0.
\end{cases}$$  

(2.53)

Finally, a few remarks on the implementation of the algorithm for minor loop modeling are made. As indicated by Bo and Lagoudas (1999c), proper transformation history must be kept. The values of $\xi$ and $Y_n$ for each reversal point must be stored, as well as the value of the parameter $C_n$. However, some of the memory for transformation history is wiped out by subsequent transformation. The wiping out algorithm (Bo and Lagoudas, 1999c) is as follows:

- For the forward phase transformation if the values of $\xi$ at previous forward-to-reverse transformation reversal points are smaller than the current value of $\xi$ then the transformation history memory corresponding to those minor loops is
wiped out;

- For the reverse phase transformation if the values of $\xi$ at previous reverse-to-forward transformation reversal points are greater than the current value of $\xi$ then the transformation history memory corresponding to those minor loops is wiped out;

This wiping out algorithm enforces the property that if the current $n$th order branch goes beyond the previous reversal point $\xi_{n-1}^r$ of the $(n-1)$st branch then the $n$th order branch is reduced to $(n-2)$nd order branch.

2.7. Estimation of Material Parameters

As a final step to characterizing the thermomechanical behavior in this section the determination of the material parameters entering the model is discussed. Three groups of material parameters are identified. First, the parameters which are necessary to describe a stable transformation cycle are determined. In the context of the current model the stable transformation cycle is defined as a thermomechanical loading cycle during which no plastic strains are developed and the material parameters remain constant. It should be mentioned that the above definition is realistic for the stable material response. However, during the first cycles there is measurable plastic strain. The effect of this plastic strain on the determination of the material parameters will be discussed in a sequel. The second group includes the material parameters which describe the behavior of SMA under cycling loading. These are the material parameters governing the evolution of plastic strains as well as the evolution of the material parameters from the first group. Finally, the third group encompasses the parameters governing the SMA behavior during minor hysteresis loops. The material parameters will be determined using uniaxial tests. Therefore, the one-dimensional reduction of
2.7.1. One-Dimensional Reduction of the Model

During uniaxial loading the stress tensor has one non-zero component. Thus, the components of the stress tensor are given by:

\[ \sigma_{11} = \sigma \neq 0, \quad \sigma_{ij} = 0 \quad \text{for all other } i, j. \quad (2.54) \]

In the equation above \( \sigma \) is the applied uniaxial stress. The transformation and plastic strain components are given by

\[ \varepsilon_{11}^t = \varepsilon^t, \quad \varepsilon_{22}^t = \varepsilon_{33}^t = -\frac{1}{2} \varepsilon^t, \quad \varepsilon_{ij}^t = 0 \quad \text{for all other } i, j, \quad (2.55) \]

\[ \varepsilon_{11}^p = \varepsilon^p, \quad \varepsilon_{22}^p = \varepsilon_{33}^p = -\frac{1}{2} \varepsilon^p, \quad \varepsilon_{ij}^p = 0 \quad \text{for all other } i, j, \quad (2.56) \]

where \( \varepsilon^t \) and \( \varepsilon^p \) are the uniaxial transformation and plastic strains. Assuming isotropic elastic properties, the constitutive equations (2.9) in the one-dimensional form become

\[ \varepsilon_{11} = \varepsilon = S \sigma + \bar{\alpha} (T - T_0) + \varepsilon^t + \varepsilon^p, \quad (2.57) \]

where \( \varepsilon \) is the uniaxial total strain, \( \bar{\alpha} \) is the thermal expansion coefficient and \( S \) is the elastic compliance given by

\[ S = \frac{1}{E}, \quad (2.58) \]

where \( E \) is the Young’s elastic modulus.

The evolution equations for the transformation and plastic strain become

\[ \dot{\varepsilon}^t = \Lambda \dot{\xi}, \quad (2.59) \]

\[ \dot{\varepsilon}^p = \Lambda^p \dot{\xi}^d. \quad (2.60) \]

The uniaxial components of the transformation and plastic direction tensors are given
by

$$\Lambda = \Lambda_{11} = \begin{cases} H^{\text{cur}} \frac{\sigma_{\text{eff}}}{|\sigma_{\text{eff}}|}, & \dot{\xi} > 0, \\ \frac{\sigma_{\text{max}}}{\xi_{\text{max}}}, & \dot{\xi} < 0, \end{cases}$$

(2.61)

$$\Lambda^p = \Lambda^p_{11} = \begin{cases} C^p_1 \exp \left[ -\frac{\zeta}{C_2} \frac{\sigma_{\text{eff}}}{|\sigma_{\text{eff}}|} \right], & \dot{\xi} > 0, \\ C^p_1 \exp \left[ -\frac{\zeta}{C_2} \frac{\sigma_{\text{max}}}{\xi_{\text{max}}} \right], & \dot{\xi} < 0. \end{cases}$$

(2.62)

The uniaxial effective stress $\sigma_{\text{eff}}$ is defined as

$$\sigma_{\text{eff}} = \sigma + \alpha,$$

(2.63)

where the back stress $\alpha$ is given by

$$\alpha = -\frac{3}{2} \frac{\dot{\varepsilon}^t}{|\varepsilon|^t} \sum_{i=1}^{N^b} D^b_i (H^{\text{cur}} \xi)^{(i)}.$$

(2.64)

The expression for the drag stress $\eta$ is the same as given by equation (2.30)

$$\eta = -D^d_1 [ - \ln(1 - \xi) ]^\frac{1}{m_1} + D^d_2 \xi.$$

(2.65)

The transformation function is given by

$$\Phi = \begin{cases} \pi - Y = 0, & \dot{\xi} > 0, \\ -\pi - Y = 0, & \dot{\xi} < 0, \end{cases}$$

(2.66)

where the thermodynamic driving force $\pi$ is given by

$$\pi = \frac{1}{2} \sigma^2 \Delta S + \sigma \Delta \bar{\alpha} (T - T_0) + \sigma_{\text{eff}} \Lambda + \eta$$

$$- \rho \Delta c \left[ T - T_0 - T \ln \left( \frac{t}{T_0} \right) \right] + \rho \Delta s_0 (T - M^{0s}) + Y.$$

(2.67)

The quantity $\Delta S$ is the difference between the elastic compliances of the austenitic and martensitic phases and is given by

$$\Delta S = \frac{1}{E^M} - \frac{1}{E^A}.$$
and $\Delta \bar{\alpha}$ is the difference between the thermal expansion coefficients of the austenite and martensite.

The uniaxial tangent stiffness and tangent thermal modulus are given by

$$L = E - \frac{\chi E^2 \partial_\sigma \Phi}{\chi E \partial_\sigma \Phi - \partial_\xi \Phi}, \quad (2.69)$$

$$\Theta = E \left[ -\chi \frac{E \bar{\alpha} \partial_\sigma \Phi}{\chi E \partial_\sigma \Phi - \partial_\xi \Phi} - \bar{\alpha} \right], \quad (2.70)$$

where the quantity $\chi$ is given by

$$\chi = \sigma \Delta S + \Delta \bar{\alpha}(T - T_0) + \Lambda + \text{sign}(\dot{\xi}) \frac{H_{\text{cur}}}{H} \Lambda^p. \quad (2.71)$$

The derivatives of the transformation function with respect to stress, temperature and the martensitic volume fraction are given by

$$\partial_\sigma \Phi = \sigma \Delta S + \Delta \bar{\alpha}(T - T_0) + \Lambda, \quad (2.72)$$

$$\partial_T \Phi = \sigma \Delta \bar{\alpha} + \rho \Delta c \ln \left( \frac{T}{T_0} \right), \quad (2.73)$$

$$\partial_\xi \Phi = -\frac{3}{2} \frac{\varepsilon^t}{|\varepsilon^t|} \Lambda \sum_{i=1}^{N^h} i H_{\text{cur}} D_i^b (H_{\text{cur}} \xi)^{(i-1)}$$

$$- \frac{1}{m_1 (1 - \xi)} D_1^d \left[ - \ln(1 - \xi) \right]^{1 - m_1} + D_2^d. \quad (2.74)$$

The determination of the material parameters of all of the three groups is described in detail in the following subsections. The tests which are necessary to be performed will be discussed and a parametric study for selected material parameters will be performed. The material parameters for NiTi reported by Bo et al. (1999) and shown in Table I will be used during the parametric study.
Table I. Material parameters for NiTi SMA characterizing a stable transformation cycle (Bo et al., 1999).

<table>
<thead>
<tr>
<th>Physical constants</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$E^A = 70.0$ GPa</td>
<td>$\alpha^A = 11.0 \times 10^{-6}$ K$^{-1}$</td>
</tr>
<tr>
<td>$E^M = 30.0$ GPa</td>
<td>$\alpha^M = 6.6 \times 10^{-6}$ K$^{-1}$</td>
</tr>
<tr>
<td>$\rho c^A = 2.12$ MJ/(m$^3$K)</td>
<td>$\nu = 0.33$</td>
</tr>
<tr>
<td>$\rho c^M = 2.12$ MJ/(m$^3$K)</td>
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<table>
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<tr>
<th>Parameters characterizing the phase transformation</th>
<th></th>
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</thead>
<tbody>
<tr>
<td>$M^{og} = 311.0$ K</td>
<td>$\rho \Delta s_0 = -0.422$ MJ/(m$^3$K)</td>
</tr>
<tr>
<td>$H = 0.069$</td>
<td>$Y = 6.0$ MJ/m$^3$</td>
</tr>
<tr>
<td>$D^b_1 = 3.40 \times 10^3$ MPa</td>
<td>$D^d_1 = 8.0$ MPa</td>
</tr>
<tr>
<td>$D^b_2 = -2.23 \times 10^5$ MPa</td>
<td>$D^d_2 = 1.7$ MPa</td>
</tr>
<tr>
<td>$D^b_3 = 8.32 \times 10^6$ MPa</td>
<td>$m_1 = 3.5$</td>
</tr>
<tr>
<td>$D^b_4 = -1.50 \times 10^8$ MPa</td>
<td></td>
</tr>
<tr>
<td>$D^b_5 = 1.03 \times 10^9$ MPa</td>
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<table>
<thead>
<tr>
<th>Minor loop parameter</th>
<th></th>
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</thead>
<tbody>
<tr>
<td>$\gamma = 3.0$</td>
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</table>
2.7.2. Material Parameters for a Stable Transformation Cycle

This group of material parameters include the elastic compliance tensors of both austenite martensite phases $S^A$ and $S^M$, their thermal expansion coefficient tensors $\alpha^A$ and $\alpha^M$ and specific heat $c^A$ and $c^M$. The martensitic start temperature $M_{0s}$, maximum transformation strain $H$, the difference between the specific entropy per unit volume $\rho \Delta s_0$, the material parameter $Y$ which provides a measure of the internal dissipation during phase transformation and the parameters associated with the back and drag stresses are also included in this group of parameters.

To determine the elastic compliance tensors $S^A$ and $S^M$, it is assumed that the SMA material behaves isotropically at macroscale. This assumption is reasonable because of the random orientation of the grains in a polycrystalline SMA. Therefore, it is only necessary to find the Young’s elastic moduli and Poisson’s ratios $E^A$, $E^M$, $\nu^A$ and $\nu^M$ of both phases. To determine the elastic constants a uniaxial pseudoelastic test must be performed. The elastic stiffness $E^A$ is determined by calculating the initial slope of the stress-strain curve for a uniaxial pseudoelastic test as shown in Figure 11. The elastic stiffness of the martensite phase $E^M$ is given by the slope of the stress-strain curve at the point of initial unloading (see Figure 11). It has been generally assumed in the literature that the Poisson’s ratios of austenite and martensite are equal and a typical value of $\nu^A = \nu^M = 0.33$ has been reported (Lagoudas and Bo, 1999; Lagoudas et al., 1996).

The thermal expansion coefficient tensors $\alpha^A$ and $\alpha^M$ are fully represented by two scalar constants $\alpha^A$ and $\alpha^M$. These constants can be estimated by measuring the slope of strain-temperature curve under constant stress at high temperature for the austenitic phase and low temperature for the martensitic phase. The specific heat constants $c^A$ and $c^M$ can be obtained from a calorimetric test. Note that these con-
Fig. 11. Schematic of a uniaxial pseudoelastic test.

stakenst (α^A, α^M, c^A, c^M) are not needed to model stress-induced phase transformation under constant temperature, but they become important when temperature changes.

The martensitic start temperature M₀s can be obtained from a DSC test. Detailed description of the DSC setup and test is given by Bo et al. (1999). The maximum transformation strain H is obtained by performing a pseudoelastic uniaxial test. Its value is estimated by extending the unloading part of the stress-strain curve using the elastic stiffness of the martensitic phase E^M, as shown in Figure 11.

As mentioned above, during the initial loading cycles observable plastic strain can develop. One proposed way to separate the plastic strain from the transformation strain is to subtract a portion of the residual plastic strain from the measured value of the transformation strain. Since the plastic strain develops during both forward and
reverse transformation, the subtracted value must be adjusted to take into account the plastic strain developed during the reverse phase transformation. As experimentally observed and reflected in the evolution equation for the plastic strain, initially the rate of accumulation of the plastic strain can be approximated by a linear function. Therefore, it is reasonable to assume that the amount of the plastic strain developed during the forward phase transformation is equal to one-half of the total residual plastic strain after one cycle. Thus, in presence of plastic strains, the value of the maximum transformation strain $H$ is obtained by extending the unloading part of the stress-strain curve and subtracting one-half of the total residual strain from the obtained number.

The material parameter $\rho \Delta s_0$ can also be obtained from the pseudoelastic stress-strain curve, schematically shown in Figure 11. Using equations (2.66) and (2.67) for the uniaxial isothermal stress loading the transformation function $\Phi$ at the onset of phase transformation ($\xi = 0$) is given by

$$\Phi = \frac{1}{2}(\sigma^{Ms})^2 \Delta S + \sigma^{Ms} H_{\text{cur}} + \rho \Delta s_0 (T - M_0^{Ms}).$$  \hspace{1cm} (2.75)

Then, using the transformation condition $\Phi = 0$ the following expression for $\rho \Delta s_0$ is obtained

$$\rho \Delta s_0 = -\frac{\frac{1}{2}(\sigma^{Ms})^2 \Delta S + \sigma^{Ms} H_{\text{cur}}}{T - M_0^{Ms}}. \hspace{1cm} (2.76)$$

Note that the value of $H_{\text{cur}}$ used in equation (2.76) should be calculated for the corresponding value of stress, which in this case is equal to $\sigma^{Ms}$. A slightly different procedure for determination of $M_0^{Ms}$ and $\rho \Delta s_0$ is reported by Bo et al. (1999). In their work, the quantity $\rho \Delta s_0$ is calculated from the DSC test and is related to the latent heat released during forward phase transformation and absorbed during reverse phase transformation. The martensitic start temperature $M_0^{Ms}$ is calculated in their work.
Fig. 12. Effect of the parameter $\rho \Delta s_0$ on the stress-strain response during forward phase transformation.

using strain-temperature curve obtained during an isobaric experiment.

To demonstrate the effect of the value of $\rho \Delta s_0$ on the stress-strain response, loading cases with different numerical values of $\rho \Delta s_0$ are simulated. The results of the parametric study are shown in Figure 12 where only the loading part is shown. It can be seen that with increasing magnitude of $\rho \Delta s_0$ the value of stress for the onset of the transformation also increases. Therefore, it can be seen that the parameter $\rho \Delta s_0$ is connected to the slope of the transformation line on the stress-temperature phase diagram (see Figure 1).

The material parameter $Y$ can also be calculated using a pseudoelastic stress-strain curve. The value of $Y$ is related to the total area $A$ enclosed by the hysteresis
Fig. 13. Effect of the parameter $Y$ on the size of the hysteresis loop.

The effect of the parameter $Y$ on the stress-strain response is shown in Figure 13. The unloading parts of the stress-strain curves for different values of $Y$ are shown in the figure while the loading parts are the same for all values of $Y$. It can be seen that with the increase of the value of $Y$ the reverse phase transformation starts at lower values of the applied stress. This, in effect, causes the increase of the area of the hysteresis loop, as seen in Figure 13.

As mentioned earlier in Section 2.3.2 [cf. equation (2.24)] the effective back stress is used to calculate the value of the current transformation strain $H^{\text{cur}}$. Thus,
an experimental result showing the dependance of $H_{\text{cur}}$ on the value of the applied stress $\sigma$ is utilized to obtain the back stress parameters $D^b_i$. To obtain this dependance several isobaric tests with thermally-induced phase transformation must be performed for different values of the applied stress. Each test gives one value of the current maximum transformation strain $H_{\text{cur}}$ corresponding to the value of the applied stress (see Figure 14). Then, the back stress parameters $D^b_i$ are obtained using the condition that the effective stress $\sigma_{\text{eff}}$ at $\xi = 1.0$ vanishes. Therefore, a least-square fit of the following equation is performed

$$\sigma = \frac{3}{2} \frac{\varepsilon_{\text{t}}}{|\varepsilon_{\text{t}}|} \sum_{i=1}^{N^b} D^b_i (H_{\text{cur}})^{(i)}.$$

After the value of $H_{\text{cur}}$ reaches the value of the maximum transformation strain $H$ it is assumed that further increase of the stress does not yield further increase of $H_{\text{cur}}$. After that point the value of $H_{\text{cur}}$ is considered to be constant and equal to $H$.

Note that sometimes it is difficult to obtain experimental curves for $\sigma$ vs. $H_{\text{cur}}$. In case that this data is unavailable, a typical curve, similar to the one shown in Figure 14 can be used. The results shown in Figure 14 have been reported by Lagoudas and Bo (1999) and similar results have also been observed by other researchers. Since for a stress-induced martensite the values of stress are expected to be high enough to induce complete detwinning of the martensitic variants, the errors introduced by this approximation are expected to be relatively small. For temperature-induced phase transformation, however, this experimental data is critical for the accuracy of the model, since small variations in stress may cause large variations of $H_{\text{cur}}$.

To estimate the material parameters entering the expression for the drag stress $\eta$ the tangent stiffness during an isothermal uniaxial pseudoelastic test is used. Assuming that all of the material parameters, except the drag stress parameters, are known, the tangent stiffness $\mathcal{L}$ given by equation (2.69) becomes a function of the
Fig. 14. Normalized maximum transformation strain for thermally induced phase transformation versus the applied stress: experimental data for NiTi SMA (Lagoudas and Bo, 1999) and a polynomial least-square fit. A polynomial of degree 5 is used.

drag stress parameters $D_1^d$, $D_2^d$ and $m_1$ and the martensitic volume fraction $\xi$:

$$
\mathcal{L}(\xi; D_1^d, D_2^d, m_1) = E - \frac{E^2(\sigma \Delta S + H_{\text{cur}})^2}{DEN},
$$

(2.79)

where the denominator is given by

$$
DEN = E(\sigma \Delta S + H_{\text{cur}})^2 + \frac{3}{2}(H_{\text{cur}})^2 \sum_{i=1}^{N^b} i D_i^b (H_{\text{cur}} \xi)^{(i-1)} + \frac{1}{m_1(1 - \xi)} D_1^d [- \ln(1 - \xi)]^{\frac{1-m_1}{m_1}} - D_2^d.
$$

(2.80)

The experimental values of the uniaxial tangent stiffness are obtained by per-
forming a pseudoelastic test. Thus, having obtained the experimental values of the tangent stiffness, a least-square fit of equation (2.79) is performed to obtain the drag stress parameters $D^d_1$, $D^d_2$ and $m_1$. Note, that the internal parameter $\xi$ cannot be directly measured. Based on numerous numerical experiments performed using the current model it has been found that it is reasonable to assume a linear relationship between the rate of total strain and the rate of the martensitic volume fraction during transformation.

