Constitutive modeling of superelastic shape memory alloys considering rate dependent non-mises tension-torsion behavior

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entitled

Constitutive Modeling of Superelastic Shape Memory Alloys Considering Rate Dependent Non-Mises Tension-torsion Behavior

by

Masood Taheri Andani

Submitted to the Graduate Faculty as partial fulfillment of the requirements for the Master of Science Degree in Mechanical Engineering

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The University of Toledo
August 2013
Shape memory alloys (SMAs) are a type of smart materials which have unique features known as superelasticity and shape memory effects. The origin of SMA characteristics is a reversible martensitic phase transformation between austenitic phase and martensitic phase. The interest in the mechanical behavior of SMAs is rapidly growing with the increasing number of potential industrial and medical applications. Accurate and practical mathematical models are essential in order to successfully design SMA devices.

Within this work is the presentation of a general 3D model capable of capturing the multiaxial behavior of superelastic shape memory alloys (SMAs) under quasi-static isothermal or dynamic loading conditions. A semi-analytical framework is developed to numerically implement the model. An extended experimental study is conducted on NiTi thin walled tubes to investigate the performance of the model. The proposed approach is shown to be able to capture the non-Mises thermomechanical response of NiTi under complex tension-torsion loading conditions. The effect of loading sequence and loading rate is also experimentally studied. The main motivation of the present study is to develop a platform for analyzing and designing biomedical devices with SMA actuator under combined tension-torsion loading conditions.

The torsional stiffness of NiTi is shown to be adjustable by applying an extra axial
load. This will lead to developing desirable torque response in NiTi tubes and rods by varying the axial load. A possible application of this technique in the form of an assistive device is discussed.
To my loving parents, who raised me.
Acknowledgments

I would like to begin by acknowledging Allah for giving me the wisdom and capability to start and complete this work. I am also very thankful to my lovely parents Jafar and Afsaneh for their unbelievable love and emotional support over the past two years.

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<td>A</td>
<td>Austenite</td>
</tr>
<tr>
<td>$A_f$</td>
<td>Austenite finish temperature at zero stress</td>
</tr>
<tr>
<td>AFO</td>
<td>Ankle Foot Orthosis</td>
</tr>
<tr>
<td>$A_s$</td>
<td>Austenite start temperature at zero stress</td>
</tr>
<tr>
<td>C</td>
<td>Celsius</td>
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<tr>
<td>FE</td>
<td>Finite Element</td>
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<td>fwd</td>
<td>Forward transformation</td>
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<td>GPa</td>
<td>Gigapascals</td>
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<td>K</td>
<td>Kelvin</td>
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<tr>
<td>M</td>
<td>Martensite</td>
</tr>
<tr>
<td>$M_f$</td>
<td>Martensite finish temperature at zero stress</td>
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<tr>
<td>mm</td>
<td>Millimeter</td>
</tr>
<tr>
<td>MPa</td>
<td>Megapascals</td>
</tr>
<tr>
<td>$M_s$</td>
<td>Martensite start temperature at zero stress</td>
</tr>
<tr>
<td>N</td>
<td>Newton</td>
</tr>
<tr>
<td>NiTi</td>
<td>Nitinol</td>
</tr>
<tr>
<td>Pa</td>
<td>Pascal</td>
</tr>
<tr>
<td>rev</td>
<td>Reverse transformation</td>
</tr>
<tr>
<td>SE</td>
<td>Superelastic effect</td>
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<tr>
<td>SMA</td>
<td>Shape memory alloy</td>
</tr>
<tr>
<td>SME</td>
<td>Shape Memory Effect</td>
</tr>
<tr>
<td>UMAT</td>
<td>User Material</td>
</tr>
<tr>
<td>3D</td>
<td>Three dimensional</td>
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## List of Symbols

\[ \sigma \quad \text{Cauchy stress tensor} \]
\[ \varepsilon \quad \text{total strain tensor} \]
\[ \varepsilon^e \quad \text{elastic strain tensor} \]
\[ \varepsilon^t \quad \text{transformation strain tensor} \]
\[ \varepsilon^{th} \quad \text{thermal expansion strain tensor} \]
\[ S \quad \text{compliance tensor} \]
\[ \alpha \quad \text{effective thermal expansion tensor} \]
\[ T \quad \text{temperature} \]
\[ T_0 \quad \text{reference temperature} \]
\[ \xi \quad \text{martensitic volume fraction} \]
\[ \Lambda \quad \text{transformation tensor} \]
\[ \Gamma \quad \text{transformation identity tensor} \]
\[ k_s \quad \text{effective stress coefficient} \]
\[ k_e \quad \text{effective strain coefficient} \]
\[ \sigma^e_0 \quad \text{critical stress in uniaxial tension} \]
\[ \tau^t_0 \quad \text{critical stress in pure torsion} \]
\[ \varepsilon^e_0 \quad \text{critical strain in uniaxial tension} \]
\[ \gamma^s_0 \quad \text{critical strain in pure torsion} \]
\[ \Omega \quad \text{effective stress identity tensor} \]
\[ H \quad \text{maximum axial transformation strain} \]
\[ \sigma' \quad \text{deviatoric stress tensor} \]
\[ \bar{\sigma} \quad \text{effective stress} \]
\[ \mathbf{I} \quad \text{identity tensor} \]
\[ \rho \quad \text{density} \]
\[ G \quad \text{Gibbs free energy} \]
\[ c \quad \text{effective specific heat} \]
\[ M \quad \text{moment} \]
\[ F \quad \text{force} \]
\[ s_0 \quad \text{effective entropy at reference state} \]
\[ u_0 \quad \text{effective specific internal energy at reference state} \]
\[ \lambda \quad \text{austenite state} \]
\[ M \quad \text{martensite state} \]
\( f(\xi) \) ........ hardening function
\( \rho b^M \) ........ constant to define hardening
\( \rho b^A \) ........ constant to define hardening
\( \mu_1 \) ........ constant to define hardening
\( \mu_2 \) ........ constant to define hardening
\( \partial \) ........ partial differentiation
\( \pi \) ........ thermodynamic force
\( \Phi \) ........ transformation function
\( Y \) ........ measure of internal energy dissipation
\( q \) ........ heat flux
\( \hat{g} \) ........ internal heat generation
\( f^{\text{fwd}}(T) \) ..... function used to capture entropy and energy changes during forward transformation
\( f^{\text{rev}}(T) \) ..... function used to capture entropy and energy changes during reverse transformation
\( \gamma \) ........ shear strain
\( \nu \) ........ Poisson’s ratio
\( ^\circ \) ........ degrees of rotation
\( k \) ........ thermal conductivity
\( h \) ........ heat convection coefficient
\( r \) ........ radius of an annular region
\( d \) ........ diameter
\( R_0 \) ........ outer radius
\( L \) ........ length
\( G_M \) ........ shear modulus in martensite
\( G_A \) ........ shear modulus in austenite
\( E_M \) ........ modulus in martensite
\( E_A \) ........ modulus in austenite
\( C_A \) ........ slope of the austenite transformation bands on the phase diagram
\( C_M \) ........ slope of the martensite transformation bands on the phase diagram
\( \Delta t \) ........ time increment
\( \Delta r \) ........ radius increment
\( \xi^{t-r} \) ........ martensite volume fraction at the beginning of reverse transformation
\( \varepsilon^{t-r} \) ........ strain at the beginning of reverse transformation
\( \kappa \) ........ equivalent internal heat generation
\( Nu \) ........ Nusselt number
\( Ra \) ........ Rayleigh number
\( Pr \) ........ Prandtl number
\( Gr \) ........ Grashof number
\( g \) ........ gravitational acceleration
\( \beta \) ........ volume coefficient of expansion
$T_\infty$ ........ ambient temperature
$\nu_a$ ........ kinematic viscosity of air
$m$ ........... mass
$C_p$ ........ heat capacity
$P$ ........... dissipated power
$\Delta Q$ ....... latent heat
Chapter 1

Introduction

1.1 Shape memory alloys

Shape memory alloys (SMAs) can recover large amounts of deformation (axial strain of 10%) under specific thermo-mechanical conditions. The key feature of these alloys is the ability to undergo large seemingly plastic strains and subsequently recover these strains when a load is removed or the material is heated. This unique property is the basis for various applications for these materials from automotive actuators to medical devices. In 1932, the first alloy to exhibit the shape memory effect (AuCd) was discovered by Arne Ölander [1]. This alloy could not survive large stresses or strains and was never developed into an actuator. In 1961, while searching for high corrosion resistant materials a group of researchers stumbled upon another SMA. The alloy was comprised of Nickel and Titanium (NiTi) and was discovered at the US Naval Ordinance Laboratory (NOL), thus the original name for the material became NiTiNOL [2]. Consequently, several other metal combinations have been found to exhibit this effect. Alloys such as Ag-Cd, Au-Cd, Cu-Sn, In-Ti, Ni-Al, Ni-Ti, Mn-Cu all exhibit shape memory tendencies. Despite the subsequent discoveries, NiTi however has proven to be the most promising alloy for many applications [3, 4, 5, 6]. This superiority is due to its greater ductility, larger recoverable motion,
excellent corrosion resistance, stable transformation temperatures, biocompatibility and ease of electrical heating. In addition to the distinctive properties of shape memory effect (SME) and superelasticity (SE) as will be discussed later, NiTi exhibits good resistance to wear and corrosion, have superior energy absorption capacity, and are often biocompatible. These properties make this alloy a good candidates for a variety of applications from aerospace and automotive to biomedical applications. NiTi has been used for actuation, energy absorbing, and sensing. As actuators, NiTi offers several advantages for system miniaturization such as excellent power to mass ratio, maintainability, reliability, and clean and silent actuation. There are disadvantages such as low energy efficiency due to conversion of heat to mechanical energy and difficulties in control due to hysteresis, nonlinearities, parameter uncertainties, and in the challenge of measuring state variables such as temperature.

1.1.1 Phase transformation in SMAs

The underlying reason for the unique properties of SMAs is in their crystalline structure. Their crystal structure undergoes a solid-solid phase transformation when cooled from its stiff, high temperature austenite (A) phase to its softer, low temperature martensite (M) structure. This inherent phase transformation can be stress or temperature induced. The stress-temperature-transformation plot is a schematic representation of the transformation regions for shape memory alloys. The lines in the plot show the phase boundaries that separate the two solid phases of an alloy. Usually a stress-temperature-transformation plot shows the temperature along the abscissa and stress along the ordinate. The mechanism in which the crystalline structure of the austenite phase transforms to martensite phase is called lattice distortion and the transformation is called martensitic transformation. The martensite crystal can also be formed as a twinned, detwinned, or reoriented form. The reversible transformation of the material from austenite, which is known as the parent phase to martensite
makes the special thermo-mechanical behavior of shape memory alloys. A widely accepted stress-temperature-transformation plot of shape memory alloy materials is shown in Figure 1-1. As described earlier, shape memory alloys can exhibit a shape memory effect or pseudoelasticity. The type of the effect depends on the chemical composition of the alloy, the processing history and of course the ambient temperature. Both effects and the special thermo-mechanical properties of shape memory alloys are described in the following sections.

Figure 1-1: Stress-temperature-transformation plot of a shape memory material depicts the stable area for each crystalline structure. Crystal transformation takes place as the result of variation in stress and temperature.

1.1.2 Shape memory effect

Shape memory effect is the ability of these alloys to recover a certain amount of unrecovered strain upon heating. This phenomenon takes place when the material is loaded such that the structure reaches the detwinned martensite phase and then unloaded while the temperature is below the austenite start temperature ($A_s$). Heating the material at this stage will lead to strain recovery and the material will...
regain its original shape. This phenomenon can be better displayed in the combined stress-strain temperature diagram as shown in Figure 1-2.

![Figure 1-2: Shape memory effect path in stress-strain-temperature space](image)

Starting from point A material is initially in the austenite phase. Cooling down the alloy to a temperature below its martensite finish temperature ($M_f$) will result in the twinned martensite crystal, point B. At this point loading the alloy at the same temperature will lead the crystal to transform to the detwinned martensite phase at point C. This stress-strain path is nonlinear because of the transformation phenomenon. Unloading the applied stress at the same temperature will result in linear strain recovery to point D and remains in the detwinned martensite phase and a residual strain. By heating the alloy above the austenite start temperature ($A_s$) at point E, the transformation from detwinned martensite to austenite phase starts. This transformation recovers the residual strain, which will be fully recovered at point F where the alloy passes the Austenite finish temperature. The stress-temperature-crystalline structure pattern during shape memory effect is depicted on the transformation diagram (Figure 1-3) for more clarity.
1.1.3 Superelasticity