To illustrate the effect of the drag stress parameters on the stress-strain results, a parametric study for different values of $D^d_1$ and $D^d_2$ has been performed. The loading part of the pseudoelastic stress-strain curve for different values of $D^d_1$ is shown in Figure 15. It can be seen from the figure that the transformation hardening increases with the increase of the value of $D^d_1$. In addition, the value of $D^d_1$ has a very strong effect on the initial transformation hardening. The effect of the parameter $D^d_2$ on the stress-strain results is shown in Figure 16. It can be seen that higher value of the parameter $D^d_2$ leads to smaller slope of the stress-strain curve. This parameter, however, has very little effect on the initial transformation hardening. The effect of $D^d_2$ can be explained by comparing the expression for the drag stress in the current model to the one given by Lagoudas et al. (1996) for a model with a polynomial hardening function. If the parameter $D^d_1$ is taken to be zero, then the parameter $D^d_2$ corresponds to the linear hardening parameter in the model by Lagoudas et al. (1996). Therefore, it has the same effect for all values of $\xi$ and its value equally affects the slope of the stress-strain curve during the phase transformation.

2.7.3. Material Parameters for Cyclic Loading

This group of parameters includes the parameters $C^p_1$ and $C^p_2$, entering the expression for $\Lambda^p$ (2.62) and constants $\lambda_1$–$\lambda_5$, which determine the evolution of the material pa-
Fig. 15. Effect of the parameter $D^d_1$ on the stress-strain response during forward phase transformation.

Parameters during cyclic loading. To understand the physical meaning of the constants $C^p_1$ and $C^p_2$, equation (2.60) can be integrated to find the following expression for $\varepsilon^p$ as a function of $\zeta^d$:

$$\varepsilon^p = C^p_1 C^p_2 \left( 1 - \exp \left( -\frac{\zeta^d}{C^p_2} \right) \right).$$

(2.81)

As seen from equation (2.81) the product of $C^p_1$ and $C^p_2$ gives the maximum (saturation) value of the plastic strain. Further, recall that for stress-induced martensite $\zeta^d = 2N$. Therefore, $C^p_2$ can be estimated by enforcing the condition that after a given number of cycles the plastic strain approaches its maximum value, or more
Fig. 16. Effect of the parameter $D_2^d$ on the stress-strain response during forward phase transformation.

Precisely, $C_2^p$ can be found from the condition

$$\exp \left[ -\frac{2N_{sat}^p}{C_2^p} \right] = \delta,$$  \hspace{1cm} (2.82)

where $N_{sat}^p$ is the number of cycles to reach the saturation value of plastic strain and $\delta$ is a small number.$^3$

Next, parameters $\lambda_1$, $\lambda_2$ are considered. Only the estimation of $\lambda_1$ is explained in detail, due to the similarity between the equations containing this set of parameters. It can be seen from equation (2.39) that $\lambda_1$ determines the number of cycles $N_{sat}^b$ until $D_i^b$ reach their final values. Thus, it can be found using the following equation,

\hspace{1cm}$^3$Reasonable values for $\delta$ are in the range from 0.01 to 0.1
similar to equation (2.82):

$$\exp \left[ -2N_{\text{sat}}^b \lambda_1 \right] = \delta. \quad (2.83)$$

The same procedure is used to find the parameter $\lambda_2$.

2.7.4. Material Parameters for Minor Loop Modeling

Only one material parameter enters this last group. This is the constant $\gamma$, appearing in equation (2.49) and dictating the size of the minor hysteresis loop. A smaller value of $\gamma$ leads to smaller area occupied by the minor loop, while larger value increases the area. An experimental stress-strain curve with one minor loop is sufficient to estimate the value of $\gamma$. A typical value of $\gamma$ is in the range of 1 to 4. To illustrate the effect of this parameter on the shape of the minor loop branches, the results for different values of $\gamma$ are shown in Figure 17.
Fig. 17. Effect of the parameter $\gamma$ on the minor loop curvature. The minor loops occur due to incomplete forward phase transformation.
CHAPTER III

NUMERICAL IMPLEMENTATION AND CORRELATION WITH EXPERIMENTAL DATA FOR DENSE SMAS

In this chapter the numerical implementation of the thermomechanical constitutive model for dense SMAs will be presented. The structure of the governing equations of the SMA constitutive model is very similar to the structure of the equations characterizing rate-independent plasticity in metals. Therefore, as shown by Qidwai and Lagoudas (2000a) the numerical algorithms developed for integrating constitutive equations characterizing plasticity can be successfully applied to integrate the equations for the SMAs. The approach taken in this work is to implement a return-mapping for the dense SMA constitutive model, presented in Chapter II. The development of the algorithm is based on the work of Qidwai and Lagoudas (2000a) with special care taken to account for the development of plastic strains. The algorithm used in the current work is an implementation of the closest point projection return mapping algorithm.

The comparison of the model simulations with the available experimental results for dense SMAs undergoing cycling loading is also presented in this chapter. The material parameters for the SMA are estimated using the data presented in the literature.

3.1. Summary of the Dense SMA Constitutive Model Equations

For convenience the SMA constitutive equations presented in Chapter II are summarized here. The strain \( \varepsilon \) is given by

\[
\varepsilon = S : \sigma + \bar{\alpha}(T - T_0) + \varepsilon^t + \varepsilon^p.
\]  

(3.1)
The evolution equations for the transformation strain $\varepsilon^t$ and the plastic strain $\varepsilon^p$ are given by

$$
\dot{\varepsilon}^t = \Lambda \dot{\xi},
$$

$$
\dot{\varepsilon}^p = \Lambda^p \dot{\zeta},
$$

where $\Lambda$ and $\Lambda^p$ are defined as

$$
\Lambda = \left\{ 
\begin{array}{ll}
\frac{3}{2} H^\text{cur} \frac{\sigma^\text{eff}}{\sigma^\text{cur}} & \dot{\xi} > 0, \\
\frac{\varepsilon_{\text{max}}^t}{\varepsilon_{\text{max}}^t} & \dot{\xi} < 0,
\end{array}
\right.
$$

$$
\Lambda^p = \left\{ 
\begin{array}{ll}
\frac{3}{2} C_p \exp \left[ -\frac{\zeta^d}{C_2} \right] \frac{\sigma^\text{eff}}{\sigma^\text{cur}}, & \dot{\xi} > 0, \\
C_1 \exp \left[ -\frac{\zeta^d}{C_2} \right] \frac{\varepsilon_{\text{max}}^p}{\varepsilon_{\text{max}}^p}, & \dot{\xi} < 0,
\end{array}
\right.
$$

and $\zeta^d$ is given by

$$
\zeta^d = \int_0^t |\dot{\zeta}^d(\tau)| d\tau.
$$

The effective stress $\sigma^\text{eff}$ is defined in terms of the applied stress $\sigma$ and the back stress $\alpha$ as

$$
\sigma^\text{eff} = \sigma + \alpha.
$$

The transformation function $\Phi$ is defined as

$$
\Phi = \left\{ 
\begin{array}{ll}
\pi - Y, & \dot{\xi} > 0, \\
-\pi - Y, & \dot{\xi} < 0,
\end{array}
\right.
$$

In the above equation $\pi$ is the thermodynamic force conjugate to $\xi$ and is given by

$$
\pi = \frac{1}{2} \frac{\sigma}{\sigma} : \Delta S : \sigma + \sigma : \Delta \alpha(T - T_0) + \sigma : \frac{\partial \varepsilon^t}{\partial \xi} + \alpha : \frac{\partial \varepsilon^t}{\partial \xi} + \eta \\
- \rho \Delta c \left[ T - T_0 - T \ln \left( \frac{T}{T_0} \right) \right] + \rho \Delta S_0 (T - M^0) + Y.
$$

Expressions for the back stress $\alpha$ and the drag stress $\eta$ are given in Section 2.3.4. The evolution of the martensitic volume fraction $\xi$ is constrained by the Kuhn–Tucker conditions

$$\dot{\xi} \geq 0, \quad \Phi \leq 0, \quad \Phi \dot{\xi} = 0,$$
$$\dot{\xi} \leq 0, \quad \Phi \leq 0, \quad \Phi \dot{\xi} = 0. \quad (3.10)$$

Thus the final system of algebraic and differential equations consists of equations (3.1)–(3.3) which is constrained by equation (3.10).

3.2. Closest Point Projection Return Mapping Algorithm for SMA Constitutive Model

To proceed with the solution of the above posed problem it is first assumed that the strain and temperature histories $\varepsilon(t)$ and $T(t)$ are given. In addition, the initial conditions for $\xi$, $\varepsilon^t$ and $\varepsilon^p$ are also known. The main idea of the return mapping algorithms is to divide the problem into two parts. The first step is to obtain a thermoelastic prediction, assuming that the transformation and plastic strains do not change. During the second step, if the predicted thermoelastic state violates the transformation condition, a transformation correction problem is solved to restore consistency (Qidwai and Lagoudas, 2000a). During the transformation correction the evolution equations for the transformation and plastic strains are discretized as

$$\varepsilon^t_{n+1} = \varepsilon^t_n + (\xi_{n+1} - \xi_n) \left[ \beta \Lambda_{n+1} + (1 - \beta) \Lambda_n \right], \quad (3.11)$$
$$\varepsilon^p_{n+1} = \varepsilon^p_n + (\zeta^d_{n+1} - \zeta^d_n) \left[ \beta \Lambda^p_{n+1} + (1 - \beta) \Lambda^p_n \right], \quad (3.12)$$

where $\beta \in [0, 1]$ and subscript $n$ indicates functional evaluation at time $t_n$. Different values of $\beta$ will result in different integration algorithms. In this work $\beta$ is chosen to be equal to 1 which results in backward Euler integration rule. The resulting algorithm
is referred to as the closest point projection return mapping algorithm (Qidwai and Lagoudas, 2000a). The stress-strain relation (3.1) for the case of $\beta = 1$ is also written as

$$\sigma_{n+1} = S_{n+1}^{-1} : \left( \epsilon_{n+1} - \epsilon_{n+1}^t - \epsilon_{n+1}^p - \bar{\alpha}_{n+1}(T_{n+1} - T_0) \right).$$

(3.13)

The main steps of the algorithm are described in detail in a sequel.

3.2.1. Thermoelastic Prediction

During the thermoelastic prediction step the following operations are performed:

$$\epsilon_{n+1} = \epsilon_n + \Delta \epsilon_{n+1},$$

(3.14a)

$$T_{n+1} = T_n + \Delta T_{n+1},$$

(3.14b)

$$\epsilon_{n+1}^{(0)} = \epsilon_n^{(0)},$$

(3.14c)

$$\epsilon_{n+1}^{(0)} = \epsilon_n^{(0)},$$

(3.14d)

$$\xi_{n+1}^{(0)} = \xi_n^{(0)},$$

(3.14e)

where $\Delta \epsilon_{n+1}$ and $\Delta T_{n+1}$ are the (known) total strain and temperature increments for the $(n + 1)$st time step. The superscript is introduced to indicate the current iteration number, which for the case of $(0)$ means evaluation of the quantities from the previous time step. The value of the stress is obtained as

$$\sigma_{n+1}^{(0)} = S_{n}^{-1} : \left[ \epsilon_{n+1} - \epsilon_{n+1}^{(0)} - \epsilon_{n+1}^{p(0)} - \bar{\alpha}_n(T_{n+1} - T_0) \right].$$

(3.15)

The corresponding value of the transformation function $\Phi$ is evaluated as

$$\Phi_{n+1}^{(0)} = \Phi(\sigma_{n+1}^{(0)}, T_{n+1}, \xi_{n+1}^{(0)}).$$

(3.16)

At this point if the value of the transformation function satisfies the transformation criterion $\Phi_{n+1}^{(0)} \leq 0$ than the thermoelastic trial state is the final, that is, no
phase transformation occurs at this time increment. However, if the transformation
criterion is violated, i.e., $\Phi_{n+1}^{(0)} > 0$ then a transformation correction is performed.
The transformation correction is performed by solving equations (3.11)–(3.13) with
initial guess given by equations (3.14), (3.15) and constrained by the Kuhn–Tucker
conditions (3.10). During the transformation correction the values of total strain $\varepsilon_{n+1}$
and temperature $T_{n+1}$ do not change. Only the values of the internal state variables
and the stress are updated.

3.2.2. Transformation Correction

To proceed with the transformation correction step, the following transformation and
plastic residuals are defined for the $k$th iteration as

$$
R_{t}^{(k)}_{n+1} = -\varepsilon_{n+1}^{(k)} + \varepsilon_{n}^{t} + \Lambda_{n+1}^{(k)}(\varepsilon_{n}^{(k)} - \xi_{n}) = 0, \tag{3.17}
$$
$$
R_{p}^{p(k)}_{n+1} = -\varepsilon_{n+1}^{p(k)} + \varepsilon_{n}^{p} + \Lambda_{n+1}^{p(k)}|\varepsilon_{n+1}^{d(k)} - \xi_{n}^{d}| = 0. \tag{3.18}
$$

The transformation (consistency) condition is given by

$$
\Phi_{n+1}^{(k)} = \Phi(\sigma_{n+1}^{(k)}, T_{n+1}, \xi_{n+1}^{(k)}) = 0. \tag{3.19}
$$

Equations (3.17)–(3.19) are solved using Newton–Raphson method. Keeping in
mind that during the transformation correction the total strain and temperature are
constant, the linearized forms of equations (3.17)–(3.19) using Taylor series expansion
become

$$
R_{t}^{(k)}_{n+1} - \Delta\varepsilon_{n+1}^{(k)} + \Delta\Lambda_{n+1}^{(k)}(\varepsilon_{n+1}^{(k)} - \xi_{n}) + \Lambda_{n+1}^{(k)}\Delta\varepsilon_{n+1}^{(k)} = 0, \tag{3.20}
$$
$$
R_{p}^{p(k)}_{n+1} - \Delta\varepsilon_{n+1}^{p(k)} + \Delta\Lambda_{n+1}^{p(k)}|\varepsilon_{n+1}^{d(k)} - \xi_{n}^{d}| + \Lambda_{n+1}^{p(k)}\Delta|\varepsilon_{n+1}^{d(k)} - \xi_{n}^{d}| = 0, \tag{3.21}
$$
$$
\Phi_{n+1}^{(k)} + \partial_{\sigma}^{(k)}\Phi_{n+1}^{(k)}: \Delta\sigma_{n+1}^{(k)} + \partial_{\xi}^{(k)}\Phi_{n+1}^{(k)}\Delta\xi_{n+1}^{(k)} = 0. \tag{3.22}
$$

Next, the increment of the stress-strain constitutive relation (3.13) is taken which
yields

\[ \Delta S_{n+1} : \sigma_{n+1}^{(k)} + S_{n+1} : \Delta \sigma_{n+1}^{(k)} = -\Delta \alpha_{n+1}(T_{n+1} - T_0) + \Delta \varepsilon_t^{(k)} - \Delta \varepsilon_p^{(k)}. \]  

(3.23)

The increments of the elastic compliance tensor \( \Delta S_{n+1} \) and the thermal expansion coefficient tensor \( \Delta \bar{\alpha}_{n+1} \) are expressed using their evaluations [cf. equation (2.2)] in terms of the increment of the martensitic volume fraction \( \xi \) as

\[ \Delta S_{n+1} = \Delta S \Delta \xi_{n+1}, \quad \Delta \bar{\alpha}_{n+1} = \Delta \bar{\alpha} \Delta \xi_{n+1}. \]  

(3.24)

Using equations (3.24) and (3.23) the following expression for the increment of the transformation strain \( \Delta \varepsilon_t^{(k)} \) is obtained:

\[ \Delta \varepsilon_t^{(k)} = -S_{n+1} : \Delta \sigma_{n+1}^{(k)} - \Delta \varepsilon_p^{(k)} - \left[ \Delta \bar{\alpha}(T_{n+1} - T_0) + \Delta S : \sigma_{n+1}^{(k)} + \Lambda_{n+1}^{(k)} \right] \Delta \xi_{n+1}. \]  

(3.25)

The increment of the transformation direction tensor \( \Delta \Lambda_{n+1}^{(k)} \) is given by

\[ \Delta \Lambda_{n+1}^{(k)} = \partial_{\sigma} \Lambda_{n+1}^{(k)} : \Delta \sigma_{n+1}^{(k)}. \]  

(3.26)

Equations (3.25) and (3.26) are substituted into equation (3.20) to obtain

\[ \left[ S_{n+1}^{(k)} + \partial_{\sigma} \Lambda_{n+1}^{(k)}(\xi_{n+1}^{(k)} - \xi_n) \right] : \Delta \sigma_{n+1}^{(k)} = -\left( R_{n+1}^{(k)} + \Delta \varepsilon_p^{(k)} + \left[ \Delta \bar{\alpha}(T_{n+1} - T_0) + \Delta S : \sigma_{n+1}^{(k)} + \Lambda_{n+1}^{(k)} \right] \Delta \xi_{n+1}^{(k)} \right). \]  

(3.27)

The increment of the plastic direction tensor \( \Delta \Lambda_{n+1}^{p(k)} \) which enters equation (3.21) is given by

\[ \Delta \Lambda_{n+1}^{p(k)} = \partial_{\sigma} \Lambda_{n+1}^{p(k)} : \Delta \sigma_{n+1}^{(k)} + \partial_{\xi} \Lambda_{n+1}^{p(k)} : \Delta \xi_{n+1}^{(k)}, \]  

(3.28)
Thus, using equations (3.28), (3.29) expression (3.21) becomes

\[
\Delta \left[ \xi_{n+1}^{d(k)} - \xi_n^d \right] = \Delta \left[ \left( \frac{H^{\text{cur}} \xi}{H} \right)_{n+1}^{(k)} - \left( \frac{H^{\text{cur}} \xi}{H} \right)_n^{(k)} \right]
\]

\[
= \text{sign} \left( \left( \frac{H^{\text{cur}} \xi}{H} \right)_{n+1}^{(k)} - \left( \frac{H^{\text{cur}} \xi}{H} \right)_n^{(k)} \right) \frac{H^{\text{cur}}}{H} \Delta \xi_{n+1}^{(k)}. \quad (3.29)
\]

Thus, using equations (3.28), (3.29) expression (3.21) becomes

\[
R_{n+1}^{p(k)} - \Delta \varepsilon_{n+1}^{p(k)} + \partial_\sigma R_{n+1}^{p(k)} : \Delta \sigma_{n+1}^{(k)} + \partial_\xi R_{n+1}^{p(k)} : \Delta \xi_{n+1}^{(k)} = 0, \quad (3.30)
\]

where the quantities \( \partial_\sigma R_{n+1}^{p(k)} \) and \( \partial_\xi R_{n+1}^{p(k)} \) are defined as

\[
\partial_\sigma R_{n+1}^{p(k)} \equiv \left[ \xi_{n+1}^{d(k)} - \xi_n^d \partial_\sigma \Lambda_{n+1}^{p(k)} \right], \quad (3.31)
\]

\[
\partial_\xi R_{n+1}^{p(k)} \equiv \left[ \xi_{n+1}^{d(k)} - \xi_n^d \partial_\xi \Lambda_{n+1}^{p(k)} + \frac{H^{\text{cur}}}{H} \text{sign} \left( \varepsilon_{n+1}^{d(k)} - \varepsilon_n^d \right) \Lambda_{n+1}^{p(k)} \right]. \quad (3.32)
\]

The increment of the plastic strain \( \Delta \varepsilon_{n+1}^{p(k)} \) is expressed using equation (3.30) and substituted into equation (3.27) to obtain

\[
\left[ S_{n+1}^{(k)} + \partial_\sigma \Lambda_{n+1}^{(k)} (\varepsilon_{n+1}^{(k)} - \varepsilon_n) + \partial_\sigma R_{n+1}^{p(k)} \right] : \Delta \sigma_{n+1}^{(k)} = - \left( R_{n+1}^{t(k)} + R_{n+1}^{p(k)} + [\Delta \alpha (T_{n+1} - T_0) + \Delta S : \sigma_{n+1}^{(k)} + \Lambda_{n+1}^{(k)} + \partial_\xi R_{n+1}^{p(k)}] \Delta \xi_{n+1}^{(k)} \right). 
\]

(3.33)

To simplify further derivations the following tensorial quantities are defined

\[
\Xi_{n+1}^{(k)} \equiv \left[ S_{n+1}^{(k)} + \partial_\sigma \Lambda_{n+1}^{(k)} (\varepsilon_{n+1}^{(k)} - \varepsilon_n) + \partial_\sigma R_{n+1}^{p(k)} \right]^{-1}, \quad (3.34)
\]

\[
\chi_{n+1}^{(k)} \equiv \Delta \alpha (T_{n+1} - T_0) + \Delta S : \sigma_{n+1}^{(k)} + \Lambda_{n+1}^{(k)} + \partial_\xi R_{n+1}^{p(k)}. \quad (3.35)
\]

which leads to the following expression for the increment of stress \( \Delta \sigma_{n+1}^{(k)} \):

\[
\Delta \sigma_{n+1}^{(k)} = -\Xi_{n+1}^{(k)} : \left[ R_{n+1}^{t(k)} + R_{n+1}^{p(k)} + \chi_{n+1}^{(k)} \Delta \xi_{n+1}^{(k)} \right]. \quad (3.36)
\]
Thus, the only unknown is the increment of the martensitic volume fraction $\Delta \xi_{n+1}^{(k)}$. The consistency condition (3.22) together with equation (3.36) is used to find
\[
\Delta \xi_{n+1}^{(k)} = \frac{\partial_\sigma \Phi_{n+1}^{(k)} : \Xi_{n+1}^{(k)} : \left[ \Phi_{n+1}^{(k)} + \Phi_{n+1}^{p(k)} \right] - \Phi_{n+1}^{(k)}}{\partial_\xi \Phi_{n+1}^{(k)} - \partial_\sigma \Phi_{n+1}^{(k)} : \Xi_{n+1}^{(k)} : \Lambda_{n+1}^{(k)}}. \tag{3.37}
\]

Once $\Delta \xi_{n+1}^{(k)}$ is found from equation (3.37) it is used to calculate the increment of stress using equation (3.36). Then the increments of plastic and transformation strain are found using equations (3.30) and (3.25).

Finally the expressions for $\partial_\sigma \Phi_{n+1}^{(k)}$, $\partial_\xi \Phi_{n+1}^{(k)}$, $\partial_\sigma \Lambda_{n+1}^{(k)}$, $\partial_\sigma \Lambda_{n+1}^{p(k)}$ and $\partial_\xi \Lambda_{n+1}^{p(k)}$ which are used in the algorithm are derived. The derivative of the transformation function with respect to stress can be obtained by differentiating equation (3.8). It follows that
\[
\partial_\sigma \Phi_{n+1}^{(k)} = \begin{cases} 
\partial_\sigma \pi_{n+1}^{(k)}, & \hat{\xi} > 0, \\
-\partial_\sigma \pi_{n+1}^{(k)}, & \hat{\xi} < 0.
\end{cases} \tag{3.38}
\]

Using equation (3.9) the derivative of the thermodynamic driving force $\pi$ with respect to stress is given by
\[
\partial_\sigma \pi_{n+1}^{(k)} = \Delta \alpha (T_{n+1} - T_0) + \Delta S : \sigma_{n+1}^{(k)} + \Lambda_{n+1}^{(k)}. \tag{3.39}
\]

Similarly the derivative of the transformation function with respect to the martensitic volume fraction is
\[
\partial_\xi \Phi_{n+1}^{(k)} = \begin{cases} 
\partial_\xi \alpha_{n+1}^{(k)} : \Lambda_{n+1}^{(k)} + \partial_\xi \eta_{n+1}^{(k)}, & \hat{\xi} > 0, \\
-\partial_\xi \alpha_{n+1}^{(k)} : \Lambda_{n+1}^{(k)} - \partial_\xi \eta_{n+1}^{(k)}, & \hat{\xi} < 0.
\end{cases} \tag{3.40}
\]

The quantities $\partial_\xi \alpha_{n+1}^{(k)}$ and $\partial_\xi \eta_{n+1}^{(k)}$ are calculated using the expressions for $\alpha$ and $\eta$ [cf. equations (2.29), (2.30)].

Using equation (3.4) the derivative of the transformation direction tensor with respect to stress $\partial_\sigma \Lambda_{n+1}^{(k)}$ is evaluated for the case of forward phase transformation.
\( (\xi > 0) \) as
\[
\partial_\sigma \Lambda_n^{(k)} = \frac{3}{2} \partial_\sigma H_{\text{cur}} \otimes \frac{\sigma_{\text{eff}}'}{\sigma_{\text{eff}}} + \frac{3}{2} H_{\text{cur}} \partial_\sigma \left[ \frac{\sigma_{\text{eff}}'}{\sigma_{\text{eff}}} \right],
\]
where the iteration counter \( k \) and the time step number \( (n+1) \) have been omitted for perspicuity. The corresponding derivative for the case of reverse phase transformation is equal to zero. To calculate the derivative of the current maximum transformation strain with respect to stress \( \partial_\sigma H_{\text{cur}} \) recall equation (2.24). Differentiating both sides of equation (2.24) result in
\[
\partial_\sigma \bar{\sigma} = \partial_\sigma \bar{\alpha}|_{\xi=1} = \partial_{H_{\text{cur}}} \bar{\alpha}|_{\xi=1} \partial_\sigma H_{\text{cur}}.
\]
Therefore, \( \partial_\sigma H_{\text{cur}} \) is given by
\[
\partial_\sigma H_{\text{cur}} = \frac{\partial_\sigma \bar{\sigma}}{\partial_{H_{\text{cur}}} \bar{\alpha}|_{\xi=1}}.
\]
After performing standard calculations the expression for \( \partial_\sigma \bar{\sigma} \) is found to be
\[
\partial_\sigma \bar{\sigma} = \frac{3}{2} \frac{\sigma'}{\bar{\sigma}}.
\]
To calculate the second term of equation (3.41) the quantity \( \partial_\sigma \left[ \frac{\sigma_{\text{eff}}'}{\sigma_{\text{eff}}} \right] \) must be found. Again, performing standard operations the following expression is derived:
\[
\partial_\sigma \left[ \frac{\sigma_{\text{eff}}'}{\sigma_{\text{eff}}} \right] = \frac{1}{\sigma_{\text{eff}}} \left[ I - \frac{1}{3} 1 \otimes 1 - \frac{3}{2} \frac{\sigma_{\text{eff}}'}{\sigma_{\text{eff}}} \otimes \frac{\sigma_{\text{eff}}'}{\sigma_{\text{eff}}} \right].
\]
The quantity \( I \) is the most general rank four symmetric identity tensor whose components are given by
\[
I_{ijkl} = \frac{1}{2} (\delta_{ik} \delta_{j\ell} + \delta_{i\ell} \delta_{jk}).
\]
Similarly, the derivative of the plastic direction tensor with respect to stress
\[ \partial_\sigma \Lambda_{n+1}^{p(k)} \] for the case of forward phase transformation is calculated as

\[
\partial_\sigma \Lambda_{n+1}^{p(k)} = \frac{3}{2} C_1^p \exp \left[ \frac{\zeta d}{C_2^p} \right] \partial_\sigma \left[ \frac{\sigma^{\text{eff}}}{\sigma^{\text{eff}}} \right],
\]

while the corresponding derivative for the case of reverse phase transformation is again equal to zero. The derivative of \( \Lambda_{n+1}^{p(k)} \) with respect to \( \xi \) is given by

\[
\partial_\xi \Lambda_{n+1}^{p(k)} = \begin{cases} 
-\frac{3 C_1^p}{2 C_2^p} \exp \left[ -\frac{\zeta d}{C_2^p} \right] \frac{H^{\text{cut}}}{H} \frac{\sigma^{\text{eff}}}{\sigma^{\text{eff}}}, & \xi > 0, \\
\frac{C_1^p}{C_2^p} \exp \left[ -\frac{\zeta d}{C_2^p} \right] \frac{H^{\text{cut}}}{H} \frac{\dot{\varepsilon}^{\text{max}}}{\dot{\varepsilon}^{\text{max}}}, & \xi < 0.
\end{cases}
\]

### 3.2.3. Consistent Tangent Stiffness and Thermal Moduli Tensors

The solution of the constitutive equations for the SMA involves calculating the stress increment for a given strain and temperature increment at each time step. This procedure makes use of the tangent stiffness tensor and the thermal tangent moduli tensor, appearing in the linearized problem. An example of such a situation is a displacement-based finite element method formulation which uses Newton’s method to solve the resulting non-linear equations. As mentioned by Qidwai and Lagoudas (2000a) the tangent tensors used by the global Newton’s method must be obtained in a manner consistent with the integration algorithm. The use of the continuum tangent tensors, derived in Section 2.4 would lead to a loss of the quadratic convergence of Newton’s iterative method (Simo and Taylor, 1985). Therefore, in this section the consistent tangent moduli tensors which are calculated at the end of the transformation correction iterative procedure and are passed to the global Newton’s method are derived.
The total differential of the stress-strain relation (3.13) result in
\[ \Delta S : \sigma_{n+1} d\xi_{n+1} + S_{n+1} : d\sigma_{n+1} = d\varepsilon_{n+1} - d\varepsilon^t_{n+1} - d\varepsilon^p_{n+1} \]
\[ - \bar\alpha_{n+1} dT_{n+1} - \Delta\bar\alpha (T_{n+1} - T_0) d\xi_{n+1}. \]  
(3.49)

The differential of the flow rules for the transformation and plastic strains [cf. equations (3.11), (3.12)] result in
\[ d\varepsilon^t_{n+1} = \Lambda_{n+1} d\xi_{n+1} + (\xi_{n+1} - \xi_n) \partial_\sigma \Lambda_{n+1} : d\sigma_{n+1}, \]  
(3.50)
\[ d\varepsilon^p_{n+1} = \partial_\xi R^p_{n+1} : d\sigma_{n+1} + \partial_\xi R^p_{n+1} d\xi_{n+1}, \]  
(3.51)
where the quantities \( \partial_\sigma R^p_{n+1} \) and \( \partial_\xi R^p_{n+1} \) are defined by equations (3.31), (3.32). The substitution of equations (3.50) and (3.51) into equation (3.49) eventually leads to
\[ d\sigma = \Xi_{n+1} : \left[ d\varepsilon - \bar\alpha_{n+1} dT_{n+1} - \chi_{n+1} d\xi_{n+1} \right], \]  
(3.52)
where \( \Xi_{n+1} \) and \( \chi_{n+1} \) are defined by equations (3.34), (3.35). Next, the consistency condition is written in the following form:
\[ d\Phi_{n+1} = \partial_\sigma \Phi_{n+1} : d\sigma_{n+1} + \partial_\xi \Phi_{n+1} d\xi_{n+1} + \partial_T \Phi_{n+1} dT_{n+1} = 0. \]  
(3.53)
Equation (3.52) together with equation (3.53) give the following expression for \( d\xi_{n+1} \):
\[ d\xi_{n+1} = \frac{\partial_\sigma \Phi_{n+1} : \Xi_{n+1} : [d\varepsilon - \bar\alpha_{n+1} dT_{n+1}] + \partial_T \Phi_{n+1} dT_{n+1}}{\partial_\sigma \Phi : \Xi_{n+1} : \chi_{n+1} - \partial_\xi \Phi}. \]  
(3.54)
Upon substituting equation (3.54) into equation (3.52) the following expression for \( d\sigma_{n+1} \) is obtained:
\[ d\sigma_{n+1} = \left[ \Xi_{n+1} - \frac{\Xi_{n+1} : \chi_{n+1} \otimes \partial_\sigma \Phi : \Xi_{n+1}}{\partial_\sigma \Phi : \Xi_{n+1} : \chi_{n+1} - \partial_\xi \Phi} \right] : d\varepsilon_{n+1} \]
\[ + \Xi_{n+1} : \left[ \chi_{n+1} \frac{\partial_\sigma \Phi : \Xi_{n+1} : \bar\alpha_{n+1} - \partial_T \Phi_{n+1}}{\partial_\sigma \Phi : \Xi_{n+1} : \chi_{n+1} - \partial_\xi \Phi} - \bar\alpha_{n+1} \right] dT_{n+1}. \]  
(3.55)
The consistent tangent stiffness tensor $\mathbf{L}_{n+1}$ and the consistent tangent thermal moduli tensor $\mathbf{\Theta}_{n+1}$ are defined as

\[
\mathbf{L}_{n+1} \equiv \frac{d\mathbf{\sigma}_{n+1}}{d\mathbf{\varepsilon}_{n+1}} = \mathbf{\Xi}_{n+1} - \mathbf{\Xi}_{n+1} : \mathbf{\chi}_{n+1} \otimes \frac{\partial \mathbf{\Phi}}{\partial \mathbf{\sigma}} : \mathbf{\Xi}_{n+1} - \frac{\partial \mathbf{\Phi}}{\partial \varepsilon_{n+1}},
\]

\[
\mathbf{\Theta}_{n+1} \equiv \frac{d\mathbf{\sigma}_{n+1}}{d\mathbf{T}_{n+1}} = \mathbf{\Xi}_{n+1} : \left[ \mathbf{\chi}_{n+1} \frac{\partial \mathbf{\Phi}}{\partial \mathbf{\sigma}} : \mathbf{\Xi}_{n+1} - \mathbf{\Xi}_{n+1} : \frac{\partial \mathbf{\Phi}}{\partial \varepsilon_{n+1}} - \frac{\partial \mathbf{\Phi}}{\partial \xi_{n+1}} - \mathbf{\alpha}_{n+1} \right].
\]

(3.56) (3.57)

3.2.4. Update of the Material Parameters

As explained in Section 2.5 the material parameters are updated only at the points of reversal of the phase transformation. To update them, the evolution equations (2.41)–(2.44) are utilized. These equations require knowledge of two parameters, which are the accumulated martensitic volume fraction $\zeta$ and accumulated detwinned martensitic volume fraction $\zeta^d$. Therefore, these variables must be made available and must be updated at each increment. To accomplish this, after the convergence of the return mapping iterative procedure, the values of $\zeta$ and $\zeta^d$ are calculated using their values from the previous increment and the newly found values of the increment of the martensitic volume fraction $\Delta \xi_{n+1}$ and the current maximum transformation strain $H_{\text{cur}}^\text{n+1}$.

3.2.5. Summary of the Numerical Algorithm for Dense SMA Constitutive Model

A summary of all steps of the numerical algorithm for the fully dense SMA are presented in Table II. The notation used in the summary is the same as the one used throughout this section, i.e., the current step number is $n + 1$ and all the quantities from the previous $n$th step are known.
Table II. Summary of the closest point projection numerical algorithm for dense SMA

1. Let $k = 0$, $\varepsilon_{n+1} = \varepsilon_n + \Delta \varepsilon_{n+1}$, $T_{n+1} = T_n + \Delta T_{n+1}$, $\varepsilon_{n+1}^{(t)} = \varepsilon_t^{(n)}$, $\varepsilon_{n+1}^{(p)} = \varepsilon_{n+1}^{(p)}$

\[ \xi_{n+1}^{(0)} = \xi_n, \quad S_{n+1}^{(0)} = S_n, \quad \alpha_{n+1}^{(0)} = \alpha_n. \]

2. Calculate $\sigma_{n+1}^{(k)}$, $\Phi_{n+1}^{(k)}$, $R_{t,n+1}^{(k)}$, $R_{p,n+1}^{(k)}$

\[
\sigma_{n+1}^{(k)} = S_{n+1}^{(k)} \cdot \left[ \varepsilon_{n+1} - \varepsilon_{n+1}^{(t)(k)} - \varepsilon_{n+1}^{(p)(k)} - \alpha_{n+1}^{(k)}(T_{n+1} - T_0) \right]
\]

\[
\Phi_{n+1}^{(k)} = \Phi(\sigma_{n+1}^{(k)}, T_{n+1}; \xi_{n+1}^{(k)})
\]

\[
R_{t,n+1}^{(k)} = -\varepsilon_{n+1}^{(t)(k)} + \varepsilon_{n+1}^{(t)} + \alpha_{n+1}^{(k)}(\xi_{n+1}^{(k)} - \xi_n)
\]

\[
R_{p,n+1}^{(k)} = -\varepsilon_{n+1}^{(p)(k)} + \varepsilon_{n+1}^{(p)} + \alpha_{n+1}^{(k)} \left| \xi_{n+1}^{(d)} - \xi_{n+1}^{(d)} \right|
\]

If $\Phi_{n+1}^{(k)} < 0$ OR $|\Delta \xi_{n+1}^{(k)}| < TOL 1$ then go to 8.

3. Check for reversal of the loading direction.

If the loading direction is reversed update the material parameters.

4. Calculate $\Xi_{n+1}^{(k)}$ and $\chi_{n+1}^{(k)}$

\[
\Xi_{n+1}^{(k)} = \left[ S_{n+1}^{(k)} + \partial_\sigma \Lambda_{n+1}^{(k)}(\xi_{n+1}^{(k)} - \xi_n) + \partial_\sigma R_{p,n+1}^{(k)} \right]^{-1}
\]

\[
\chi_{n+1}^{(k)} = \Delta \alpha(T_{n+1} - T_0) + \Delta S : \sigma_{n+1}^{(k)} + \alpha_{n+1}^{(k)} + \partial_\xi R_{p,n+1}^{(k)}
\]

5. Calculate the increments of the martensitic volume fraction $\Delta \varepsilon_{n+1}^{(k)}$

stress $\Delta \sigma_{n+1}^{(k)}$, transformation strain $\Delta \varepsilon_{n+1}^{(t)(k)}$ and plastic strain $\Delta \varepsilon_{n+1}^{(p)(k)}$

\[
\Delta \varepsilon_{n+1}^{(k)} = \frac{\partial_\sigma \Phi_{n+1}^{(k)} : \Xi_{n+1}^{(k)} : \left[ R_{t,n+1}^{(k)} + R_{p,n+1}^{(k)} \right] - \Phi_{n+1}^{(k)}}{\partial_\xi \Phi_{n+1}^{(k)} - \partial_\sigma \Phi_{n+1}^{(k)} : \Xi_{n+1}^{(k)} : \chi_{n+1}^{(k)}}
\]

\[
\Delta \sigma_{n+1}^{(k)} = -\Xi_{n+1}^{(k)} : \left[ R_{t,n+1}^{(k)} + R_{p,n+1}^{(k)} + \chi_{n+1}^{(k)} \Delta \varepsilon_{n+1}^{(k)} \right]
\]

\[
\Delta \varepsilon_{n+1}^{(p)(k)} = -R_{p,n+1}^{(k)} - \partial_\sigma R_{p,n+1}^{(k)} : \Delta \sigma_{n+1}^{(k)} - \partial_\xi R_{p,n+1}^{(k)} : \Delta \xi_{n+1}^{(k)}
\]

\[
\Delta \varepsilon_{n+1}^{(t)(k)} = -S_{n+1} : \Delta \sigma_{n+1}^{(k)} - \Delta \varepsilon_{n+1}^{(p)(k)} - \left[ \Delta \alpha(T_{n+1} - T_0) + \Delta S : \sigma_{n+1}^{(k)} \right] \Delta \varepsilon_{n+1}^{(k)}
\]
6. Update martensitic volume fraction, transformation and plastic strains, elastic compliance tensor and thermal expansion coefficient tensor:

\[
\begin{align*}
\xi_{n+1}^{(k+1)} &= \xi_{n+1}^{(k)} + \Delta \xi_{n+1}^{(k)} \\
\varepsilon_{n+1}^t(k+1) &= \varepsilon_{n+1}^t(k) + \Delta \varepsilon_{n+1}^t(k) \\
\varepsilon_{n+1}^p(k+1) &= \varepsilon_{n+1}^p(k) + \Delta \varepsilon_{n+1}^p(k) \\
S_{n+1}^{(k+1)} &= S^A + \xi_{n+1}^{(k+1)} \Delta S \\
\bar{\alpha}_{n+1}^{(k+1)} &= \bar{\alpha}^A + \xi_{n+1}^{(k+1)} \Delta \bar{\alpha}
\end{align*}
\]

7. Set iteration counter \( k = k + 1 \). Go to 2.

8. Calculate consistent tangent stiffness tensor \( \mathbf{L}_{n+1} \) and thermal moduli tensor \( \mathbf{\Theta}_{n+1} \):

\[
\begin{align*}
\mathbf{L}_{n+1} &= \Xi_{n+1} - \frac{\Xi_{n+1}: \mathbf{X}_{n+1} \otimes \partial \Phi : \Xi_{n+1}}{\partial \Phi : \Xi_{n+1} : \mathbf{X}_{n+1} - \partial \Phi} \\
\mathbf{\Theta}_{n+1} &= \Xi_{n+1} : \left[ \mathbf{X}_{n+1} \frac{\partial \Phi : \Xi_{n+1} : \bar{\alpha}_{n+1} - \partial \Phi : \Xi_{n+1} : \mathbf{X}_{n+1} - \partial \Phi}{\partial \Phi : \Xi_{n+1} : \mathbf{X}_{n+1} - \partial \Phi} \right] - \bar{\alpha}_{n+1}
\end{align*}
\]

9. Update \( \zeta_{n+1} \) and \( \dot{\zeta}_{n+1}^d \):

\[
\begin{align*}
\zeta_{n+1} &= \zeta_n + |\Delta \zeta_{n+1}| \\
\dot{\zeta}_{n+1}^d &= \dot{\zeta}_n + \frac{H_{\text{cur}}}{H} |\Delta \zeta_{n+1}|
\end{align*}
\]

The numerical algorithm presented in this chapter is implemented as a user material subroutine (UMAT) which is used by the FEM package ABAQUS (HKS, 1997). All of the essential steps of finite element analysis — mesh generation, assembly of the equations and their solution, the global Newton’s method to resolve the nonlinearity, etc. — are handled by ABAQUS. When the analyses involve an SMA material, the UMAT is called by ABAQUS. The internal state variables (\( \xi, \varepsilon^t, \varepsilon^p \), etc.) for each integration point are stored in a designated array and updated after each call to the subroutine.
3.3. Test Cases for Numerical Implementation

To test the numerical implementation of the model for dense SMAs and to demonstrate the capabilities of the model, different boundary-value problems (BVPs) are presented in this section. First, a uniaxial isothermal pseudoelastic case is presented. The second BVP represents a uniaxial thermally-induced transformation under constant stress. Finally, the third BVP involves a torsion-compression loading of a cylindrical SMA specimen. The material parameters for all of the three cases are the ones given by Bo et al. (1999) and are presented in Table I.