Pseudoelastic or superelastic behavior is the ability of SMAs to recover large amount of strains through mechanical loading/unloading. Figure 1-4 shows a typical superelastic stress-strain response of SMAs. The superelastic thermo-mechanical behavior starts from temperatures above austenite finish temperature (Af) where the material is fully austenite (point A) and continues in loading by an applied force to make the detwinned martensite crystal form (point B). During this (forward) transformation from austenite to martensite the transformation strain is generated. Upon unloading, the generated strain is fully recovered in the (backward) transformation and the original form is achieved (point C). The stress-temperature-crystalline structure cycle of such behavior is shown on the transformation plot in Figure 1-5.
Figure 1-4: Superelastic stress-strain response of SMAs

Figure 1-5: Superelasticity in phase diagram

Training an SMA refers to the process of repeatedly loading/unloading the material until its response becomes consistent. Once trained the hysteretic response
of the material stabilizes and the inelastic strain saturates and disappears. Figure 1-6 shows the cyclic mechanical loading of a superelastic NiTi wire. At the end of the first cycle, a permanent plastic strain remains in the material. The additional permanent strain associated with each consecutive cycle begins to gradually decrease until it practically ceases to further accumulate. Training is a recommended process to be conducted on every off-the-shelf NiTi component before practical application to avoid an inconsistent strain response.

![Stress-Strain Diagram](image)

Figure 1-6: Training is required to be conducted on SMA to stabilize its cyclic response

### 1.1.4 Applications

Shape memory alloy (SMA) actuators are attractive due to their many potential applications in mechanical, electrical, medical and aerospace systems. SMAs have many advantages over conventional actuation methods. Their significantly reduced
weight, size, complexity and noiseless operation make them suitable as actuators for a wide range of applications from micro robotics to medical application and aerospace systems. Their benefits over other smart materials such as piezoelectric materials, electrostrictive materials and magnetostrictive materials include their high force to weight ratio, and large displacement capabilities. Shape memory alloy actuators can replace conventional actuators thanks to the large mechanical strains induced by heating and cooling. Large mechanical stress is consequently produced when SMA elements are heated or cooled beyond critical temperatures. SMA actuators can apply up to 600 MPa. As an example, a 0.1 mm diameter NiTi wire can therefore apply a force of 4.7 N. This means that the wire can lift up an object about 100,000 times its own weight. Another advantage that SMA actuators have over conventional actuators is that they can be made compact and simplistic. There are many advantages to employ SMA wires as actuators in various applications. In the following, possible loading and actuation modes of SMA devices are discussed. Example(s) are also presented for each mode to better show the mechanism of the actuation.

**One-way and two-way actuators**

One-way shape memory effect refers to the ability of an SMA deformed at a low temperature to recover the deformation when heated to a higher temperature. In this behavior, the austenite shape is memorized due to self-accommodated structure of martensite variants. One-way shape memory is the most frequently utilized SMA behavior in practice. In actuation applications, however, the shape memory behavior is never used in this fashion. Instead, an external biasing force always exists on SMA actuators during thermal cycling. During transformation, the associated shape change causes SMA to push against the biasing force, thus doing mechanical work. There is another shape memory behavior where SMAs can exhibit repeatable shape changes without a biasing mechanical load. Instead the SMA will alternate between
memorized shapes when subjected to a cyclic thermal load. In this case the SMA memorizes a martensite shape different from the austenite shape. This behavior is called the two-way shape memory effect. In this mode, when the SMA is cooled from austenite to martensite, instead of adapting to a self-accommodated structure, some variants of the martensite are favored and the martensite adopts a shape different from that of the self-accommodated structure. Two-way shape memory effect is caused by internal stresses that develop in the SMA from plastic deformation in martensite usually through aging for precipitation under stress and/or under constraint, which is called training.

Most of the SMA actuators utilize these alloys in the wire form. The SMA actuators are designed to use the shape memory effect in creating motion and force. When an SMA wire is heated, the material applies a large amount of force and displacement while returning to a memorized length. Joule heating is an effective and simple way for actuating SMA components. So far, most of developed SMA actuators operate in simple axial loading with small displacements. However, it is possible to overcome these drawbacks through design optimization. Figure 1-7 shows a simple mechanism used by Elahinia and Afsharioun [7] to create a rotational motion by actuating an SMA wire. The arm mechanism converts the small axial deformation of the wire to a large rotational displacement and the bias spring makes the cyclic motion possible.

Utilizing SMAs in the form of springs is another solution to overcome the deformation limitations of these materials. Spring type SMA actuators provide large deformation in addition to smooth, silent, and clean motion compared to traditional types of actuators. This kind of actuator is particularly appropriate for robotic applications where size and weight are critical. Moghaddam et al. [8] designed a lightweight biped using two SMA based actuators. Figure 1-8 shows a configuration of this device. The experiments conducted on a prototype of the device demonstrated a promising capability of the SMA springs in providing a flexible motion under un-
wanted turbulences.

![Figure 1-7: SMA rotary actuator [7]](image)

It is well-established that using SMA actuators drastically can reduce the number of moving mechanical parts, simplify the assembly procedure and reduce manufacturing costs. These benefits have caused researchers to use SMAs to design less expensive and compact actuators. The automotive is a large potential market for these types of actuators. Williams et al. [9] designed an SMA external side mirror actuator. As shown in Figure 1-9, the mirror is primarily made of a modified ball and socket joint and four SMA wires. The spring-loaded joint provides mirror stability between actuation. At the time of actuation, the force of the SMA wires disengages the joint.

![Figure 1-8: Configuration of a biped actuated by SMA springs [8]](image)
to provide friction-free motion. This joint passively provides a larger range of motion with smaller actuation force. The actuation force, unlike in the first generation mirror [10], is not used to overcome friction. This feature of the joint, additionally, mitigates the disturbances such as aerodynamic forces and variation in environment temperature. The proposed actuator provides a two degree of freedom by rotating the mirror about its two axes.