3.3.1. Uniaxial Isothermal Pseudoelastic Loading

The schematic of the BVP for this loading case is shown in Figure 18. The domain is chosen to be a unit cube (1×1×1 m). Since the stress is constant in the whole domain during the loading, a finite element mesh of only one linear element is chosen. Initially, the material is in stress-free state. During the first step of the loading, the stress is increased to 600 MPa which results in stress-induced phase transformation. During the unloading step a reverse phase transformation occurs. The stress-strain response of the material for this case is shown in Figure 19 for two different temperatures: 70°C and 80°C.

In the case of loading at $T = 70^\circ$C it can be seen that the forward phase transformation starts at the value of applied stress approximately equal to 210 MPA and the transformation is completed at 510 MPA. At the point of completion of the forward transformation the value of the transformation strain is equal to the value of the maximum transformation strain $H = 0.069$. The onset of the reverse phase transformation is at 350 MPa and the transformation is completed at 40 MPa. During the reverse phase transformation, the transformation strain changes from its maximum value to
Fig. 18. Schematic of the BVP for uniaxial pseudoelastic SMA response; (a) geometry and boundary conditions; (b) loading history.

zero. The change in the temperature leads to change of the stress values at which the transformation occurs. The onset of the transformation for $T = 80^\circ C$ occurs at the value of the applied stress approximately equal to 265 MPa and the transformation is completed at 565 MPa. The reverse transformation initiates at 405 MPa and it is completed at 100 MPa.

The loading was performed incrementally and the total load was divided into 100 loading increments. The unloading was also performed using 100 increments. The value of the tolerance $TOL_1$ (see Table II) was chosen to be $1.0 \times 10^{-8}$. For this value of the tolerance and the number of loading increments the number of Newton iterations performed for each of the eight integration points during the transformation correction step was in the range between 4 and 6. The numerical calculations were performed on a single processor DIGITAL™ Alpha 600AU workstation running Digital UNIX V4.0E. The total CPU time to complete the numerical calculations was 14.2 sec.
3.3.2. Uniaxial Isobaric Thermally-Induced Transformation

Thus BVP describes a thermal cycle of a uniaxial SMA specimen under constant applied stress. The schematic of the BVP and the loading history are shown in Figure 20. Initially the material is isothermally loaded to a given stress level which is then kept constant. The first loading step involves cooling of the SMA from the initial temperature of 100°C to the final temperature of 0°C. During this loading step a forward phase transformation occurs and the transformation strain develops. The final value of the transformation strain after the completion of the phase transformation is dictated by the level of the applied stress and is equal to the current maximum transformation strain $H_{\text{cur}}$. To illustrate the dependance of $H_{\text{cur}}$ on the applied stress, cases with different values of the applied stress are performed. During
the second loading step the material is heated back to 100°C and the transformation strain is recovered.

Fig. 20. Schematic of the BVP for uniaxial isobaric thermally-induced transformation; (a) geometry and boundary conditions; (b) loading history.

The results for the loading cases are shown in Figure 21. Two different effects of the level of the applied stress on the results are observed. First, as mentioned above, the maximum transformation strain during the phase transformation increases with the increase of the value of the applied stress. The second effect is the shift of the initial transformation temperature: the transformation starts at higher temperature for higher value of the applied stress. This shift of the transformation temperatures can be explained by recalling the expression for the transformation function, given by equations (3.8) and (3.9). As seen from equation (3.9) with higher value of the applied stress the transformation criterion will be satisfied for higher temperature.

3.3.3. Torsion-Compression Loading

While both of the previous loading cases were uniaxial, the model is also capable of handling three-dimensional loading cases. To demonstrate such loading cases, the
Fig. 21. Strain versus temperature for different values of the applied stress.

response of a cylindrical SMA bar subjected to combined torion-compression and torsion followed by compressive loading is modeled. The schematic of the BVPs is shown in Figure 22. The specimen is chosen to have a diameter of 13 mm and length of 35 mm.\(^1\) The domain is discretized using eight-node quadratic axisymmetric elements with a twist degree of freedom (elements CGAX8, for details see HKS, 1997). Since there is no stress variation in the axial direction, only one layer of elements is used in that direction with a length of 1.75 mm, while 5 elements are used in the radial direction, as shown in Figure 22c. The maximum value of the applied rotation (see Figure 22) is taken to be \(\theta_{\text{max}} = 0.02\) rad \((\approx 1.15^\circ)\), which corresponds to 11.4 rad/m

\(^1\)The dimensions are chosen to correspond to the dimensions of a porous SMA bar which will be presented in Section 5.2.2
rotation \((\approx 1.8 \text{ full revolutions per meter length})\), while the maximum value of the displacement in the axial direction is taken to be \(u_{z}^{\text{max}} = -0.125 \text{ mm}\), corresponding to axial compressive strain of \(\varepsilon_{zz} = 0.071\). Both compression and rotation boundary conditions are applied on the top surface of the specimen, while the bottom surface is held fixed in the \(z\)- and \(\theta\)-directions. Traction-free boundary condition in the radial direction is applied. The numerical simulations are performed at a temperature of \(60^\circ\text{C}\).

![Fig. 22. Schematic of the BVP for multiaxial loading of an SMA bar; (a) geometry; (b) loading history; (c) finite element mesh and boundary conditions.](image)

First the results for the sequential torsion-compression loading are presented. During the first loading step when the bar is subjected to torsion a nonhomogeneous stress state is created. As the stress increases the critical stress for the onset of the phase transformation is first reached at the outer surface of the bar. The phase transformation front then propagates towards the center of the bar. To illustrate this, the contour plot of the martensitic volume fraction for the cross-section of the bar at the end of the torsional loading (when the value of the loading parameter is equal to
Fig. 23. Contour plot of the martensitic volume fraction in the SMA bar at the end of the torsional loading.

0.5) is shown in Figure 23. It can be seen that the lines of constant value of $\xi$ form concentric circles.

The history of the axial and shear stress components during both loading steps is shown in Figure 24. The average values of these quantities are shown for the element indicated in Figure 24. During the initial torsional loading the shear stress linearly increases until a critical value is reached. At this point (at the value of the loading parameter of $\approx 0.1$) the phase transformation initiates. During the first loading
Fig. 24. History of the axial and shear stress components during sequential torsion-compression loading.

step the axial stress component remains zero. During the second loading step the phase transformation continues until it is fully completed (at the value of the loading parameter of ≈ 0.9). The axial stress increases while the shear stress is partially relaxed. After the completion of the phase transformation the material is fully in the martensitic phase and behaves linearly.

To explain the partial relaxation of the shear stress during the compressive axial loading, consider the shear and axial components of the transformation strain, shown in Figure 25. It is seen that during the second loading step, when a compressive loading is applied, the shear component of the transformation strain continues to increase. This is caused by the choice of the functional form of the transformation direction tensor $\Lambda$, given by equation (2.22). Since the shear component of the stress is non-zero, the shear component of the transformation strain keeps developing during the second loading step, albeit with a smaller rate. On the other hand, since the applied rotation and, therefore, the total strain, is kept constant during the
Fig. 25. History of the axial and shear transformation strain components during sequential torsion-compression loading.

Compressive loading, the shear component of the stress decreases according to the constitutive equation (2.9).

The history of the axial and shear stress components for the simultaneous torsion-compression loading case are presented in Figure 26. The results for this loading case resemble superposition of the results under compression and torsion applied independently. The stresses increase linearly until a critical value is reached and transformation initiates (the value of the loading parameter approximately equal to 0.05). Then the transformation proceeds until the material is fully transformed at the value of the loading parameter approximately equal to 0.9. After the transformation is completed, the response of the material is again linear with the elastic properties of the martensite.
3.4. Correlation with Experimental Data

The experimental results for NiTi undergoing cyclic loading will be simulated in this section. The experimental data for one of the NiTi alloys reported by Strnadel et al. (1995b) and presented in Section 2.1 will be used. Two types of tests were performed by Strnadel et al. (1995b): the first type involved cycling, during which the material is loaded to the same value of strain during each cycle and the second type involved cycling performed to a given constant value of stress. Both types of tests have been performed at a temperature higher than the austenitic finish temperature $A_{0f}$. The data for alloy “A”, which refers to one of the six tested alloys in the original publication (Strnadel et al., 1995b) and has the composition Ti-50.9at%Ni. The experimental results for alloys “A” for loading cases are shown on the top of Figure 8. Based on the dimensions of the specimen and the reported elongation the maximum value of strain during the first cycling test is estimated to be equal to $\varepsilon_{\text{max}} = 0.04$. The maximum value of the stress during the second test is reported to
be $\sigma_{\text{max}} = 550\text{MPa}$. Twenty loading-unloading cycles with a constant maximum value of strain have been performed, while the number of cycles with a constant maximum value of strain is 50.

First the material parameters for the alloy are determined based on the experimental graphs and reported data. The procedure described in Section 2.6 is used. The obtained parameters are given in Table III. It should be mentioned that there is no data on the dependance of the current maximum transformation strain $H_{\text{cur}}$ on the value of the applied stress. Therefore, the data shown in Figure 14 is used to obtain the back stress coefficients $D^{b}_{i}$. The coefficients are obtained for the value of the maximum transformation strain for high values of stress $H = 0.038$) as reported by Strnadel et al. (1995b). A polynomial of degree 5 is used in the expression for the back stress. Based on the experimental results the back stress parameters are assumed to be the same for both the initial and the final state of the material and are given by $D^{b}_{1} = 6.18 \times 10^{3} \text{MPa}$, $D^{b}_{2} = -7.37 \times 10^{5} \text{MPa}$, $D^{b}_{3} = 4.98 \times 10^{7} \text{MPa}$, $D^{b}_{4} = -1.63 \times 10^{9} \text{MPa} \text{ and } D^{b}_{5} = 2.03 \times 10^{10} \text{MPa}$.

The initial set of material parameters has been determined using the initial transformation cycle for the case of loading to a maximum value of stress, while the final set has been determined from the stress-strain response after 50 cycles (see Figure 8). In addition, as seen from Table III the parameters $\lambda_{1}$ and $\lambda_{2}$ have been selected to be the same. Their value has been determined such that the material parameters reach their saturation values after 50 cycles. As seen from Table III, not all of the parameters change their values during the transformation cycling. Based on the experimental results the maximum transformation strain is assumed to be constant. Only the initial value of the martensitic start temperature is reported in the work by Strnadel et al. (1995b) and thus here it is also assumed to remain constant. Four of the parameters — $\alpha^{A}$, $\alpha^{M}$, $c^{A}$, $c^{M}$ — are taken from the work of Lagoudas and
Table III. Material parameters for NiTi alloy “A”.

Parameters remaining constant during cyclic loading

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E^A$</td>
<td>46.0 GPa</td>
<td>$\alpha^A$</td>
<td>$11.0 \times 10^{-6}$ K$^{-1}$</td>
</tr>
<tr>
<td>$E^M$</td>
<td>25.0 GPa</td>
<td>$\alpha^M$</td>
<td>$6.0 \times 10^{-6}$ K$^{-1}$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.33</td>
<td>$\rho c^A$</td>
<td>2.12 MJ/(m$^3$K)</td>
</tr>
<tr>
<td>$m_1$</td>
<td>3.5</td>
<td>$\rho c^M$</td>
<td>2.12 MJ/(m$^3$K)</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>3.5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Parameters changing during transformation cycling

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Initial set</th>
<th>Final set</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_0^{os}$</td>
<td>242.3 K</td>
<td>242.3 K</td>
</tr>
<tr>
<td>$H$</td>
<td>0.038</td>
<td>0.038</td>
</tr>
<tr>
<td>$\rho \Delta s_0$</td>
<td>$-0.24$ MJ/(m$^3$K)</td>
<td>$-0.17$ MJ/(m$^3$K)</td>
</tr>
<tr>
<td>$Y$</td>
<td>5.0 MJ/m$^3$</td>
<td>3.0 MJ/m$^3$</td>
</tr>
<tr>
<td>$D_1^d$</td>
<td>5.0 MPa</td>
<td>6.0 MPa</td>
</tr>
<tr>
<td>$D_2^d$</td>
<td>5.22 MPa</td>
<td>4.0 MPa</td>
</tr>
</tbody>
</table>

Parameters characterizing the response during cyclic loading

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1^p$</td>
<td>$3.6 \times 10^{-3}$</td>
<td>$\lambda_1$</td>
<td>0.25</td>
</tr>
<tr>
<td>$C_2^p$</td>
<td>18.0</td>
<td>$\lambda_2$</td>
<td>0.25</td>
</tr>
</tbody>
</table>
Bo (1999). Since both works (Lagoudas and Bo, 1999; Strnadel et al., 1995b) deal with NiTi alloys it is expected that these physical constants will be close for alloys with only slight change in the composition. As explained earlier in Section 2.7.2, the values of these constants have no effect on the results when the temperature during the loading-unloading cycle remains constant.

### 3.4.1. Response of NiTi SMA to Constant Maximum Stress Cycling

The response of the material for the constant maximum stress cycling loading is presented in Figure 27. Only the stress-strain curves for the first and 50th (last) loading cycle are shown. It can be seen that the transformation response after 50 cycles has stabilized and the plastic strain developed during the last cycle is negligible. The transformation loop has significantly evolved during the cyclic loading. First, the value of stress for the onset of phase transformation is much lower for the last loading cycle compared to the one for the first cycle. Also, the transformation hardening during the last cycle is significantly higher than the hardening during the first cycle. The area enclosed by the transformation hysteresis loop is smaller for the last cycle than the area enclosed by the initial loop.

The plastic strain for this loading case has saturated after 50 cycles. The graph showing its evolution during the cycling is shown in Figure 28. Further transformation cycling will result in a negligible change of the plastic strain and the shape of the transformation loop. As seen from Figure 27, the modeling results are in very good agreement with the experimental observations. It must be pointed out that the modeling results are not predictions but simulations of the experiment, since the experimental data has been used to estimate the material parameters.
3.4.2. Response of NiTi SMA to Constant Maximum Strain Cycling

The response of the material during constant maximum strain cycling is shown in Figure 29. Three stress-strain curves are presented: the initial stress-strain curve (first cycle) as well as the stress-strain curves for the 10th cycle. It is observed from the figure that as the number of cycles increases, the value of stress at the maximum value of strain $\varepsilon_{\text{max}}$ decreases. In addition, the area enclosed by the hysteresis loop also decreases. Two factors acting in concert are responsible for these effects. First, the accumulation of the residual strain contributes for the smaller hysteresis area as well as for the lower value of stress. The second factor is the evolution of the material parameters with the number of cycles. Since the value of stress for the onset of the phase transformation decreases, then the same value of strain for a later cycle will correspond to a lower value of stress than that for an earlier cycle.

The evolution of the residual plastic strain for this loading case is shown in
Figure 28. Plastic strain evolution during constant maximum stress cycling.

Figure 30. It is observed that the plastic strain has not reached a saturation value and continues to increase. This can be explained by the fact that this type of cycling results in incomplete phase transformation, and, therefore, it would take much more cycles for the plastic strain to saturate than complete transformation cycles. As shown in Figure 31 the maximum value of the martensitic volume fraction achieved during each subsequent loading cycle $\xi_{\text{max}}$ significantly decreases ($\xi_{\text{max}} = 0.56$ for the first cycle, while $\xi_{\text{max}} = 0.28$ for the 10th cycle). This incomplete phase transformation results in minor hysteresis loop branches during unloading.

In contrast to the previous case, the modeling results presented for constant maximum strain cyclic loading are predictions, since the experimental data for this loading case has not been used to calibrate the model. The comparison of the model-
Fig. 29. Stress-strain response of NiTi SMA to cycling up to a constant maximum value of strain: curves for the first and 10th cycles.

...ing results with the experimental curves, presented in Figures 29 and 30 shows that the results for constant maximum strain cycling are in relatively good agreement. Both the stress-strain responses as well as the plastic strain evolution are predicted with good accuracy. Also, the shape of the minor hysteresis loops predicted by the model is very close to the shape of the experimental loops.

3.4.3. Response of an SMA Torque Tube

In this section the capabilities of the model to handle loading cases beyond uniaxial loading are tested by simulating an SMA torque tube. The material parameters for NiTi SMA presented in Table III are used in the numerical calculations. The following
dimensions of the tube are used: outer diameter $d_o = 6.34\,\text{mm}$ and inner diameter $d_{in} = 5.0\,\text{mm}$. The reason for selecting these dimensions is to model a tube which geometrically resembles tubes available commercially.\(^2\)

Based on the small thickness of the tube wall only one quadratic element in radial direction is used. In addition, since the stress is constant in the axial direction, one element in the axial direction is sufficient to obtain accurate results. To obtain appropriate aspect ratio, the length in the axial direction has been chosen to be $0.67\,\text{mm}$, equal to the wall thickness. An axisymmetric finite element with a rotational degree of freedom (element CGAX8 from the ABAQUS element library, see HKS,\(^2\)

\(^2\)The diameters used here have also been used by Qidwai (1999) and are based on the specifications of torque tubes manufactured by Memry Corp.
Fig. 31. Maximum value of the martensitic phase transformation $\xi_{\text{max}}$ during constant maximum strain cycling.

1997) was used. The schematic of the mesh and the boundary conditions is shown in Figure 32. The bottom part of the tube is fixed and rotation is applied to the top part. The maximum value of the applied rotation is $1.4 \times 10^{-2}$ rad. The rotation is applied cyclically in both direction. The loading history for one full cycle is also shown in Figure 32. Ten full rotational loading/unloading cycles in both directions have been applied.

The stress-strain response of the tube is shown in Figure 33 where the average shear stress in the finite element is plotted versus the average shear strain. The results shown in the figure indicate the evolution of the transformation loop with the number of loading cycles. One significant difference, observed between these results
and the uniaxial results presented in Sections 3.4.2 and 3.4.1 is the value of the plastic strain at the end of the cycling test. While the final value of the plastic strain in the uniaxial test is equal to the value of the accumulated plastic strain, the final value in the case of torsional loading is significantly smaller. The explanation for this fact is in the nature of the cycling loading. The loading for the uniaxial results is not reversed, therefore, the plastic strain accumulates only in one direction (direction of the loading). In the case of torsional cycling loading with the loading history shown in Figure 32c the direction of the loading is reversed during each cycle. Therefore, during each half of the loading cycle the direction of the plastic strain accumulation is
also reversed. The result of this effect, as shown in Figure 34 is the almost complete cancellation of the resulting total plastic strain. It should be noted, however, that even in the absence of observable plastic strain the material still changes during the cycling. As seen from Figure 33 the hysteresis loop evolves during the cycling loading. Thus, the microstructural changes caused by the cyclic loading are taken into account by evolving the material parameters and updating the internal state variables.

Fig. 33. Stress-strain response of NiTi SMA tube subjected to cycling torsional loading: *average* shear stress over *average* shear strain.
Fig. 34. Plastic strain evolution in NiTi SMA tube during cycling torsional loading.
CHAPTER IV

MODELING OF POROUS SHAPE MEMORY ALLOYS USING MICROMECHANICAL AVERAGING TECHNIQUES

In this chapter\(^1\) a thermomechanical constitutive model for porous SMAs is developed. The current work uses micromechanical averaging methods in incremental formulation to establish a macroscopic constitutive model for the porous SMA material using the properties of the dense SMA and information about pore shape, orientation and volume fraction. Analytical expressions for the overall elastic and tangent stiffness of the porous SMA material are derived as well as an evolution equation for the overall inelastic strain. The derivations are first given for the more general case of a two-phase composite with rate-independent constituents. After the general expressions are derived, the properties of the porous SMA material are obtained by using the constitutive model for dense SMA to model the matrix, and treating the inhomogeneities as elastic phases with stiffness equal to zero.

4.1. Modeling of a Composite with Inelastic Matrix and Inelastic Inhomogeneities

The development of the model starts by considering a two-phase composite material with both matrix and inhomogeneities undergoing inelastic deformations. Let the Cauchy stress in the matrix be denoted by \(\mathbf{\sigma}^m\), the linearized strain be \(\mathbf{\varepsilon}^m\) and the inelastic strain be \(\mathbf{\varepsilon}^{in,m}\). The matrix is characterized by its elastic stiffness \(\mathbf{L}^m\) (compliance \(\mathbf{M}^m = (\mathbf{L}^m)^{-1}\)) and tangent stiffness \(\mathbf{T}^m\). Similarly, let the stress in the inhomogeneities be \(\mathbf{\sigma}^i\), the strain be \(\mathbf{\varepsilon}^i\) and the inelastic strain be \(\mathbf{\varepsilon}^{in,i}\). The inho-

mogeneities are characterized by the elastic stiffness $L^i$ (compliance $M^i = (L^i)^{-1}$), and tangent stiffness $T^m$. Let the volume fraction of the matrix phase be $c^m$ and the volume fraction of the inhomogeneities be $c^i = 1 - c^m$. The composite is characterized by its effective elastic stiffness $L$, tangent stiffness $T$ and effective stress, strain and inelastic strain $\Sigma$, $E$ and $E^{in}$.

The approach taken in this work follows the standard micromechanical techniques for composites undergoing inelastic deformations found in the literature (Hill, 1965; Hutchinson, 1970; Tandon and Weng, 1988). However, the current work takes into account not only the development of inelastic strains in the phases but also the change in the stiffness of the phases during loading/unloading, as well as their transformation characteristics.

4.1.1. Constitutive Models for the Matrix and the Inhomogeneities

In this work the matrix will be the SMA, which will be modelled by a rate-independent inelastic constitutive model with internal state variables. The model developed earlier in Chapter II will be utilized here. Note that any other SMA constitutive model can also be applied. One of the characteristics of SMAs is the change in the elastic stiffness with phase transformation, in addition to the inelastic strain induced by the martensitic phase transformation. Starting from the Hooke’s law for the elastic strain

$$\sigma^m = L^m : \varepsilon^{el,m} = L^m : (\varepsilon^m - \varepsilon^{in,m}),$$

the rate of the stress in the matrix is given by

$$\dot{\sigma}^m = \dot{L}^m : \varepsilon^{el,m} + L^m : \dot{\varepsilon}^{el,m} = \dot{L}^m : (\dot{\varepsilon}^m - \dot{\varepsilon}^{*m}),$$

where $\dot{\varepsilon}^{*m}$ is defined by

$$\dot{\varepsilon}^{*m} \equiv \dot{\varepsilon}^{in,m} + \dot{M}^m : \sigma^m.$$
The second term on the right-hand-side of equation (4.3) above reflects the change of the elastic stiffness of the matrix during the loading. To better understand its physical meaning consider the one-dimensional case schematically shown in Figure 35.

As shown on the figure, initially the material is at state ① and is characterized by stress $\sigma^m$, total strain $\varepsilon^m$ and elastic compliance $M^m$. The total strain is decomposed into the elastic strain $\varepsilon^{el,m}$ and inelastic strain $\varepsilon^{in,m}$. An increment of load brings the material to state ② where it is characterized by stress $\sigma^m + \Delta \sigma^m$, total strain $\varepsilon^m + \Delta \varepsilon^m$ and elastic compliance $M^m + \Delta M^m$ (see Figure 35). The value of the elastic strain at state ② is

$$\varepsilon^{el,m} + \Delta \varepsilon^{el,m} = (M^m + \Delta M^m)(\sigma^m + \Delta \sigma^m),$$  

(4.4)

and the following expression for $\Delta \sigma^m$ is obtained:

$$\Delta \sigma^m = L^m(\Delta \varepsilon^{el,m} - \Delta M^m \sigma^m - \Delta M^m \Delta \sigma^m),$$  

(4.5)

which in the limit of the loading increment approaching zero reduces to the 1-D version of equation (4.2).

The stress increment in the matrix can also be obtained using the tangent stiffness of the matrix as

$$\dot{\sigma}^m = T^m : \dot{\varepsilon}^m.$$  

(4.6)

A specific expression for the tangent stiffness $T^m$ will not be given in the current derivation. Suffices it to say that $T^m$ will be calculated according to the given constitutive model for the SMA matrix.

The constitutive equations for the inhomogeneities are given by

$$\sigma^i = L^i : (\varepsilon^i - \varepsilon^{in,i}).$$  

(4.7)
The rate form of equation (4.7) is very similar to equation (4.2):

\[ \dot{\sigma}^i = L^i : (\dot{\varepsilon}^i - \dot{\varepsilon}^{*i}), \]  

where \( \dot{\varepsilon}^{*i} \) reflects both the change in the inelastic strain and a possible change of the elastic stiffness during the loading/unloading of the inhomogeneities and is defined as

\[ \dot{\varepsilon}^{*i} \equiv \dot{\varepsilon}^{in,i} + \dot{\mathbf{M}}^i \sigma^i. \]  

Similarly as in the case of the matrix, the stress increment in the inhomogeneities can be calculated using the tangent stiffness of the inhomogeneities \( \mathbf{T}^i \):

\[ \dot{\sigma}^i = \mathbf{T}^i : \dot{\varepsilon}^i. \]  

Note, that in certain special cases one or both of terms \( \dot{\mathbf{M}}^m \) and \( \dot{\mathbf{M}}^i \) can be equal to zero. One example would be plastic deformation of the corresponding phase with no change in the elastic stiffness. Another example would be an SMA phase with
equal elastic stiffness for both austenite and martensite.

To simplify further derivations the rate form of the constitutive equations for both phases can be written in a generic form as

\[
\dot{\sigma} = \mathbf{L} : (\dot{\varepsilon} - \dot{\varepsilon}^*) ,
\]

(4.11)

where \( \dot{\varepsilon}^* \) is equal to \( \dot{\varepsilon}^{*m} \) in the matrix and \( \dot{\varepsilon}^{*i} \) in the inhomogeneities and \( \mathbf{L} \) is equal to \( \mathbf{L}^m \) in the matrix and \( \mathbf{L}^i \) in the inhomogeneities.

4.1.2. Macroscopic Composite Behavior

The macroscopic constitutive law for the composite is proposed as

\[
\Sigma = \mathbf{L} : (\mathbf{E} - \mathbf{E}^{in}) ,
\]

(4.12)

where \( \Sigma \) and \( \mathbf{E} \) are the overall stress and strain tensors defined as

\[
\Sigma = \langle \sigma \rangle = \frac{1}{V} \int_V \sigma dV ,
\]

(4.13)

\[
\mathbf{E} = \langle \varepsilon \rangle = \frac{1}{V} \int_V \varepsilon dV ,
\]

(4.14)

\( \mathbf{E}^{in} \) is the macroscopic inelastic strain tensor and \( \mathbf{L} \) is the overall elastic stiffness tensor.

The rate form of equation (4.12) is given by

\[
\dot{\Sigma} = \mathbf{L} : (\dot{\mathbf{E}} - \dot{\mathbf{E}}^*) ,
\]

(4.15)

where \( \dot{\mathbf{E}}^* \) is defined as

\[
\dot{\mathbf{E}}^* \equiv \dot{\mathbf{E}}^{\text{in}} + \dot{\mathbf{M}} : \Sigma .
\]

(4.16)

An alternative formulation which involves stress and strain rates and the macro-
scopic tangent stiffness of the composite $T$ is

$$\dot{\Sigma} = T : \dot{E}. \quad (4.17)$$

To fully characterize the macroscopic composite response, expressions for $L$, $T$ and the evolution of $E^{in}$ must be derived. In the following, these expressions will be derived using micromechanical averaging techniques.

To connect the macroscopic stress and strain rates to the respective microscopic ones the following *instantaneous* strain and stress concentration factors $A(x)$ and $B(x)$ are defined as (assuming that the local strain is driven by the macroscopic strain):

$$\dot{\varepsilon} = A(x) : \dot{E}, \quad (4.18)$$

$$\dot{\sigma} = B(x) : \dot{\Sigma}. \quad (4.19)$$

Tensors $A(x)$ and $B(x)$ are generic and take different values in different phases such that

$$A(x) = \begin{cases} 
A^m(x), & x \in V^m; \\
A^i(x), & x \in V^i;
\end{cases} \quad (4.20)$$

$$B(x) = \begin{cases} 
B^m(x), & x \in V^m; \\
B^i(x), & x \in V^i.
\end{cases} \quad (4.21)$$

To proceed with the derivations, first an expression for the macroscopic elastic stiffness $L$ will be obtained. For the case of elastic response there is no change in the stiffness of neither phase and there is no change in the values of the inelastic strain in neither of the phases. Then, equation (4.15) is written as

$$\dot{\Sigma} = \frac{1}{V} \int_V \dot{\sigma} dV = \frac{1}{V} \int_{V^m} L^m : \dot{\varepsilon}^m dV + \frac{1}{V} \int_{V^i} L^i : \dot{\varepsilon}^i dV. \quad (4.22)$$
Assuming that the elastic stiffness in each of the phases depends only on the average value of the stress in each phase, equation (4.22) becomes

\[ \dot{\Sigma} = (c^m L^m A^{el,m} + c^i L^i A^{el,i}) : \dot{\mathbf{E}}. \]  

(4.23)

Note that equation (4.23) is derived for the elastic loading (unloading) case and \( A^{el,m} \) and \( A^{el,i} \), appearing in this equation are the average elastic strain concentration factors:

\[ A^{el,m} = \frac{1}{V_m} \int_{V_m} A^{el}(x) dV, \]  

(4.24)

\[ A^{el,i} = \frac{1}{V_i} \int_{V_i} A^{el}(x) dV. \]  

(4.25)

They differ from the instantaneous strain concentration factors defined by equation (4.18) and must be calculated assuming elastic behavior of the composite phases. The overall elastic stiffness \( \mathbf{L} \) is expressed from equation (4.23) as

\[ \mathbf{L} = c^m L^m A^{el,m} + c^i L^i A^{el,i}. \]  

(4.26)

The expression for the elastic stiffness (4.26) is well-known and presented in the literature (see, for example the works of Benveniste, 1987; Hill, 1963; Weng, 1984).

Next, an expression for the overall tangent stiffness \( \mathbf{T} \) is derived. The derivation follows the same procedure as in the previous case of the elastic stiffness \( \mathbf{L} \). Using equation (4.17) and equations (4.18) and (4.19) results in:

\[ \dot{\Sigma} = \frac{1}{V} \int_{V_m} \mathbf{T}^m : \mathbf{\dot{\varepsilon}}^m dV + \frac{1}{V} \int_{V_i} \mathbf{T}^i : \mathbf{\dot{\varepsilon}}^i dV \]

\[ = (c^m \mathbf{T}^m \mathbf{A}^m + c^i \mathbf{T}^i \mathbf{A}^i) : \dot{\mathbf{E}}, \]  

(4.27)

where \( \mathbf{A}^m \) and \( \mathbf{A}^i \) are the average instantaneous strain concentration factors for the matrix and the inhomogeneities, respectively. Note, that in the derivation of the
above equation it has been assumed that the tangent stiffness of each phase is a function of the average value of stress in that phase only. Therefore, the macroscopic tangent stiffness of the composite is given in terms of the tangent stiffness of the two phases and the average instantaneous strain concentration factors as

\[ T = c^m T^m A^m + c^i T^i A^i. \]  \hspace{1cm} (4.28)

In the case of elastic behavior of both of the phases the above expression for the macroscopic tangent stiffness will take the same form as the expression for the macroscopic elastic stiffness [cf. equation (4.26)].

The next step in establishing the macroscopic constitutive behavior of the composite is the derivation of an evolution equation for the macroscopic inelastic strain \( \mathbf{E}^{in} \). To derive the evolution equation, first equations (4.18) and (4.19) are substituted into equation (4.11), which results in

\[ \mathbf{B}(x) : \dot{\Sigma} = \mathbf{L} : (\mathbf{A}(x) : \dot{\mathbf{E}} - \dot{\mathbf{e}}^*). \]  \hspace{1cm} (4.29)

Multiplying equation (4.15) by \( \mathbf{B}(x) \) gives

\[ \mathbf{B}(x) : \dot{\Sigma} = \mathbf{B}(x) \mathbf{L} : (\dot{\mathbf{E}} - \dot{\mathbf{E}}^*). \]  \hspace{1cm} (4.30)

Combining equations (4.29) and (4.30) leads to

\[ \mathbf{B}(x) \mathbf{L} : (\dot{\mathbf{E}} - \dot{\mathbf{E}}^*) = \mathbf{L} : (\mathbf{A}(x) : \dot{\mathbf{E}} - \dot{\mathbf{e}}^*). \]  \hspace{1cm} (4.31)

Taking the volume average of equation (4.31) over the whole volume \( V \) and taking into account the fact that the average of \( \mathbf{B}(x) \) over \( V \) is equal to the identity tensor yields

\[ \mathbf{L} : (\dot{\mathbf{E}} - \dot{\mathbf{E}}^*) = (\mathbf{L} \mathbf{A}(x)) : \dot{\mathbf{E}} - (\mathbf{L} : \dot{\mathbf{e}}^*). \]  \hspace{1cm} (4.32)
Consider the two volume averaged terms on the right-hand-side in equation (4.32). The first term is evaluated as

\[ \langle \mathcal{L} \mathcal{A}(x) \rangle = \frac{1}{V} \int_{V} \mathcal{L} \mathcal{A}(x) dV \]

\[ = c^m L^m A^m + c^i L^i A^i. \tag{4.33} \]

The evaluation of the second term leads to

\[ \langle \mathcal{L} : \dot{\varepsilon}^* \rangle = \frac{1}{V} \int_{V} \mathcal{L} : \dot{\varepsilon}^* dV \]

\[ = \frac{1}{V} \int_{V^m} L^m : \dot{\varepsilon}^{*m} dV + \frac{1}{V} \int_{V^i} L^i : \dot{\varepsilon}^{*i} dV \]

\[ = c^m L^m : \langle \dot{\varepsilon}^{*m} \rangle_m + c^i L^i : \langle \dot{\varepsilon}^{*i} \rangle_i. \tag{4.34} \]

The subscripts \( m \) and \( i \) indicate that the volume averages are taken over the matrix and inhomogeneities phases \( V^m \) and \( V^i \), respectively. Using equations (4.33) and (4.34), equation (4.32) is rewritten as

\[ L : (\dot{\mathbf{E}} - \dot{\mathbf{E}}^*) = c^m L^m : (A^m : \dot{\mathbf{E}} - \langle \dot{\varepsilon}^{*m} \rangle_m) + c^i L^i : (A^i : \dot{\mathbf{E}} - \langle \dot{\varepsilon}^{*i} \rangle_i), \tag{4.35} \]

which leads to the following expression for \( \dot{\mathbf{E}}^* \)

\[ \dot{\mathbf{E}}^* = \dot{\mathbf{E}} - c^m M L^m : (A^m : \dot{\mathbf{E}} - \langle \dot{\varepsilon}^{*m} \rangle_m) \]

\[ - c^i M L^i : (A^i : \dot{\mathbf{E}} - \langle \dot{\varepsilon}^{*i} \rangle_i). \tag{4.36} \]

and finally from (4.16) to an expression for \( \dot{\mathbf{E}}^{\text{in}} \):
\[
\dot{E}^{in} = \dot{E} - c^m ML^m : (A^m : \dot{E} - \langle \dot{\varepsilon}^m \rangle_m )
\]
\[
- c^i ML^i : (A^i : \dot{E} - \langle \dot{\varepsilon}^i \rangle_i )
\]
\[
- \dot{ML} : (E - E^{in}).
\] (4.37)

The above equation is a first order ODE for \( E^{in} \). Since the coefficients of this equation (overall elastic compliance, elastic stiffness of the phases as well as the concentration factors) change during the phase transformation, they ultimately depend on \( E^{in} \). Thus this equation is non-linear and cannot be integrated directly for given history of the overall strain \( E \).

Thus, expressions for the overall elastic stiffness \( L \), overall tangent stiffness \( T \) and the evolution of the overall inelastic strain \( E^{in} \) are derived using the constitutive behavior of the phases. Equations (4.26), (4.28) and (4.37) are general in nature and can be used for any composite with rate-independent inelastic phase behavior.

The above derived equations are generalized for the case of a composite with any number of phases in the sequel. The number of phases will be characterized by a finite set of volume fractions \( \{c^j\} \) or by a distribution function related to the orientation, shape and material parameters. The derivation is straightforward and is omitted here for brevity; only the final expressions are shown. Thus, the expressions for the elastic stiffness, the tangent stiffness and the inelastic strain increment become

\[
L = c^m L^m A^{el,m} + \{ L^i A^{el,i} \},
\] (4.38)

\[
T = c^m T^m A^m + \{ T^i A^i \},
\] (4.39)
\[ \dot{E}^{in} = \dot{E} - c^m \mathbf{M} \mathbf{L}^m : (\mathbf{A}^m : \dot{\mathbf{E}} - \langle \dot{\varepsilon}^* \rangle_m) \]

\[ - \dot{\mathbf{M}} \{ \{ \mathbf{L}^i \mathbf{A}^i \} \} : \dot{\mathbf{E}} + \dot{\mathbf{M}} : \{ \{ \mathbf{L}^i : \dot{\varepsilon}^* \} \} - \dot{\mathbf{M}} : \Sigma. \]  

(4.40)

The double curly brackets in the above equations (4.38)–(4.40) indicate the appropriate average with respect to variables, identifying the phases. For a finite number of distinct phases (shape, orientation, material properties) \( N \) the averages become

\[ \{ \{ \mathbf{L}^i \mathbf{A}^{el,i} \} \} = \sum_{j=1}^{N} c_j^i \mathbf{L}^i_j \mathbf{A}^{el,i}_j \]  

(4.41a)

\[ \{ \{ \mathbf{T}^i \mathbf{A}^i \} \} = \sum_{j=1}^{N} c_j^i \mathbf{T}^i_j \mathbf{A}^i_j \]  

(4.41b)

\[ \{ \{ \mathbf{L}^i : \dot{\varepsilon}^* \} \} = \sum_{j=1}^{N} c_j^i \mathbf{L}^i_j : \langle \dot{\varepsilon}^* \rangle_j \]  

(4.41c)

For a parameterization of the phases accounting for different orientation the following evaluation results

\[ \{ \{ \mathbf{L}^i \mathbf{A}^{el,i} \} \} = c^i \int_{0}^{2\pi} \int_{0}^{\pi} \rho(\varphi, \theta) \mathbf{L}^i(\varphi, \theta) \mathbf{A}^{el,i}(\varphi, \theta) \sin \theta d\varphi d\theta \]

\[ \{ \mathbf{L}^i \mathbf{A}^{el,i} \} = c^i \frac{\int_{0}^{2\pi} \int_{0}^{\pi} \rho(\varphi, \theta) \mathbf{L}^i(\varphi, \theta) \mathbf{A}^{el,i}(\varphi, \theta) \sin \theta d\varphi d\theta}{\int_{0}^{2\pi} \int_{0}^{\pi} \rho(\varphi, \theta) \sin \theta d\varphi d\theta} \]  

(4.42)

and similarly for \( \{ \{ \mathbf{T}^i \mathbf{A}^i \} \} \) and \( \{ \{ \mathbf{L}^i : \dot{\varepsilon}^* \} \} \). In the first set of equations above \( c^i_j \) is the volume fraction of \( j^{th} \) phase and \( \mathbf{L}^i_j \) and \( \mathbf{A}^{el,i}_j \) are the corresponding elastic stiffness tensor and elastic strain concentration factor. For the case of distribution of phases \( \rho(\varphi, \theta) \) is the orientation distribution function and the integration is performed over a unit sphere. In the most general case the function \( \rho \) may indicate not only the distribution of phase orientations but also of shapes and, possibly, of material properties. In this general case the integration must be performed over the whole space of possible orientations, shapes and material properties. While interesting from
an academic point of view, this case is beyond the scope of the current work. However, the averaging over the inhomogeneity orientations for randomly distributed phases (i.e., $\rho(\varphi, \theta) = 1$) will be reconsidered later in Section 4.2.1.