Figure 1-9: Configuration of an SMA mirror actuator [9]

Superelastic devices

Superelastic SMAs are beneficial in passive applications where large recoverable deformations are required. SMAs can provide almost constant level of force (stress) over a large range of strain (up to 10%). Dental archwires, brassieres, springs, cell phone antennae, and many other applications use the pseudoelastic property of SMA to increase the durability and performance of consumer goods such as those aforementioned [11]. An innovative application for superelastic Nitinol is the retrograde blade which is designed to cut bone. As shown in Figure 1-10, the blades undergo large bending deformations without considerable residual deformation.
Another application is an intervertebral cage, developed using superelastic Nitinol hinges under torsional loading (Figure 1-11) [12]. The cage was built using additive manufacturing out of medical grade titanium. Elliptical shape rods were employed so that residual torque at closure is possible. An intervertebral cage is a spacer that is used when two vertebrae are fused together to alleviate low back pain. In Figure 1-12, two individual cage segments are shown being assembled. The two segments are “over-rotated” (panel a) and the two parts are made to come together (panel b). The cage is then straightened and put in its pre-deployment condition (panel b). After deployment, the superelasticity of the nitinol causes the cage to go from the constrained straight form to the oval closed form (panel c).
Figure 1-11: An intervertebral cage was developed using superelastic NiTi elliptical shape rods as hinges [12]

Figure 1-12: The assembly and deployment configuration of the intervertebral cage [12]

**Antagonistic actuators**

A distinct actuation approach is possible based on combining the two distinct properties of SMAs: shape memory effect (SM) and superelasticity (SE). A SM member in conjunction with a SE element would make an antagonistic manner actuator, such that they force each other in the opposite directions. The SM component would
control the actuation while the SE element provides the required actuation force and large actuation stroke. The function of the actuator is as follows: assuming that the actuator is supposed to work between two temperatures; low temperature ($T_l$) and high temperature ($T_h$). The SE member is always in austenite phase either at low temperature or high temperature. This means that its austenite finish temperature is lower than both low and high temperatures ($A_{f SE}^i < T_l$ $A_{f SE}^i < T_h$). On the other hand, the SM element is initially in its martensite phase but transforms to austenite at high temperature. To this end, the SM material should be selected such that it’s martensite finish temperature ($M_{f SM}^i$) is higher than the low temperature and its austenite finish temperature ($A_{f SM}^i$) is lower than high temperature ($T_l < M_{f SM}^i$ and $T_h > A_{f SM}^i$). The SE and SM elements original shapes are set such that in low temperature, the SE element is stronger and the assembly stays toward the SE element, which is set to be the inactivated form of the actuator. At high temperature, the SM element passes its austenite temperature and moves the assembly toward its original shape that is set to be the activated form of the device.

The described antagonistic actuator could be assembled in many different ways. An interesting configuration is having the SM element as a flat wire and SE element as a ring shaped wire. By wrapping the flat wire around the round member, a smart antagonistic actuator would be resulted. Figure 1-13(a) and Figure 1-13(b) respectively display the initial shape set or memorized forms of the SE and SM elements before assembly.

When the two members are assembled at a low temperature, they apply force to each other in a way that the SM at wire tries to enclose the ring while the SE element tends to keep the ring open. Depending on the material properties of the two components, an equilibrium position will be obtained. Figure 1-14(a) displays the equilibrium or neutral position of the device at low temperature. By heating the SM element either by changing the thermal environmental condition or by resistant
heating, the assembly tends toward the shape set form of the SM member which likes to enclose the ring as shown in Figure 1-14(b). By cyclic heating and cooling these two configurations can be perfectly repeated. It’s worth mentioning that the actuation stroke and shape generally depend on the material properties and shape set forms of the SM and SE elements and thus there are numerous actuation possibilities with the antagonistic method.

Figure 1-13: Initial memorized shapes of the members before assembly in an antagonistic actuator

Figure 1-14: Smart antagonistic actuator assembly
Tissue clamps are widely used to hold the body organs during the surgery. The conventional devices are usually large, heavy and hard to control. A smart tissue clamp is designed based on the introduced antagonistic actuation method. This novel device is light and small, with a large actuation stroke and the ability of remote controllable releasing. A prototype of the smart tissue clamp was fabricated and experimentally evaluated in the Dynamic and Smart Systems Laboratory at The University of Toledo. The shape memory wire was heated and the temperature of the device was measured by an infrared camera (Micro Epsilon). Figure 1-15(a) shows the device before the actuation of the SM wire at room temperature. As soon as the SM wire is heated, it starts to release the clamp as shown in Figure 1-15(b). By cyclic heating and cooling, the clamping and releasing configurations would be repeated.

Figure 1-15: Experimental evaluation of the smart antagonistic tissue clamp

1.1.5 Multi-axial loading behavior

So far, in most of the developed SMA based devices, SMA wire or tube is subjected to simple uniaxial tension or pure torsion loading/unloading conditions. In these simple cases, the SMA element would provide a unique stress-strain hysteresis-like profile
which is associated with the force/torque requirement of the device at a constant temperature. But there are also potential applications, in which the required force/torque profiles are more complex than simple hysteresis loops resulted from simple tension or torsion loading/unloading. In such cases, using combined tension-torsion loading paths might be a solution to achieve a more versatile response. Another driving force is that today’s development in the manufacturing and processing techniques of SMAs [13] is leading to the freedom in fabrication of complex SMA parts and structures with loading modes other than simple tension or torsion.

Although there is a significant interest in modeling the superelastic behavior of shape memory alloys and particularly NiTi, the experimental data, which are used to develop and evaluate the models, are in most cases associated to simple uniaxial tests. In order to develop reliable models, which may be used to simulate general 3D structures subjected to complex loading conditions, it is of paramount importance to use multiaxial experiments.

There have been extensive studies on the superelastic behavior of NiTi shape memory alloys since the late 1980’s. Although, most of the mechanical experiments found in the literature were performed under a uni-axial loading state, some experimental works in 2-D conditions also appear in the literature. Sittner et al. [14, 15] conducted out of phase non-proportional box and triangle tension-torsion experiments on Cu-based SMAs. They also demonstrated the path dependency of the SMA mechanical response in the tension-torsion states. Rogueda et al. [16] conducted similar studies for NiTi. Extensive proportional and non-proportional biaxial tests were also performed by Lim and McDowell [17], McNaney et al. [18], Helm and Haupt [19], and Grabe and Bruhns [20]. Loading direction (axial or torsional) as well as loading sequence was shown to affect the macroscopic behavior of SMAs. More specifically, the Von Mises equivalence for describing the macroscopic behavior proved to be insufficient when used to predict the tension-torsion response.
1.1.6 Loading rate dependency (thermo-mechanical coupling)

It is well established that increasing the strain rate causes a significant temperature change in the material due to the produced/absorbed latent heat during the phase transformation [21]. It is known that the forward phase transformation (A $\rightarrow$ M) is exothermal and the reverse transformation (M $\rightarrow$ A) is endothermal. Therefore, during the forward transformation, the temperature of the SMA increases making austenite more stable and during the reverse phase change the temperature of the SMA decreases making martensite more stable. This temperature evolution results in different stress plateaus (and different slopes of plateaus) in the dynamic loading conditions, which also leads to different values of hysteresis loop area and energy dissipation. This phenomenon is depicted in Figure 1-16 for a typical Nitinol wire under uniaxial loading with two loading rates corresponding to strain rates of 0.01/s (fast) and $2.5 \times 10^{-4}$/s (slow). As shown in this figure, the transformation finish stresses and the slopes of the phase transformation plateaus increase with increasing strain rate.

![Figure 1-16: Evolution of the mechanical response at different loading rates](image-url)
There are several works in the literature that investigate the latent heat effect on the thermomechanical response of SMAs. They generally present a platform which couples the constitutive equations of SMA with the heat balance equation. Auricchio et al.[22] presented a rate dependent uniaxial constitutive model to represent the thermo-mechanical behavior of SMAs in seismic applications. Their model is based on a single internal scalar variable, the martensite fraction, for which different rate-independent evolutionary equations are proposed. The constitutive model is thermo-mechanically coupled with a thermal energy balance equation to capture the latent heat effect. They compared the stress-strain response of their model with the experiment under a dynamic uniaxial loading condition, but they didn’t report the temperature variation during the test. In a similar work, Vitiello et al. [23] used the one-dimensional Tanaka’s model [24] in conjunction with the energy balance equation to take into account the latent heat effect. The solution was restricted to very slender cylinders with small Biot numbers. In this special case, temperature non-uniformity in the cross-section can be neglected, and the governing equations are simplified by assuming a uniform temperature distribution at each time increment. In another work, Messner et al. [25] studied the local increase in temperature near a moving phase transformation front due to the latent heat of phase transformation in one-dimensional SMAs subjected to tensile loading. They modeled the effect of phase transformation latent heat by a moving heat source. A constant value is considered for the latent heat generated by phase transformation. This assumption is unrealistic for polycrystalline SMAs because the amount of generated heat is specified by a set of coupled equations and depends on variables such as stress and martensitic volume fraction. Morin et al. [26] modified the Zaki-Moumni model for SMAs [27] by including the heat equation and provided a general coupled three-dimensional model. Their model is in qualitative agreement with the experimental results at high strain rates.
1.2 Constitutive modeling of SMAs

There have been many attempts to mathematically model the SMA material features over the past three decades. The resulting models can be divided into two different groups: micro models and phenomenological macro models. In general, micro-mechanical based models [28, 29, 30] utilize information about the microstructure of the SMA to predict the macroscopic response. They are very useful to understand the fundamental phenomenon, although they are not easily applicable at the real engineering applications. On the other hand, phenomenological models [24, 31, 32, 33, 34, 35, 36, 37, 38] are built on phenomenological thermodynamics and/or directly curve fitting experimental data. Many are based on the common phase diagram of SMA transformation where the transition regions of martensite to parent phase or parent phase to martensite transformation are determined experimentally and plotted in stress-temperature space. Researchers typically use the martensite volume fraction as an internal variable and different mathematical functions to describe a smooth transition. These kinds of models are generally more suitable for engineering applications due to their simplicity and fast computations, but they can only describe the global mechanical response while all the microscopic details are ignored; because the phase diagram is built on experimental data, the models are also quite accurate.

Based on continuum thermodynamics with internal variables, several three-dimensional macroscopic phenomenological models have been proposed, in the literature, with success. Numerous methods have been developed to employ these mathematical models for the analysis of SMA structures. The Finite Element Method (FEM) as a strong numerical approach has been proposed in several works [39, 40, 41, 42] for the analysis of SMA-based devices. Exact and analytical solutions have also been studied in recent years. They are computationally less expensive and as a result provide faster
simulations. Additionally exact models are more readily applicable in real time simulations and control of SMA actuators. Mirzaefar et al. [43] has conducted a study to find the exact solution for torsional behavior of shape memory alloy rods. They simplified the 3-D Boyd and Lagoudas model [33] to a 1-D shear form. This way, they developed an exact form for the relationship between the applied torque and the angular displacement. In another work by the same group [44], a semi-analytical analysis is conducted on the behavior of shape memory thick-walled cylinders under internal pressure. Similar analytical works [45, 46, 47] have been conducted for solving the moment due to stress distribution of an SMA beam.

1.3 Objectives

The main objective of this work is to provide a general 3D modeling approach for superelastic SMAs to address the discrepancies observed between the experimental data and the predictions of the available models in capturing the SMA response under complex loading patterns.

The rate dependent nature of SMAs as well as their non-Mises response must be addressed in the developed approach. A complete set of experiments are required to verify the model. The model should be implemented in a numerical platform to be applicable for engineering purposes.

1.4 Approach

In order to accomplish the objectives set forth as for the current study, a 3D rate dependent constitutive model was first developed based on the experimental observations for NiTi which revealed the non-Mises effective response of the material in combined tension-torsion loading histories. The developed mathematical platform
is general and applicable to different complex 3D loading conditions.

A semi-analytical platform was coded in MATLAB for solving the developed coupled nonlinear governing equations. Initial thermal conditions, loading rate and total twist angle and axial displacement are considered as inputs to the model. The model predicts the stress-strain response of the SMA element as well as its temperature evolution during the simulated loading/unloading pattern.

Several sets of mechanical tests were conducted on NiTi tubes to evaluate the capability of the model in capturing the thermal and mechanical responses of SMAs tube under various quasi-static isothermal and dynamic loading conditions. The model predicts the material response with good accuracy in all cases.

1.5 Contribution

The contribution of the work is the successful simulation of the thermo-mechanical behaviors of superelastic shape memory alloys subjected to complex mechanical loading patterns. The presented modeling method can be used to design SMA biomedical actuators when combined loading histories are required. This model has been employed in the design procedure of an SMA ankle foot orthosis and an intervertebral cage developed in the Dynamic and Smart Systems Laboratory at the University of Toledo [12] [48].

1.6 Publications

Journals

- Taheri Andani, M., Alipour, A., Eshghinejad, A. and Elahinia, M., “Modifying the torque-angle behavior of rotary SMA actuators through axial loading: A semi-analytical study of biaxial behavior”, Journal of Intelligent Material Sys-
tems and Structures, 2013.


- Taheri Andani, M. and Elahinia, M., “A rate-dependent tension-torsion constitutive model for superelastic Nitinol under non-proportional loading; a departure from Von Mises equivalency”, Smart Materials and Structures, (submitted)


Intellectual property


Proceedings


• Taheri Andani, M. and Elahinia, M., “Modeling and Simulation of Medical Devices Undergoing Complex Thermo-Mechanical Loadings”, Shape Memory and Superelastic Technologies Conference and Exposition (SMST), May 21-24, 2013, Prague, Czech Republic.