The derivation of the macroscopic constitutive equations presented here can be compared to the results presented by Cherkaoui et al. (2000) for a composite with elasto-plastic matrix and SMA fibers. However, there are two distinctions which must be pointed out. First, in their work the inelastic behavior introduced by plasticity in the matrix is separated from the inelasticity due to phase transformation. Thus, the composite is characterized by the overall elasto-plastic tangent stiffness that excludes the transformation strains, while in this work the tangent stiffness incorporates both plasticity and phase transformation. The second difference is in the way of connecting the local increments of stress and strain to the global ones. Their concentration factors are defined as (see equations (15) and (16) in the paper by Cherkaoui et al., 2000):

$$\dot{\varepsilon} = \hat{A}(x) : \dot{E} + a(x), \quad (4.43)$$

$$\dot{\sigma} = \hat{B}(x) : \dot{\Sigma} + b(x), \quad (4.44)$$

where $\hat{A}(x)$ and $\hat{B}(x)$ are instantaneous elasto-plastic strain concentration factors. Thus, the effect of the transformation strain is taken into account by introducing tensors $a(x)$ and $b(x)$. In practice, however, it would be difficult to separate the nonlinearity due to plasticity from the one due to the phase transformation. In addition, mechanically induced phase transformation will result in $a(x)$ and $b(x)$ being proportional to the increment of the effective strain and stress, $\dot{E}$ and $\dot{\Sigma}$, respectively, as introduced by equations (4.18) and (4.19).
4.1.3. Evaluation of the Strain Concentration Factors

The Mori–Tanaka method will be used in this work to calculate the concentration factors. One of the reasons for choosing the Mori–Tanaka method is the fact that in porous SMAs the matrix is readily identified. Another reason is its relative simplicity, compared to the self-consistent method, which is implicit. For the case of ellipsoidal inhomogeneities the Mori–Tanaka estimate of $A^i$ (see Lagoudas et al., 1991) is given by

$$A^i = \left[ I + c^m S^E (T^m)^{-1} (L^i - T^m) \right]^{-1}. \quad (4.45)$$

where $T^m$ is the matrix tangent stiffness and $S^E$ is the Eshelby tensor, which is defined for the shape of inhomogeneities and the matrix tangent stiffness. Using the well-known identity $c^m A^m + c^i A^i = I$ the average strain concentration factor for the matrix is given by

$$A^m = \frac{1}{c^m} (I - c^i A^i). \quad (4.46)$$

The estimates of the average elastic strain concentration factors $A^{el,m}$ and $A^{el,i}$ used in the evaluation of the macroscopic elastic stiffness $L$ are obtained by using the matrix elastic stiffness $L^m$, i.e.,

$$A^{el,i} = \left[ I + c^m S^{E,el} M^m (L^i - L^m) \right]^{-1}, \quad (4.47)$$

$$A^{el,m} = \frac{1}{c^m} (I - c^i A^{el,i}). \quad (4.48)$$

$S^{E,el}$ in the equation above us the Eshelby tensor evaluated using the elastic stiffness of the matrix.
4.2. Application to Porous Shape Memory Alloys

The above developed theory will be applied in modeling the constitutive response of porous SMAs. To apply the theory for this case, it is first assumed that the inhomogeneities behave elastically and their constant elastic stiffness in the limit approaches zero, i.e., \( L^i = 0 \). It should be noted that even though in the case of \( L^i = 0 \) the elastic compliance of the inhomogeneities \( M^i \) is not defined, but it is still possible to formally follow all derivations presented in Section 4.1.

For porous SMAs the inelastic strain in the inhomogeneities \( \varepsilon^{in,i} \) vanishes and the inelastic strain in the SMA matrix consists of the transformation strain and the plastic strain, i.e., \( \varepsilon^{in,m} = \varepsilon^{t,m} + \varepsilon^{p,m} \). The macroscopic inelastic strain \( E^{in} \) reduces to the sum of the macroscopic transformation strain \( E^t \) and the macroscopic plastic strain \( E^p \).

Equation (4.26) for the macroscopic elastic stiffness \( L \) for porous SMAs has the form

\[
L = c^m L^m A^{el,m},
\]

(4.49)

where \( L^m = (M^m)^{-1} \) with its evaluation given in Chapter II as

\[
M^m = M^A + \xi (M^M - M^A),
\]

(4.50)

where \( M^A \) and \( M^M \) are the elastic compliance tensors for the austenitic and the martensitic phases, respectively.

The equation for the macroscopic tangent stiffness \( T \) becomes

\[
T = c^m T^m A^m.
\]

(4.51)

\( A^m \) and \( A^{el,m} \) are evaluated from equations (4.46), (4.48) and the strain concentration
factors for the pores are given by

\[ A^i = \left[ I - c^m S^E \right]^{-1}, \quad A^{el,i} = \left[ I - c^m S^{E,el} \right]^{-1}. \]  \hspace{1cm} (4.52)

The tangent stiffness tensor for the SMA matrix \( T^m \) appearing in equation (4.49) has been derived using the SMA constitutive model in Section 2.4. For the isothermal case considered here the tangent stiffness \( T^m \) becomes

\[ T^m \equiv \frac{d\sigma^m}{d\varepsilon^m} = L^m : \chi \otimes L^m : \partial_\sigma \Phi - \partial_\sigma \Phi : L^m : \chi - \partial_\xi \Phi. \]  \hspace{1cm} (4.53)

The quantity \( \chi \) has been introduced in Section 2.4 and in this particular case it is given by

\[ \chi = \Lambda + \text{sign}(\dot\xi) \frac{H_{\text{cur}}}{H} \Lambda^p + \Delta M^m : \sigma^m. \]  \hspace{1cm} (4.54)

The evolution equation for the macroscopic inelastic strain (4.37) is simplified after substituting the expression for the elastic stiffness (4.49) and becomes

\[ \dot{\dot{E}}^m = (I - (A^{el,m})^{-1} A^m) : \dot{E} + (A^{el,m})^{-1} : \langle \dot{\varepsilon}^* m \rangle_m - \dot{M} : \Sigma. \]  \hspace{1cm} (4.55)

Using the SMA constitutive model the local rate of inelastic strain \( \dot{\varepsilon}^* m \) is written as

\[ \dot{\varepsilon}^* m = \dot{\varepsilon}^{tm} + \dot{\varepsilon}^{lp} + \dot{M}^m : \sigma^m = \chi \dot{\xi}, \]  \hspace{1cm} (4.56)

with \( \chi \) defined by equation (4.54). The rate of the martensitic volume fraction \( \dot{\xi} \) is expressed using equation (2.35) and substituting the expression for the strain increment in the matrix in terms of the overall strain increment \( \dot{E} \) and the instantaneous strain concentration factor \( A^M \) as

\[ \dot{\xi} = \frac{\partial_\sigma \Phi : L^m A^m : \dot{E}}{\partial_\sigma \Phi : L^m : \chi - \partial_\xi \Phi}. \]  \hspace{1cm} (4.57)
4.2.1. Pore Shape Selection

Porous SMAs have been produced by different fabrication techniques as mentioned in the introduction, resulting in different pore sizes, shapes and orientations. As an example, consider micrographs of a porous NiTi SMA sintered from elemental powders (Vandygriff et al., 2000), shown in Figure 36. It can be seen from Figure 36 that the pores have a random distribution and irregular shapes. Similar observations in terms of microstructure have been reported for porous SMAs produced from elemental powders using different techniques (Lagoudas et al., 2000b; Li et al., 1998; Tangaraj et al., 2000). To be able to utilize the Eshelby solution for ellipsoidal inhomogeneities, one should try to approximate the pores by ellipsoids of different sizes, shapes and orientations. However, this will result in many different orientations, as well as shapes and sizes. To incorporate such a large number of pores will be computationally very demanding and not practically feasible, since the constitutive model for the SMA requires an incremental implementation and the averaging process needs to be performed at each load increment for all phases.

In seeking a simplification to the above problem, the possibility of replacing the different shapes, sizes and orientations by only one representative pore geometry is investigated. Noting that the absolute size does not enter in the Eshelby solution and by assuming that all pores can be represented by a single ellipsoidal shape, the remaining parameter, i.e., the orientation of the pores is investigated. Based on microscopic evaluations of porous SMAs fabricated using elemental powders under isostatic conditions, the distribution of pore orientations is approximated by a random distribution function.

Based on the above assumptions the effective properties of a composite with randomly orientated ellipsoidal inhomogeneities will be obtained. As a starting point
the effective elastic properties are studied first. Equation (4.38) is used to find the elastic stiffness $\mathbf{L}$ of a composite with an elastic matrix with stiffness $\mathbf{L}^m$ and a distribution of elastic ellipsoidal inhomogeneities with stiffness $\mathbf{L}^i$, which for the case of porous SMAs will eventually be taken to be zero. The Mori–Tanaka estimate of the elastic strain concentration factor $A^{el,i}$, which now depends on the orientation of the inhomogeneities is given by the following equation (for details see (Benveniste, 1987)):

$$A^{el,i}(\varphi, \theta) = \tilde{A}(\varphi, \theta) \left[ c^{ii} \mathbf{I} + \{ \tilde{A} \} \right]^{-1},$$

(4.58)
where $\tilde{A}$ is defined as:

$$
\tilde{A}(\varphi, \theta) = \left[ I + S^{E,el}(L^m)^{-1}(L^i - L^m) \right]^{-1}
$$

(4.59)

and $S^{E,el}$ is the Eshelby tensor evaluated using the matrix stiffness $L^m$ and the shape of inhomogeneities. Equations (4.58)–(4.59) are substituted into equation (4.38) and the expression $c^m A^{el,m} + \{\{\tilde{A}^{el,i}\}\} = I$ [analogical to equation (4.48)] is used to eliminate the matrix strain concentration factor. Thus, assuming isotropic elastic properties for the matrix and inhomogeneities, the following expression for the effective elastic stiffness is obtained:

$$
L = L^m + (L^i - L^m) \{\{\tilde{A}\}\} \left[ c^m I + \{\{\tilde{A}\}\} \right]^{-1}.
$$

(4.60)

For random distribution of ellipsoids $\{\{\tilde{A}\}\}$ is given by equation (4.42)

$$
\{\{\tilde{A}\}\} = \frac{c^i}{4\pi} \int_0^\pi \int_0^{2\pi} \tilde{A}(\varphi, \theta) \sin \theta d\varphi d\theta.
$$

(4.61)

Thus, the averaging indicated by the double curly brackets is performed over all possible orientations of the ellipsoid. Initially, the tensor $\tilde{A}$ is found in the local coordinate system of the inhomogeneity and is then expressed in the global coordinate system (see Figure 37). The two coordinate systems are related to each other by the rotation $Q$.\(^2\) For the case shown in Figure 37a the local coordinate system can be obtained by Body-1-2-3 rotation (for details see Kane et al., 1983) and the matrix representation of $Q$ is given by

\(^2\)The components of $\tilde{A}(\varphi, \theta)$ are explicitly given by $\tilde{A}_{ijkl}(\varphi, \theta) = Q_{mi}Q_{nj}\tilde{A}_{mnpq}Q_{pk}Q_{q\ell}$. 


Fig. 37. (a) Global and local coordinate system; (b) principal axes of the ellipsoidal inhomogeneity in the local coordinate system.

\[
Q = \begin{bmatrix}
\sin \theta \cos \varphi & -\cos \theta \cos \varphi & \sin \varphi \\
\sin \theta \sin \varphi & -\cos \theta \sin \varphi & -\cos \varphi \\
\cos \theta & \sin \theta & 0
\end{bmatrix}.
\] (4.62)

The same rotation tensor has been used by Christensen (1991) in his work on modeling the elastic response of fibrous composites with random fiber orientation.

Results obtained for two different inhomogeneity shapes — prolate spheroids and cylinders — are compared with the results for spherical inhomogeneities. For the case of prolate spheroids two of the principal axes of the ellipsoid are selected to be equal \((a_2 = a_3)\) while the third axis is selected to be \(a_1 = 2a_2\) (see Figure 37b). For the case of cylindrical inhomogeneities the ratio \(a_1/a_2\) is set to a very large number. The averaging procedure described above has been implemented for the case of a porous SMA material \((L = 0)\). The value of the Young’s modulus used in the above calculation was taken to be \(E = 70\text{GPa}\) and the value of Poisson’s ratio \(\nu = 0.33\).
Fig. 38. Normalized effective elastic Young’s modulus for porous SMA.

The averaging procedure results in isotropic effective material properties due to the randomness of the orientation of the inhomogeneities. Results for the effective Young’s modulus and effective bulk modulus are presented here. The values of these material parameters are normalized by the corresponding matrix properties. The values of the normalized effective Young’s modulus for different pore volume fractions are plotted in Figure 38 and the normalized effective bulk modulus is plotted in Figure 39. It is observed from these figures that there is a very slight difference between the results for different pore shapes and there is a very good agreement, especially between the results for the case of spherical pores and prolate spheroids.

A different approach for obtaining the effective properties of a composite with random orientation of fibers has been presented by Christensen (1991). In his work the averaging over all the possible fiber orientations is performed after obtaining the effective properties of the composite with single fiber orientation. Using the present notation, Christensen’s approach would be equivalent to calculating the effective stiff-
The effective elastic stiffness calculated using equation (4.63) is also isotropic. However, it is noted that this method does not take into account the interactions among inhomogeneities with different orientations. To compare the differences between the two approaches the Young’s modulus of elasticity is calculated using equation (4.63) and equation (4.60) for the case of random distribution of prolate spheroids and the results are plotted in Figure 40. The same set of parameters as in Figures 38 and 39 is used. It can be seen from Figure 40 that for the current choice of parameters the results of both methods are very close. This may be a reason why one would choose to use equation (4.63), which is somewhat simpler, since it requires only one averaging. However, equation (4.60) does not carry a significant additional computational overhead and accounts for the interactions among inhomogeneities with different orientations.
Fig. 40. Normalized effective Young’s modulus calculated using the present approach [equation (4.60)] compared with the Young’s modulus calculated using the approach by Christensen (1991) [equation (4.63)].

The results presented here are normalized and, therefore, are valid for all possible values of the matrix stiffness. Thus, it is expected that the same result will hold if one uses the tangent stiffness of the phases to obtain the effective properties of a porous SMA undergoing a phase transformation.

Therefore, based on the above discussion, a spherical pore shape will be used to represent the porosity in an SMA with a random distribution of pores. This shape gives adequate representation of porosity and at the same time its use will greatly reduce computational costs. Thus, a spherical pore shape will be used in all further numerical calculations in this work.

4.2.2. Transformation Response

The determination of the transformation response of porous SMAs involves the solution of equations (4.51) and (4.55) to obtain the values of the macroscopic stress
Σ and inelastic strain $E^{in}$ for a given history of the overall strain $E$. To achieve this, the tangent stiffness of the SMA matrix needs to be evaluated at every strain increment. Due to the non-linearity of the problem, a numerical algorithm is utilized in this work. A two-level numerical implementation is necessary: on the macroscopic level the non-linearity is associated with the dependence of the strain concentration factor $A^i$ (and, therefore, $A^m$) on the value of tangent stiffness of the SMA matrix; on the microscopic level the non-linearity is due to the non-linear constitutive SMA model. The numerical implementation is described in detail in Chapter V.

To demonstrate the capabilities of the model numerical calculations for porous SMA undergoing phase transformation have been performed. As a starting point first the response during stable transformation cycle is modeled. To accomplish this task, the material parameters for the SMA matrix are selected to correspond to NiTi characterized in the work of Bo et al. (1999). These material parameters are presented in Table I. Note that these parameters are for stable transformation cycle.

As a representative example numerical evaluations for the isothermal pseudoelastic response of porous NiTi SMA were performed. The temperature was set to be 343 K. The numerical calculations were performed for an SMA prismatic bar under uniaxial loading (see Figure 41). The numerical results were produced using a mesh of two 3-D eight node solid elements, while identical results were obtained for a mesh of eight 3-D elements, since both stress and strain are uniform. The axial effective stress-strain response of the bar for various levels of porosity $c^p = 1 - c^m$ is shown in Figure 42.

The results of Figure 42 indicate that the response of the material during trans-

---

$^3$The Eshelby tensor $S^E$ entering the expression for the strain concentration factor $A^i$ is evaluated numerically, since in the case of general loading the tangent stiffness of the SMA matrix is anisotropic. The method used for the evaluation of the Eshelby tensor is the one presented by Lagoudas et al. (1991).
formation strongly deviates from linearity which indicates that the tangent stiffness tensor $T$ continuously changes. This effect is caused by the change in the tangent stiffness of the SMA matrix $T^m$. Since the Eshelby tensor used to evaluate the instantaneous matrix strain concentration factor $A^m$ is calculated using the tangent stiffness of the matrix, it is expected that the instantaneous strain concentration factor will vary significantly during the transformation. Thus it should be updated at each loading increment.

Next the solution of equation (4.55), shown below for convenience is investigated.

$$
\dot{\mathbf{E}}^{in} = \left( \mathbf{I} - (A^{el,m})^{-1} A^m \right) : \dot{\mathbf{E}} + (A^{el,m})^{-1} : \langle \dot{\varepsilon}^m \rangle_m - \dot{\mathbf{M}} : \Sigma
$$

It can be seen from equation (4.64) that there are three terms contributing to the macroscopic inelastic strain. The first term is due to the difference between the elastic and instantaneous strain concentration factors. In the case that $A^{el,m}$ and $A^m$ are the same this term will vanish. The second term represents the effect of the
Fig. 42. Effective stress-strain response of a porous NiTi SMA bar.