**Book Chapter**

Chapter 2

A rate dependent constitutive non-Mises based model

2.1 Introduction

The model introduced in this chapter is motivated by the 3D model developed by Boyd and Lagoudas [33] and is based on the experimental observations of NiTi tubes subjected to combined tension-torsion histories. General constitutive equations are derived for both quasi-static and dynamic 3D loading conditions. Experimental effective stress/strain terms are employed in the model to include the non-Mises response of the material. A semi-analytical approach is finally discussed in order to implement the developed modeling framework. The main benefit of the resulting model is its simplicity of implementation, which paves the way for real-time actuators undergoing combined tension-torsion loading conditions. More importantly, this solution is general and valid at different temperatures and therefore valid for various combined tension-torsion loading patterns. Moreover, the small number of model parameters and the simplicity to calibrate them made this solution suitable for straightforward implementation into practical engineering applications. The proposed approach provides a reliable platform to design and analyze of SMA components under various
2.2 Development of a general 3D constitutive model

Strain decomposition

The following classic decomposition of the total strain is assumed as the first step in developing the constitutive model:

\[ \varepsilon = \varepsilon^e + \varepsilon^{th} + \varepsilon^t \]

where \( \varepsilon^e \), \( \varepsilon^{th} \) and \( \varepsilon^t \) represent the elastic strain, thermal expansion strain and inelastic strain, respectively. The first two tensors are defined as:

\[ \varepsilon^e = S : \sigma, \]

\[ \varepsilon^{th} = \alpha(T - T_0) \]

where \( S \), \( \sigma \), \( \alpha \), \( T \) and \( T_0 \) are the effective compliance tensor, Cauchy stress tensor, effective thermal expansion coefficient tensor, temperature and reference temperature, respectively. The sign \( (:) \) indicates double dot product operation between two tensors.

Transformation strain evolution

The third term in equation (2.1), \( \varepsilon^t \) is the inelastic strain caused by the martensitic transformation in the material. In the current framework, it is assumed that the evolution of the transformation strain tensor is proportionally dependent on the change in the martensite volume fraction shown by \( \xi \). The relation between the rate of transformation strain tensor and rate of martensitic volume fraction is called flow rule. The flow rule proposed in [33] is modified as follows based on the experimental
observations to capture the coupling between axial and torsional strains during the transformation:

\[ \varepsilon^t : \Gamma = \Lambda^t \dot{\xi} \]  \hspace{1cm} (2.4)

where \( \Gamma \) is a \( 6 \times 6 \) diagonal tensor, defined as:

\[ \Gamma = diag(1, 1, 1, k_s k_e, k_s k_e, k_s k_e) \]  \hspace{1cm} (2.5)

where \( k_s \) and \( k_e \) specify the extent of coupling between tension and torsion and are called effective stress coefficient and effective strain coefficient, respectively. When \( k_s \) and \( k_e \) are equal to 1, equation (2.4) would be identical to the Von Mises based flow rule presented in [33]. In order to calibrate these two parameters, a pure torsion test is necessary as well as a uniaxial tension test at the same temperature. The value of \( k_s \) is determined using the yield stresses in uniaxial tension, \( \sigma_0^s \), and in pure torsion, \( \tau_0^t \), as:

\[ k_s = \frac{\sigma_0^s}{\sqrt{3} \tau_0^t} \]  \hspace{1cm} (2.6)

and \( k_e \) is defined using the axial strain corresponding to the yield stress in pure tension, \( \varepsilon_0^s \) and the shear strain when the material begins to yield in pure torsion, \( \gamma_0^t \), in the form of:

\[ k_e = \frac{\sqrt{3} \varepsilon_0^s}{\gamma_0^t} \]  \hspace{1cm} (2.7)

**Transformation direction**

Introduced in equation (2.4), \( \Lambda^t \) is the transformation tensor which determines the transformation strain direction and relates the evolution of the martensitic fraction to the transformation strain. In the current work, the following form is proposed for this tensor:
\[
\Lambda' = \begin{cases} 
\frac{3}{2}H\Omega : \sigma' \\
\Gamma : \frac{\varepsilon^{t-r}}{\xi^{t-r}} 
\end{cases} \quad \xi > 0, \\
\Gamma : \frac{\varepsilon^{t-r}}{\xi^{t-r}} \quad \xi < 0,
\tag{2.8}
\]

where \( H, \sigma' \) and \( \sigma \) are the maximum axial transformation strain, deviatoric stress tensor and effective stress, respectively. \( \varepsilon^{t-r} \) and \( \xi^{t-r} \) are the transformation strain and martensitic volume fraction at the reversal point, which represent the state of transformation at the end of loading. As implied from equation (2.8) and as discussed in [49], the direction of the reverse phase transformation is assumed to be correlated to the mean transformation strain created in the forward transformation. \( \Omega \) is the effective stress diagonal tensor which is defined to shape an experimental based transformation surface and is written as:

\[
\Omega = \text{diag}(1,1,1,k_s^2,k_s^2,k_s^2).
\tag{2.9}
\]

An important macroscopic phenomenon reported in [14] is that the effective stress in SMAs does not obey Von Mises equivalent rule. To describe this phenomenon, the following non-Mises effective stress, introduced by Peng et al.[50], is adopted in the current work:

\[
\bar{\sigma} = \sqrt{\frac{3}{2} \sigma' : \Omega : \sigma'}.
\tag{2.10}
\]

The deviatoric stress is expressed as: \( \sigma' = \sigma - \frac{1}{3}(tr \sigma) \mathbf{I} \), where \( \mathbf{I} \) is the identity tensor.

**Thermodynamics of transformation**

Although, the state of SMA material during the transformation could be described using the introduced flow rule equation (2.4) and transformation tensor equation (2.8), an additional constraint is required to define the occurrence of transformation. To this end, the second law of thermodynamics is used in the following form proposed...
by Qidwai and Lagoudas [39]:

\[
\sigma : \dot{\varepsilon}^t - \rho \frac{\partial G}{\partial \xi} \dot{\xi} = \pi \dot{\xi} \geq 0, \tag{2.11}
\]

where \( \rho \) and \( G \) are the SMA mass density and Gibbs free energy, and \( \pi \) is the thermo-
dynamic force. The following expression is selected for the total Gibbs free energy:

\[
G(\sigma, T, \varepsilon^t, \xi) = -\frac{1}{2\rho} \sigma : S \sigma - \frac{1}{\rho} \sigma : \left[ \alpha(T - T_0) + \varepsilon^t \right] + c[(T - T_0) - T ln\left(\frac{T}{T_0}\right)] \\
- s_0 T + u_0 + \frac{1}{\rho} f(\xi), \tag{2.12}
\]

where \( c, s_0 \) and \( u_0 \) are the effective specific heat, effective specific entropy and effective
specific internal energy at the reference state, respectively. This form of Gibbs free
energy results in the following expression for \( \pi \):

\[
\pi = \sigma : \Lambda^t + \frac{1}{2} \sigma : \Delta S : \sigma + \Delta \alpha : \sigma(T - T_0) - \rho \Delta c[(T - T_0) - T ln\left(\frac{T}{T_0}\right)] \\
+ \rho \Delta s_0 T - \frac{\partial f(\xi)}{\partial \xi} - \rho \Delta u_0, \tag{2.13}
\]

An effective material property \( \mathcal{P} \) can be determined in terms of the properties for the
pure phases and the martensitic volume fraction \( \xi \) via \( \mathcal{P} = \mathcal{P}^A + \xi(\mathcal{P}^M - \mathcal{P}^A) \). The
symbol \( \Delta(\mathcal{P}) \) denotes the difference between the martensitic and austenitic phases, i.e.
\( \Delta(\mathcal{P}) = (\mathcal{P})^M - (\mathcal{P})^A \). Superscripts \( A \) and \( M \) represent the austenite and martensite
phases, respectively. For the hardening function \( f(\xi) \), the polynomial form proposed
in [33] is employed in the current work as:

\[
f(\xi) = \begin{cases} 
\frac{1}{2} \rho b^M \xi^2 + (\mu_1 + \mu_2) \xi & \dot{\xi} > 0, \\
\frac{1}{2} \rho b^A \xi^2 + (\mu_1 - \mu_2) \xi & \dot{\xi} < 0,
\end{cases} \tag{2.14}
\]

where \( \rho b^A, \rho b^M, \mu_1 \) and \( \mu_1 \) are material constants for transformation strain hardening.
To define the occurrence of transformation and for the inequality (2.11) to be always valid, the transformation function $\Phi$ is introduced as:

\[
\Phi(\sigma, T, \xi) = \begin{cases} 
\pi - Y = 0 & \dot{\xi} > 0, \\
-\pi - Y = 0 & \dot{\xi} < 0, \\
< 0 & \dot{\xi} = 0,
\end{cases}
\tag{2.15}
\]

where $Y$ is a measure of internal energy dissipation due to micro-structural changes during phase transformation. The transformation function represents the elastic domain in the stress-temperature state. In other words, when $\Phi < 0$ the material response is elastic and the martensitic volume fraction does not change ($\dot{\xi} = 0$). During the forward phase transformation ($\dot{\xi} > 0$) and the reverse phase transformation ($\dot{\xi} < 0$), the state of stress, temperature and martensitic volume fraction should remain on the transformation surface, which is characterized by $\Phi(\sigma, T, \xi) = 0$ [43].

**Thermomechanical coupling of SMAs in dynamic loading**

It has been observed [17, 51] that thermomechanical coupling is significant in SMAs. Since latent heat is produced/absorbed during the forward/reverse phase transformation, temperature evolution can occur in the material, influencing its mechanical behavior. This coupling is more significant when the transformations occur over relatively short time spans, corresponding to dynamic loading at high loading rates.

To find the general thermo-mechanical balance equation, the first law of thermodynamics (conservation of energy) in local form is combined with the second law of thermodynamics (see [51, 52] for more details) and the following relation is obtained:

\[
T\alpha : \dot{\sigma} + \rho c\dot{T} + (-\pi + T\Delta\alpha : \sigma - \rho\Delta T\ln(\frac{T}{T_0}) + \rho\Delta s_0 T)\dot{\xi} = -\text{div}(q) + \rho\dot{g}, \tag{2.16}
\]
where \( q \) and \( \hat{g} \) represent the heat flux and internal heat generation except the phase transformation latent heat, respectively. Equation (2.16) is the 3-D form of the fully coupled balance equation of SMAs. The first term on the left hand side \((T\alpha : \dot{\sigma})\) captures the temperature changes due to a change in the state of the material, while the second term on the left hand side \((\rho c\dot{T})\) is related to the heat capacity. The third term on the left hand side \(\left((-\pi + T\Delta\alpha : \sigma - \rho\Delta T\ln\left(\frac{T}{T_0}\right) + \rho\Delta s_0 T)\dot{\xi}\right)\) describes how the temperature changes during the transformation, associated with the transformation latent heat and it is related to the variation in the martensitic volume fraction. For the SMAs subjected to dynamic loading conditions, equation (2.16) should be solved simultaneously with the constitutive equation (2.1) to fully capture the thermomechanical response of the material.

The condition during phase transformation which guarantees the stress and temperature states to remain on the transformation surface is given by \( \dot{\Phi} = 0 \). Substituting (2.11) and (2.15) into this constraint, the evolution of the martensitic volume fraction is expressed as:

\[
\dot{\xi} = -\frac{(\Lambda + \Delta S : \sigma) : \dot{\sigma} + (\rho\Delta s_0)\dot{T}}{\rho\Delta s_0(M_s - M_f)}, \tag{2.17}
\]

for the forward transformation and as:

\[
\dot{\xi} = -\frac{(\Lambda + \Delta S : \sigma) : \dot{\sigma} + (\rho\Delta s_0)\dot{T}}{\rho\Delta s_0(A_s - A_f)}, \tag{2.18}
\]

for the reverse transformation. Substituting (2.17) into (2.16) and assuming \( \Delta\alpha = \Delta c = 0 \), which is valid in almost all practical cases, the following expression is obtained as the second constitutive equation for the forward phase transformation:

\[
-\frac{1}{D_{fwd}}(-Y + \rho\Delta s_0 T)(\Lambda + \Delta S : \sigma) : \dot{\sigma} + [\rho c - \frac{\rho\Delta s_0}{D_{fwd}}(-Y + \rho\Delta s_0 T)]\dot{T} = -\text{div}(q) + \rho\hat{g}, \tag{2.19}
\]
and similarly for the reverse transformation, the second constitutive equation is obtained as:

\[
- \frac{1}{D_{rev}} (Y + \rho \Delta s_0 T) (\Lambda + \Delta S : \sigma) : \dot{\sigma} + \rho c \Delta s_0 (Y + \rho \Delta s_0 T) \dot{T} = - \text{div}(q) + \rho \ddot{g},
\]

where \(D_{fwd} = \rho \Delta s_0 (M_s - M_f)\) and \(D_{rev} = \rho \Delta s_0 (A_s - A_f)\).