The contribution of each of the three terms to the macroscopic inelastic strain $E^{in}$ is examined for three different cases. The calculations for all of the three cases are performed on a uniaxial SMA bar with 50% porosity for the loading path shown in Figure 43. The difference between the three test cases is in the properties of the SMA matrix.
In the first case it is assumed that the SMA matrix undergoes phase transformation and no plastic strains are accumulated. This case describes the situation where the SMA matrix undergoes a stable transformation cycle. Therefore, the overall inelastic strain $\varepsilon^{\text{in}}$ becomes simply the overall transformation strain $\varepsilon^t$. The material properties for this test case are the same used to obtain the results shown in Figure 42 and are summarized in Table I. The temperature for this case was set to be 343 K. The normal components in the direction of the loading for each of the three terms contributing to the effective transformation strain are plotted in Figure 44. It can be seen that the contribution of the second term due to the local transformation strain is dominant for the current choice of the material parameters. The contribution of the first term is negative and lowers the value of the effective macroscopic transformation strain. It can thus be seen from the figure that the effect of the difference between the elastic and instantaneous strain concentration factors is not negligible. The third term, which reflects the effect of the effective elastic compliance change has the small-
est magnitude of the three terms. Even though the third term is positive because the elastic compliance of the SMA matrix in the martensitic phase is greater than the compliance in the austenitic phase, its contribution to the total transformation strain is negative, due to the negative sign in front of the term in equation (4.64). It is noted that at the end of the reverse transformation the two contributions of the second and the third terms cancel each other, while the contribution of the first term goes to zero. It can be shown analytically that for the case of porous SMAs the part of the second term, corresponding to the change in the stiffness in the SMA matrix, is exactly equal to the third term. However, this result is only valid for a particular choice of the phases, i.e., martensite and austenite have the same Poisson’s ratio, and it will not hold in general.

Fig. 44. Components of the macroscopic transformation strain as a function of the loading.
In the second test case it is assumed that the elastic properties of the martensite and the austenite are the same, i.e., $M^M = M^A$. Then, the rate of inelastic strain in the SMA matrix $\langle \dot{\varepsilon}_{m} \rangle_m$ becomes simply the rate of the transformation strain $\langle \dot{\varepsilon}_{t,m} \rangle_m$ in the second term, and the third term vanishes. To illustrate this special case, the results of numerical calculations are show in Figure 45 for the same porous SMA uniaxial bar with porosity of 50% as in the previous case. The material parameters for this case are the ones shown in Table III for NiTi SMA tested by Strnadel et al. (1995b). The temperature of the test was set to be 300 K. The values after the stabilization of the transformation cycle (final values) of the material parameters are used. The resulting normal strain components are shown in Figure 45. The same general trend as in the previous case is observed (see Figure 44). However, in this case the third term in equation (4.64) is zero.

The third test case is an extension of the second case and considers the situation where both transformation and plastic strain are present. Thus, the inelastic strain rate term in the SMA matrix contains both the rate of transformation strain and the rate of plastic strain. To perform the numerical calculations for this test case the same material properties as in the previous case are used (see Table III). However, to be able to model the development of plastic strains both the initial and final sets of parameters are used. Numerical simulations of one full transformation cycle are performed at a temperature of 300 K.

The results showing the contribution of the different term on the overall inelastic strain $\mathbf{E}^{in}$ are shown in Figure 46. Two effects manifesting the influence of the plastic strain on the development of the overall inelastic strain are observed. First, since the rate of the plastic strain in the matrix $\dot{\varepsilon}_{p,m}$ enters the second term in equation (4.64) it is seen that its contribution at the end of the loading-unloading cycle does not vanish. The second effect is due to the different tangent stiffness during loading and
Fig. 45. Components of the macroscopic transformation strain for the case of equal stiffness of the austenite and martensite.

unloading. The difference in the tangent stiffness is caused by the development of the plastic strain and it results in different evaluations of the instantaneous matrix strain concentration factor $A^m$ during loading and unloading. Therefore, it is seen that the total contribution of the first term [cf. equation (4.64)] at the end of the transformation cycle does not vanish. These two effects result in the development of non-zero total inelastic strain $E^m$ at the end of the loading-unloading cycle. To better illustrate the situation, the stress-strain curve for this test case is shown in Figure 47. The residual macroscopic strain at the end of the cycle (at zero applied stress) seen in the figure is caused by the two effects discussed here.
Fig. 46. Components of the macroscopic inelastic strain as a function of the loading (both plastic and transformation strains are present).
Fig. 47. Effective stress-strain response of a porous NiTi SMA bar (both plastic and transformation strains are present).
CHAPTER V

NUMERICAL IMPLEMENTATION OF THE MODEL FOR POROUS SMAS AND COMPARISON WITH EXPERIMENTAL RESULTS

In this chapter the micromechanical model presented in Chapter IV will be numerically implemented and used to simulate the experimental results for mechanical loading of porous NiTi. First the material parameters of the porous NiTi will be estimated. As a next step the test results will be simulated using the model. Finally different loading cases will be performed to test the capabilities of the model.

5.1. Numerical Implementation of the Micromechanical Model for Porous SMAs

This section addresses the implementation of the micromechanical model for porous SMAs. This implementation utilizes the earlier established procedure for numerical integration of the constitutive equations for the fully dense SMA, presented in Chapter III. The implementation presented here is valid for a displacement-based formulation (e.g., a finite element formulation) where the history of the overall strain $E(t)$ is given. Note that an additional non-linearity is introduced due to the dependence of the strain concentration factors on the current tangent stiffness in the SMA matrix. This additional difficulty is resolved by employing a direct iteration (Picard iteration) method, as described in a sequel.

The numerical implementation involves the following iterative procedure: first, the elastic stiffness of the SMA matrix is used to calculate the Eshelby tensor and the strain concentration factor $A^m$; once the current value of the strain concentration factor $A^m$ is known, it is used to obtain the strain increment in the SMA matrix $\Delta \varepsilon^m$ from the given increment of the overall strain $\Delta E$; if the phase transformation condition in the matrix is satisfied, then the return mapping algorithm presented in
Section 3.1 is then used to update the values of the stress, transformation strain, plastic strain, martensitic volume fraction and tangent stiffness in the matrix; finally, a new value of the strain concentration factor is obtained using these updated results.

The direct iteration procedure terminates after the difference between two successive values of the strain concentration factor is less than a given tolerance. At this point the obtained final values of the stress, transformation strain, plastic strain, martensitic volume fraction and the strain concentration factor are used to obtain the effective tangent stiffness and the increment of the effective inelastic strain using equations (4.51) and (4.55). The steps of the iterative procedure are summarized in Table IV.

Table IV. Implementation of the incremental micromechanical averaging method for porous SMAs.

1. Set $k = 0$, $T^{m(0)} = L^m$.
2. Calculate Eshelby tensor $S^{E(k)}$ using $T^{m(k)}$, calculate average instantaneous strain concentration factor $A^{m(k)}$:
   \[
   A^{m(k)} = \frac{1}{c^m} \left( I - (1 - c^m) \left[ I + c^m S^{E(k)} \right]^{-1} \right)
   \]
3. Calculate the increment of strain in the matrix $\Delta \varepsilon^{m(k)}$:
   \[
   \Delta \varepsilon^{m(k)} = A^{m(k)} : \Delta E
   \]
4. The return mapping algorithm for dense SMAs (Table II) is called with $\Delta \varepsilon^{m(k)}$ as its input. The output of the algorithm are the updated value of the stress in the matrix $\sigma^{m(k+1)}$, martensitic volume fraction $\xi^{(k+1)}$, transformation and plastic strain $\varepsilon^{tm(k+1)}$, $\varepsilon^{pm(k+1)}$ and the tangent stiffness tensor of the SMA matrix $T^{m(k+1)}$. 

5. Calculate Eshelby tensor $S^{E(k+1)}$ using $T^{m(k+1)}$, calculate average instantaneous strain concentration factor $A^{m(k+1)}$.

6. If $|A^{m(k+1)} - A^{m(k)}| > TOL2$ then

   set $k = k + 1$;
   go to 3.

7. Calculate the overall tangent stiffness tensor $T$ and the increment of the inelastic strain $\Delta E^{in}$:

\[
T = c^m T^m A^m
\]

\[
\Delta E^{in} = (I - (A^{el,m})^{-1} A^m) : \Delta E + (A^{el,m})^{-1} : (\Delta \varepsilon^{*m})_m - \Delta M : \Sigma
\]

Note that in the implementation of the micromechanical averaging method the strain in the SMA matrix becomes another internal state variable. It must be updated and stored at each load increment. The number of Picard iterations depends on the value of tolerance $TOL2$ and on the number of the load increments. For tolerance $TOL2 = 1.0 \times 10^{-9}$ and 100 load increments 5–8 iterations are performed before a convergence is achieved.

5.2. Uniaxial Porous NiTi Bars under Compression

Porous NiTi specimens were fabricated from elemental Ni and Ti powders using HIP-ping techniques in the Active Materials Laboratory at Texas A&M University (Vandy-griff et al., 2000). Using two slightly different processing cycles two different porous NiTi alloys were produced. The first alloy was fabricated at a temperature of $\approx 940^\circ$C and is characterized by its small pore size (on the order of 25 $\mu$m). The fabrication temperature for the second alloy was $\approx 1000^\circ$C and the sizes of its pores are sig-
nificantly larger (pores as large as 1 mm are observed). A detailed analysis of the composition of the two alloys was performed by Lagoudas and Vandygriff (2002) using Energy-Dispersive X-ray Spectrometry (EDS) and further using Wave-Dispersive X-ray Spectrometry (WDS). The analysis has revealed evidence of multiple intermetallic phases present in both large and small pore alloys. The greater part of the material for large pore alloys was identified as equiatomic NiTi. However, the material contains numerous needle-like structures having a width of approximately one-half micron. These needle-like structures were too small to be analyzed without interference from the surrounding medium. By analyzing some of the larger intersections of needle-like phases however, it is presumed by a slight increase in the percentage of Ni that the needle phases are Ni rich phases. For the small pore alloy five different phases, i.e., NiTi, Ni$_2$Ti, NiTi$_3$ and elemental Ni and Ti were identified. The apparent reason for the presence of relatively large intermetallic phase regions in the small pore alloy is the lower fabrication temperature, which leads to incomplete diffusion of the elemental powders.

The porosity of the specimens was measured by taking micrographs and estimating the ratio of the area occupied by the pores to the total area at different cross-sections. The estimate of the porosity was also verified by comparing the density of the porous NiTi material with the theoretical density of fully dense NiTi. The porosity of the small pore alloy is estimated to be equal to 50% while the porosity of the large pore alloy is equal to 42%. Micrographs of typical specimens for both small and large pore alloys are shown in Figures 48 and 49. The dark areas on the micrographs, shown in Figures 48 and 49 represent the pores, while the lighter areas are occupied by NiTi.

The porous NiTi specimens were further analyzed using differential calorimetry techniques. The DSC test curves for both small and large pore alloys are shown
Fig. 48. Microphotograph of a small pore porous NiTi specimen.

in Figures 50 and 51, respectively. The upper curves seen in Figures 50 and 51 represent the normalized heat flow into the specimen during heating and the lower curves represent the heat flow out of the specimen upon cooling. The tests indicate solid-solid phase transformation at approximately 44°C and 42°C for the small and large pore alloys during heating (martensite-to-austenite) and −12°C and 20°C during cooling (austenite-to-martensite) for the small and large pore specimens, respectively. Therefore, depending on whether the specimen was previously heated or cooled, either martensite or austenite crystalline structure can be present at room temperature (22°C). The cooling curves for both alloys show evidence of a dual peak that is indicative of an R-phase.

The fabricated porous NiTi specimens have a cylindrical shape with a nominal diameter of 13 mm and a length of 35 mm. The specimens were mechanically tested under compressive load. Load from a hydraulic MTS load frame was applied through two compression plates. An extensometer was used to take the strain measurements during testing. The specimens were tested using a cyclic loading-unloading pattern
by loading quasi-statically up to a stress and strain level and then unloading to zero stress. For each subsequent cycle, the stress and/or strain were increased with respect to the previous level. The resulting stress-strain response for a typical small pore specimen, tested at a temperature of 60°C is shown in Figure 52 and shows evidence of pseudoelastic behavior upon unloading. However, full strain recovery is not observed, which is due to plastic strain development in the SMA matrix. The typical stress-strain response for a large pore specimen also tested at 60°C is shown in Figure 53. The results for the second specimen are qualitatively similar to the result for the small pore specimen. However, certain distinctions are observed from Figures 52 and 53. The initial tangent stiffness of the austenite and martensite are different in the two specimens. The approximate stiffness of the austenite phase in the large pore specimen is approximately 15 GPa, about twice that of the small pore austenite phase stiffness of 7 GPa. This difference in the stiffness may be partially due to incomplete diffusion of the powders in the small pore specimen and the resulting partial adherence of the powder particles. The difference in the pore volume fraction
of the two types of specimens also contributes to the difference in the stiffness. Thus, while the maximum reached strain level for the two specimens is similar, the stress levels differ significantly.

When a large pore specimen is loaded to strain levels beyond 5% it starts to fail by forming microcracks, which was evident by the cracking and popping noises during loading. This failure is identified on the stress-strain curve by the decrease of the stress as the strain is increased (Figure 53). On the other hand the small pore specimens failed catastrophically, forming large cracks that propagated throughout the entire specimen, causing the specimen to break into multiple fragments.

5.2.1. Estimation of the Material Properties for Porous NiTi

Using the experimental data presented in Figures 50–53 the material parameters for both types of porous NiTi alloy are estimated in this section. First, the estimation of the parameters for the small pore NiTi alloy is presented. The procedure presented here is outlined in Section 2.7. Care must be exercised when taking into account the
Fig. 51. DSC results for large pore porous NiTi alloy.

porosity. The values of the stress appearing during the estimation of the parameters in Section 2.7 must be calculated for the SMA matrix. Therefore, to connect the stress in the matrix with the applied stress, the Mori–Tanaka method is used. Only one set of material parameters is obtained, since the experimental data is not sufficient to obtain complete two sets (initial and final, see Sections 2.5, 2.7).

First the material parameters for a transformation cycle without plastic strains are estimated. To accomplish this, the residual plastic strain after each increment is subtracted from the total strain. Thus, only the elastic/phase transformation response is obtained (see Figure 54). The material parameters are estimated for a transformation loop which is the envelope of the experimental results shown in Figure 54.

To proceed with the estimation of the material properties, it is assumed that the SMA matrix is isotropic with Poisson’s ratio $\nu^A = \nu^M = 0.33$. Next, the Young’s elastic moduli of austenite and martensite are evaluated by solving the inverse Mori–Tanaka problem for the porous material and using the experimental data. The value
Fig. 52. Stress-strain response of small pore porous NiTi alloy tested at 60°C.

of the effective Young’s modulus of the porous austenite is measured using the slope at the beginning of the loading (see Figure 54) and the corresponding value of the Young’s modulus for the austenitic matrix is evaluated from the inverse Mori–Tanaka method to be $E^A = 19.7$ GPa. Similarly, the value of the effective Young’s modulus of the porous martensite is obtained using the unloading slope of the last loading cycle (see Figure 54), which results in $E^M = 19.0$GPa. The values of the thermal expansion coefficient for martensite and austenite are taken from the work of Lagoudas and Bo (1999) and are equal to $\alpha^A = 11.0 \times 10^{-6}$ K$^{-1}$ and $\alpha^M = 6.0 \times 10^{-6}$ K$^{-1}$. Similarly, the values of the specific heat constants $c^A$ and $c^M$ are obtained from the literature (Bo
Fig. 53. Stress-strain response of large pore porous NiTi alloy tested at 60°C.

and Lagoudas, 1999a). Since the loading cases considered in this work are isothermal, the last four constants will not have any effect on the numerical results, but they are still necessary for successful runs of the numerical code.

The martensitic start temperature $M^{0s}$ is determined from the calorimetric test data, shown in Figure 50. As explained earlier, the cooling curve in Figure 50 shows evidence of a dual peak that is indicative of an $R$-phase. The second peak was used to obtain the value of the martensitic start temperatures $M^{0s} = 269.5$ K.

The experimental stress-strain curves shown in Figure 52 differ from the stress-strain response expected for NiTi. Namely, it is expected that after initial hardening
Fig. 54. Elastic/phase transformation stress-strain response of small pore porous NiTi alloy.

The pseudoelastic stress-strain curve reaches a plateau with subsequent hardening after the phase transformation is complete. However, the results shown in Figure 52 reach a plateau without exhibiting the second hardening. In addition, the value of the recovered transformation strain is smaller than expected for a NiTi alloy. Therefore, these results suggest that the material does not undergo full austenite-to-martensite phase transformation. Thus, the value of the maximum transformation strain cannot be accurately obtained using the available experimental data. To overcome this...
difficulty a value of the maximum transformation strain $H = 3\%$ which is typical for NiTi has been used in this work. Then, it follows that the maximum value of the martensitic volume fraction $\xi$ reached during the stress loading is approximately equal to 0.5. The value of the material parameter $\rho \Delta s_0$ is estimated to be equal to $-0.03 \text{ MJ/(m}^3\text{K})$ where equation (2.76) has been utilized by calculating the value of the stress in the matrix using the Mori–Tanaka method. The value of the material parameter $Y$ is estimated to be equal to $Y = 1.3 \text{ MJ/m}^3$.

There is no available data on the dependance of the current maximum transformation strain $H^{\text{cur}}$ on the value of the applied stress for this alloy. Therefore, to evaluate the drag stress parameters the data for a dense NiTi alloy shown in Figure 14 is used with an appropriate scaling such that the maximum transformation strain for high values of stress is equal to the maximum transformation strain $H = 0.03$. The back stress parameters $D_1^d$, $D_2^d$ and $m_1$ are evaluated by curve-fitting of the transformation stress-strain curve during forward transformation. The parameter governing the curvature of the minor transformation loops is estimated to be $\gamma = 4.0$. The comparison of the model simulations for one loop using the estimated parameters with the experimental stress-strain data is shown in Figure 55. It can be seen that the simulation results closely match the experimental curve.

Once the parameters for a single transformation cycle are determined, the only unknowns are the parameters connected with the development of the plastic strains. To obtain the values of the parameters $C_1^p$ and $C_2^p$ one must have data on the evolution of plastic strain with the number of cycles. Since the loading cycles performed during the experiments are not complete, to establish the values of the parameters, a slightly different procedure than the one described in Section 2.7 is used. First the model is used to establish the values of the internal parameter $\zeta^d$ at the end of each loading cycle. Next, the value of the plastic strain at the end of each loading cycle is found
Fig. 55. Comparison of the experimental elastic/phase transformation stress-strain response of small pore porous NiTi alloy with the model simulations.

from the experimental results. Thus, the relationship between the plastic strain and the accumulated detwinned martensitic volume fraction is found. Using this data and equation (2.81) the values of the parameters $C_1^p$ and $C_2^p$ are estimated. Note that the procedure presented in Section 2.7 can still be utilized if complete transformation cycles were performed. The complete set of material parameters for the small pore NiTi alloy is summarized in Table V.

The material parameters for the large pore porous NiTi alloys are estimated
Table V. Material parameters for small pore porous NiTi SMA.

<table>
<thead>
<tr>
<th>Physical constants</th>
<th></th>
<th>Parameters characterizing the phase transformation</th>
<th></th>
<th>Parameters characterizing the accumulation of plastic strain</th>
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</thead>
<tbody>
<tr>
<td></td>
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<td></td>
</tr>
<tr>
<td>$E^A = 19.7$ GPa</td>
<td>$\alpha^A = 11.0 \times 10^{-6}$ K$^{-1}$</td>
<td>$M^{0s} = 269.5$ K</td>
<td>$\rho\Delta s_0 = -0.03$ MJ/(m$^3$K)</td>
<td>$Y = 1.3$ MJ/m$^3$</td>
</tr>
<tr>
<td>$E^M = 19.0$ GPa</td>
<td>$\alpha^M = 6.6 \times 10^{-6}$ K$^{-1}$</td>
<td>$H = 0.03$</td>
<td>$D_1^d = 2.0$ MPa</td>
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</tr>
<tr>
<td>$\rho c^A = 2.12$ MJ/(m$^3$K)</td>
<td>$\nu = 0.33$</td>
<td>$D_1^b = 7.83 \times 10^3$ MPa</td>
<td>$D_2^d = -2.5$ MPa</td>
<td></td>
</tr>
<tr>
<td>$\rho c^M = 2.12$ MJ/(m$^3$K)</td>
<td></td>
<td>$D_2^b = -1.18 \times 10^6$ MPa</td>
<td>$D_3^b = 1.01 \times 10^8$ MPa</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$D_3^b = -1.18 \times 10^6$ MPa</td>
<td>$D_4^b = -4.19 \times 10^9$ MPa</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$D_5^b = 6.61 \times 10^{10}$ MPa</td>
<td>$D_4^b = -4.19 \times 10^9$ MPa</td>
<td></td>
</tr>
<tr>
<td>Minor loop parameter</td>
<td></td>
<td></td>
<td>$m_1 = 3.5$</td>
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<td>$\gamma = 4.0$</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>$C_1^p = 6.0 \times 10^{-3}$</td>
<td>$C_2^p = 1.66$</td>
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</tr>
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</table>
following the same procedure and using the data shown in Figures 51 and 53. Only the data before the occurring of the microcracking is used to estimate the material parameters. They are summarized in Table VI.

It is noted that the obtained material parameters for both small and large pore porous NiTi are different from the ones used earlier in Chapter II. This difference can be explained by the different processing parameters of the material. The material parameters in Chapter II are obtained for NiTi wires, which have a substantial amount of cold work, as well as different heat treatments from the porous SMA material, which has not been cold worked.

5.2.2. Comparison of the Experimental Results with Model Simulation

A finite element model reflecting the geometry of a typical specimen (diameter of 13 mm and length of 35 mm) is constructed. The domain is discretized using eight-node quadratic axisymmetric elements. In order to allow for both compression and combined compression-torsion loading, results of which are presented in a sequel, elements with a twist degree of freedom were used. Since the axial stress does not vary for both loading cases, only one layer of elements in the axial direction is used. The length of the elements in the axial direction is chosen to be 1.75 mm. To capture the stress variation in the radial direction, 5 elements are used. The finite element mesh and the loading history are shown in Figure 56.

The comparison of the compressive stress-strain response for the small pore NiTi alloy simulated by the model with the experimental data is shown in Figure 57. The material properties presented in Table V have been used during the numerical calculations. Overall, very good agreement between the results is obtained. Several observations are made from Figure 57. First, the effective Young’s moduli for both austenite and martensite are correctly reproduced by the model, since their values
Table VI. Material parameters for large pore porous NiTi SMA.

<table>
<thead>
<tr>
<th>Physical constants</th>
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<tr>
<td>$E^A$ = 42.0 GPa</td>
<td>$\alpha^A = 11.0 \times 10^{-6}$ K$^{-1}$</td>
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<tr>
<td>$E^M$ = 32.0 GPa</td>
<td>$\alpha^M = 6.6 \times 10^{-6}$ K$^{-1}$</td>
</tr>
<tr>
<td>$\rho c^A = 2.12$ MJ/(m$^3$K)</td>
<td>$\nu = 0.33$</td>
</tr>
<tr>
<td>$\rho c^M = 2.12$ MJ/(m$^3$K)</td>
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<table>
<thead>
<tr>
<th>Parameters characterizing the phase transformation</th>
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<tbody>
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<td>$M^{0s} = 293.0$ K</td>
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</tr>
<tr>
<td>$H = 0.03$</td>
<td>$Y = 3.0$ MJ/m$^3$</td>
</tr>
<tr>
<td>$D_1^b = 7.83 \times 10^3$ MPa</td>
<td>$D_1^d = 12.0$ MPa</td>
</tr>
<tr>
<td>$D_2^b = -1.18 \times 10^6$ MPa</td>
<td>$D_2^d = 1.0$ MPa</td>
</tr>
<tr>
<td>$D_3^b = 1.01 \times 10^8$ MPa</td>
<td>$m_1 = 3.5$</td>
</tr>
<tr>
<td>$D_4^b = -4.19 \times 10^9$ MPa</td>
<td></td>
</tr>
<tr>
<td>$D_5^b = 6.61 \times 10^{10}$ MPa</td>
<td></td>
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</table>

<table>
<thead>
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<th>Minor loop parameter</th>
<th></th>
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<tbody>
<tr>
<td>$\gamma = 1.0$</td>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>Parameters characterizing the accumulation of plastic strain</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1^p = 1.99 \times 10^{-2}$</td>
<td></td>
</tr>
<tr>
<td>$C_2^p = 1.51$</td>
<td></td>
</tr>
</tbody>
</table>
have been used for the model calibration. The slope of the stress-strain curve during the transformation is in good agreement with the experimental data. The behavior of the material during minor loops is also correctly reproduced.

Next, the comparison of the plastic strain predicted by the model with the plastic strain developed during the testing of the material is presented. As explained earlier, the evolution of plastic strain in the direction of the loading $E^p$ is presented as a function of the accumulated detwinned martensitic volume fraction $\zeta^d$. The comparison of the model simulation with the experimental data is shown in Figure 58. It can be seen that the model simulation closely follows the experimental results.

Similar results have been calculated for the large pore porous NiTi alloy using the material parameter shown in Table VI. The comparison of the numerical results with the experimental stress-strain data is shown in Figure 59. It can be seen that despite some discrepancies, the results of the numerical simulations are in good agreement with the experimental data. The plot of the plastic strain versus the accumulated detwinned martensitic volume fraction is shown in Figure 60.
Fig. 57. Stress-strain response of a small pore porous NiTi SMA bar — comparison between the experimental results and the model simulation.

One reason for the observed discrepancies may be due to the development of microcracks in the specimen during testing. As mentioned earlier, the large pore NiTi alloy under compressive testing started failing by developing microcracks. Even though attempts were made to eliminate the effect of the microcracking by considering only the results before it occurred some failure may have occurred earlier. The stress-strain response during the last three loading cycles is shown in Figure 61. It can be seen that starting with the 7th loading cycle the results of the model substantially deviate from the experimental results. It is evident from the change in the slope of the experimental stress-strain curve that there are some changes in the properties of the alloy. A micrograph of the large pore specimen after testing is shown in Figure 62. The
Fig. 58. Plastic strain $E^p$ versus accumulated detwinned martensitic volume fraction $\zeta^d$ for the small pore porous NiTi.

The figure shows that microcracks propagate through the pore walls. Thus, the change in the stiffness of the specimen after the loading can be attributed to the development of these microcracks.

One can attempt to improve the model simulations by eliminating the last two loading cycles and modifying the plastic strain evolution constants $C_1^p$ and $C_2^p$ such that a better simulation of the plastic strain is obtained. Thus, if the new values for the constants are selected to be $C_1^p = 0.052$ and $C_2^p = 0.25$ the resulting plastic strain evolution as predicted by the model is shown in Figure 63. The corresponding stress-strain response is shown in Figure 64. It can be seen from these figures that the results of the model simulations are in good agreement with the experimental observations.
Fig. 59. Stress-strain response of a large pore porous NiTi SMA bar — comparison between the experimental results and the model simulation.
Fig. 60. Plastic strain $E_p$ versus accumulated detwinned martensitic volume fraction $\zeta^d$ for the large pore porous NiTi.
Fig. 61. Stress-strain response of a large pore porous NiTi SMA bar — last three loading cycles.

Fig. 62. Microcracking of the large pore porous NiTi SMA bar during mechanical loading.
Fig. 63. Plastic strain $E^p$ versus accumulated detwinned martensitic volume fraction $\zeta^d$ for the large pore porous NiTi using the modified plastic strain evolution constants.
Fig. 64. Stress-strain response of a large pore porous NiTi SMA bar using the modified plastic strain evolution constants.
5.3. Porous NiTi Bars under Multiaxial Loading

The loading cases described above represent uniaxial loading of porous SMA bars. However, most engineering applications require the capability to handle more complex loading paths, involving multiaxial non-proportional loading. It is envisioned that the capability to model such loading cases will become increasingly important as porous SMAs are used in various new applications, such as vibration isolation of multiple degrees of freedom and biomedical applications. In addition, the modeling of complex loading paths will facilitate experimental work, which will provide results necessary for the calibration of the model, which is three dimensional.

5.3.1. Compression-Torsion Loading of Porous SMA Bars

To test the capabilities of the model, the response of the small pore NiTi porous SMA bar with 50% porosity, described in Section 5.2, is modeled under combined compression-torsion loading. Different loading cases were tested: compression-torsion, torsion-compression as well as simultaneous compression-torsion. The boundary conditions and the loading histories for these cases are shown in Figure 65 while the finite element mesh is the same as shown in Figure 56a. The maximum value of the applied rotation (see Figure 65) was taken to be $\theta^{\text{max}} = 0.02 \text{ rad} \ (\approx 1.15^\circ)$, which corresponds to $\approx 11.4 \text{ rad/m} \ (\approx 1.8 \text{ full revolutions per meter})$ rotation, while the maximum value of the displacement in the axial direction during the second loading step was taken to be $u^z_{\text{max}} = -0.125 \text{ mm}$, corresponding to macroscopic axial compressive strain of $E_{zz} = 0.071$. Both compression and rotation boundary conditions were applied on the top surface of the specimen, while the bottom surface was held fixed in the $z-$ and $\theta-$ directions. Traction-free boundary condition in the radial direction was applied. The numerical simulations were performed at temperature of
60°C. The analyses were performed on a single processor DIGITAL™ Alpha 600AU workstation. Forty eight loading increments were performed to complete both loading and unloading steps and the CPU time required to perform the computations varied between 32.0 sec for the case of combined loading to 48.7 sec for the case of torsion-compression loading.

![Diagram](image)

Fig. 65. Schematic of the BVP for compression-torsion multiaxial loading of a porous SMA bar: (a) boundary conditions; (b) loading histories.

The history of the stresses and the martensitic volume fraction for the three cases are shown in Figure 66 for an element positioned at the outer surface of the bar. It is seen that the results for the combined compression-torsion loading case resemble superposition of the results under compression and torsion applied independently, while for the case of compression-torsion the material fully transforms during the compressive loading (depending on the value of the imposed axial strain) and the response under torsion is elastic. Thus only the results for the torsion-compression loading are presented in greater detail.

The contour plot of the martensitic volume fraction in the SMA matrix at the
Fig. 66. History of the axial stress, shear stress and the martensitic volume fraction during torsion-compression loading.
Fig. 67. Contour plot of the martensitic volume fraction in the porous NiTi SMA bar at the end of the torsional loading.

end of the torsional loading (the value of loading parameter equals to 0.5) for the porous bar is shown in Figure 67. It is observed from the figure that the contours corresponding to the same value of $\xi$ are concentric circles. The maximum value of the martensitic volume fraction is $\xi = 0.67$ at the external boundary of the bar, where the shear stress is maximum, while its minimum value is $\xi = 0.0$ close to the center of the bar.

Next, the history of the stresses and the martensitic volume fraction are shown
for an element positioned at the outer surface of the bar (the element is indicated in Figure 67). For comparison purposes, the same loading case was tested on a fully dense NiTi SMA bar with the same geometry and the same material properties. The same finite element mesh of 100 quadratic axisymmetric elements as in the case of compressive loading was used. The average values of the axial and shear stress and the average value of the martensitic volume fraction versus the loading parameter for both the porous and the fully dense SMA bar are plotted on Figure 68. It can be seen from the results that initially the porous SMA material behaves elastically, with the onset of the phase transformation near the value for the loading parameter of about 0.15. The partial phase transformation continues to the end of the torsional loading (the value of the loading parameter is 0.5). Next, with the application of compressive loading, the phase transformation continues and it is fully completed close to the value of the loading parameter of 0.85. Due to the phase transformation during the compressive loading the shear stress $\Sigma_{z\theta}$ is partially relaxed, as indicated in Figure 68. Upon further loading the material behaves elastically with the elastic properties of martensite.

Similar trends are observed for the case of the dense SMA bar, but the stress values are much higher than the ones in the case of the porous bar. The results shown in Figure 68 are also compatible with the results for thin fully dense SMA tubes presented in Chapter II.
Fig. 68. History of the axial stress, shear stress and the martensitic volume fraction during torsion-compression loading.
5.3.2. Three-Dimensional Effects during Compressive Loading of Porous SMA Bars

As mentioned before, the tested porous SMA bars have nominal diameter of 13 mm and length of 35 mm. Since the length/diameter ratio is not very large, the compressive loading may result in three-dimensional stress state, due to the traction between the specimen and the compressive plates. To examine the three-dimensional effects, a boundary-value problem using the geometry of the whole bar and the appropriate boundary conditions is analyzed. The computational domain is discretized using 100 axisymmetric quadratic elements, as shown in Figure 69.

\[ u_r = u_\theta = 0, \quad u_z = \text{const} \]

Fig. 69. Schematic of the BVP for compressive loading of a porous SMA bar with constrained surfaces.

To account for the traction between the specimen and the compressive plates, the
top and bottom surfaces are constrained in the radial direction, as shown in Figure 69. In addition, the top surface is constrained in the axial direction using a multi-point constraint such that it remains planar. The compressive loading is applied on the top surface. The applied force is selected to be the same as in the case of uniaxial loading, presented in Section 5.2.1.

The material parameters for the small pore NiTi alloy are used (see Table V). For simplicity, it is assumed that no plastic strains develop. The effective stress is obtained by calculating the ratio of the applied force to the area of the bar and the effective strain is calculated as the ratio of the displacement of the top surface to the initial length of the bar. The effective stress-strain response of the porous SMA bar is shown in Figure 70, where it is also compared with the uniaxial response, presented in Section 5.2.1. It can be seen that the effective response of the bar, calculated by taking into account the three-dimensional effects, deviates from the uniaxial response.

To further examine the three-dimensional effects, the von Mises effective stress in the bar is analyzed. The contour plot of the von Mises stress at the end of the loading is plotted in Figure 71. It can be seen, that near the top and bottom surfaces the stress is very non-uniform, while it is uniform in the middle part of the bar. The non-uniformity is due to the applied constraints on the surfaces. The constraint in the radial direction results in compressive stresses being developed in the radial direction as well as in stress concentrations near the outer surface of the bar. The compressive stresses decrease the value of the von Mises effective stress near the center of the bar, as seen in Figure 71. As a result of the decrease in the effective stress, the phase transformation in these regions takes place slower than in the middle of the bar. This effect can be observed by analyzing the contour plot of the martensitic volume fraction in the porous SMA bar, shown in Figure 72. As seen from Figure 72, the values of the martensitic volume fraction are significantly lower near the top and bottom surfaces.
Fig. 70. Stress-strain response of a small pore porous NiTi SMA bar showing the three-dimensional effect during compressive loading.

of the bar. The net effect of the lower value of the martensitic volume fraction in these regions is the apparent stiffer effective response, as seen in Figure 70.
Fig. 71. Contour plot of von Mises effective stress in the porous SMA bar at the end of the compressive loading.
Fig. 72. Contour plot of the martensitic volume fraction in the porous SMA bar at the end of the compressive loading.
CHAPTER VI

CONCLUSIONS AND FUTURE WORK

6.1. Summary and Conclusions

The development of a macroscopic constitutive model for porous SMAs has been presented in this work. The model is derived using micromechanical averaging techniques. The porous SMA material is modeled as a two-phase composite with an SMA matrix and a second phase which represents the pores. The behavior of the dense SMA matrix is modeled using a rate-independent thermomechanical constitutive model with internal variables. The evaluation of the material parameters for the porous SMA material has been presented for two NiTi alloys fabricated from elemental powder sintering. The major findings and contributions of this work are summarized below.

In the first part of the current work the derivation of a three-dimensional thermomechanical constitutive model for fully dense SMAs has been presented. In the current formulation of the model the following quantities are chosen as internal state variables: martensitic volume fraction, transformation strain, plastic strain, back stress and drag stress. The evolution equations for these parameters for the case of a three-dimensional loading have been presented. It should be noted that the plastic strain adopted in this work differs from the plastic strain in regular metal plasticity. The plastic strain defined in this work is induced by the martensitic phase transformation at relatively low values of the applied stress. The evolution equations for the plastic strain have been chosen to accurately represent the case of a material undergoing stress-induced martensitic phase transformation and differ from the ones given by Bo and Lagoudas (1999a).
In addition to the development of plastic strains the model is also able to account for the evolution of the transformation loop during cyclic loading. To accomplish this, evolution equations for the material parameters have been proposed based on the ideas presented by Bo and Lagoudas (1999a). For a given material two sets of material parameters need to be established. Then, during cyclic loading, involving phase transformation, the material parameters change from the initial set to the final set according to the evolution equations for each of the parameters. Thus, after a given number of cycles, a stabilization of the material response is achieved. Using the experimental results presented in the literature it has been demonstrated that the model can accurately simulate the SMA thermomechanical response. Different boundary value problems, including multiaxial loading, have been analyzed to demonstrate the capabilities of the model.

The development of a constitutive model for porous SMAs has been accomplished in the second part of the presented research work. The methodology developed for composite material have been utilized to establish the current micromechanical model. In contrast to the methods applied in composites undergoing plastic deformations, the current model focuses on the phenomena specific to the behavior of the shape memory alloys. In particular, the development of transformation strain which is recovered upon unloading and the change in the elastic properties of the SMA during phase transformation have been addressed in the current work.

The mechanical behavior of the porous SMA material is characterized by its effective elastic and tangent stiffness and by the effective inelastic strain. Therefore, expressions for the elastic and the tangent stiffness tensors in terms of the elastic and tangent stiffness of the SMA matrix and the pore volume fraction have been derived. In addition, the pore shape also enters the expressions through the strain concentration factors, which are evaluated using the Eshelby solution. The effect of different
pore shapes on the elastic properties of the material has been investigated. It has been found that for the case of random orientation of ellipsoidal pores the mechanical behavior of the material can be modeled using a spherical pore shape. However, if a different processing technique is established which is capable of fabricating porous SMAs with oriented porosity, the model can still be used. In the case of oriented porosity the distribution function for the pore orientations must be given. An evolution equation for the macroscopic inelastic strain has also been derived. The effects of different components entering the expression for the macroscopic inelastic strain rate have been investigated and their contributions have been evaluated.

A detailed procedure for the estimation of the material parameters for both fully dense and porous SMAs has been presented. The evaluation of the material parameters is given for the case of an SMA material undergoing stress-induced martensitic phase transformation. The experimental data for two different porous NiTi alloys has been used to estimate the material parameters used by the model. The results of the numerical simulations have been compared with the experimental stress-strain response of the material and it has been concluded that the model simulations are in good agreement with the experimental observations. To demonstrate the capabilities of the model, different boundary value problems involving multiaxial loading have been simulated. The results for sequential torsion-compression loading of a porous SMA bar, which is of particular interest for potential future applications, have been presented in detail and discussed.

The numerical implementation of the constitutive model has been presented where the methods reported by Qidwai and Lagoudas (2000a) have been utilized. Particular attention was given to implementing the evolution of the plastic strain as well as the evolution of the material parameters during cyclic loading. As a part of integrating the constitutive model in a computer code with capabilities of structural
modeling, it has been numerically implemented in a user-supplied material subroutine for ABAQUS.

6.2. Future Work

Based on the results of the current research effort, several topics for future research activity can be recommended. One issue which could be addressed in future research is the different behavior of SMAs under tension and compression. To accomplish this, a different form of the transformation function must be specified, as shown by Qidwai and Lagoudas (2000b). Another issue which should be addressed is the incorporation of two-way shape memory effect into the constitutive model for the fully dense SMA. The choice of proper tensorial variable to replace the current maximum transformation strain $H_{\text{cur}}$ used in this formulation will require additional experiments. These experiments should reveal the multiaxial effects of training and facilitate the further development of the model. The development of plastic strain for material undergoing incomplete transformation cycles must also be revisited. In the current model the evolution equations for the plastic strain do not distinguish between the complete and incomplete transformation cycles, while the experimental results suggest that the development of plastic strain may differ for incomplete transformation cycles.

Different issues can also be addressed in the model for porous SMAs. The first problem that should be further researched is the development of microcracks in the porous alloys. As seen from the experimental results this is a serious problem in porous SMAs fabricated from elemental powders. It has been observed that when subjected to compressive loading the porous SMA specimens develop cracks and eventually fail. Therefore, the incorporation of a damage mechanism into the constitutive model should be considered. Another issue that may become important is the investiga-
tion of different orientation distribution functions for oriented porosity. Finally, the
dynamic loading of porous SMAs must also be addressed. The experiments and mod-
eling of the behavior of porous SMAs under impact loading will become important
as these materials find their applications in various energy absorption devices.
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