Equations (2.1) and (2.19) for the forward phase transformation and Equations (2.1) and (2.20) for the reverse phase transformation are the constitutive equations of SMAs. They capture a strong coupled relationship between the stress, strain and temperature as the thermo-mechanical terms of the material before, during and after the phase transformation and thus can describe the full thermo-mechanical response of SMAs.

### 2.2.1 Coupled Constitutive Relations For The Combined Tension-Torsion Loading

The general 3-D constitutive relations introduced in the previous section can be reduced to two sets of constitutive equations (one set for the forward phase transformation and the other one for the reverse phase transformation) for the case when a rod is under combined axial-torsional loading and unloading. In the case of prismatic circular rods, due to Saint-Venant’s formulation for torsion and with the assumption of no warpage in the cross section, we can assume that the shear strain varies linearly from the central axis toward the outer radius. On the other hand, normal or axial strain is considered constant throughout the cross section. In this case, the stress
tensor has the following form:

\[
\sigma = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \tau_{\theta z} \\ 0 & \tau_{\theta z} & \sigma_{zz} \end{pmatrix},
\]  

(2.21)

where \(\tau_{\theta z}\) and \(\sigma_{zz}\) represent the shear stress and axial stress, respectively. The deviatoric stress tensor could be written as:

\[
\sigma' = \begin{pmatrix} -\frac{\sigma_{zz}}{3} & 0 & 0 \\ 0 & -\frac{\sigma_{zz}}{3} & \tau_{\theta z} \\ 0 & \tau_{\theta z} & \frac{2\sigma_{zz}}{3} \end{pmatrix}.
\]  

(2.22)

The effective stress \(\bar{\sigma}\) for this case is reduced to:

\[
\bar{\sigma} = \sqrt{\sigma_{zz}^2 + 3k^2_\theta \tau_{\theta z}^2}.
\]  

(2.23)

The transformation tensor is expressed as:

\[
\Lambda^t_{\text{fwd}} = \frac{3H}{2\sqrt{\sigma_{zz}^2 + 3k^2_\theta \tau_{\theta z}^2}} \begin{pmatrix} -\frac{\sigma_{zz}}{3} & 0 & 0 \\ 0 & -\frac{\sigma_{zz}}{3} & k^2_\theta \tau_{\theta z} \\ 0 & k^2_\theta \tau_{\theta z} & \frac{2\sigma_{zz}}{3} \end{pmatrix},
\]

\[
\Lambda^t_{\text{rev}} = \frac{1}{\xi^{t-r}} \begin{pmatrix} \epsilon^{t-r}_{rr} & 0 & 0 \\ 0 & \epsilon^{t-r}_{\theta\theta} & k_\kappa \epsilon^{t-r}_{\theta z} \\ 0 & k_\kappa \epsilon^{t-r}_{\theta z} & \epsilon^{t-r}_{zz} \end{pmatrix}.
\]  

(2.24)

where \(\epsilon_{\theta z}, \epsilon_{zz}, \epsilon^{t-r}_{\theta z}\) and \(\epsilon^{t-r}_{zz}\) are the shear strain, axial strain, transformation shear strain at the reversal and the axial strain at the reversal, respectively. In Equation
(2.24), \( \Lambda_{\text{fwd}}^t \) is the transformation direction tensor during forward transformation and 
\( \Lambda_{\text{rev}}^t \) is the form during reverse. Substituting Equation (2.24) into Equations (2.15) 
and (2.13) and using the following relation between the constitutive model parameters 
\[
\rho \Delta u_0 + \mu_1 = \frac{1}{2} \rho \Delta s_0 (M_s + A_f), \quad \rho \Delta s_0 (A_f - M_s), \quad \mu_2 = \frac{1}{4} (\rho b^A - \rho b^M), \\
\rho b^A = -\rho \Delta s_0 (A_f - A_s), \quad \rho b^M = -\rho \Delta s_0 (M_s - M_f) 
\] (2.25) 

explicit expressions for the martensitic volume fraction in forward and reverse phase 
transformation are then obtained as:

\[
\xi_{\text{fwd}} = \frac{1}{\rho b^M} \left[ \sqrt{\sigma_{zz}^2 + 3k_s^2 \tau_{\theta z}^2 H} + \frac{1}{2} (\sigma_{zz}^2 \Delta S_{44} + \sigma_{zz}^2 \Delta S_{33}) + f_{\text{fwd}}(T) \right], 
\] (2.26) 

\[
\xi_{\text{rev}} = \frac{1}{\rho b^A} \left[ \frac{1}{\xi_{\text{fwd}}} (2k_s k_e \tau_{\theta z} \epsilon_{\theta z}^r + \sigma_{zz} \epsilon_{zz}^r) + \frac{1}{2} (\tau_{\theta z}^2 \Delta S_{44} + \sigma_{zz}^2 \Delta S_{33}) 
\right. \\
\left. + f_{\text{rev}}(T) \right], 
\] (2.27) 

where:

\[
f_{\text{fwd}}(T) = \rho \Delta c \left[ (T - T_0) - T \ln \left( \frac{T}{T_0} \right) \right] + \rho \Delta s_0 (T - M_s), 
\] (2.28) 

\[
f_{\text{rev}}(T) = \rho \Delta c \left[ (T - T_0) - T \ln \left( \frac{T}{T_0} \right) \right] + \rho \Delta s_0 (T - A_f), 
\] (2.29) 

In Equations (2.26) and (2.27), \( \Delta S_{33} = \frac{1}{E_M} - \frac{1}{E_A} \) and \( \Delta S_{44} = \frac{1}{G_M} - \frac{1}{G_A} \), where \( E \) 
and \( G \) are the Young’s modulus and shear modulus, respectively. The parameters 
\( M_s \) and \( A_f \) are the martensitic start and austenitic finish temperatures, respectively 
and the superscripts \( \text{fwd} \) and \( \text{rev} \) represent forward and reverse transformations. By 
substituting the explicit expressions of the martensitic volume fractions, Equations 
(2.26) and (2.27), into Equation (2.4) and integrating from zero to an arbitrary pseudo 
time, the transformation strain can be calculated. The constitutive Equations (2.1)
and (2.19) for the forward transformation is now reduced to three algebraic expressions as:

\[
\epsilon_{\theta z} = \frac{1 + \nu}{E_A + \xi(E_M - E_A)} \tau_{\theta z} + \frac{3k_s H \tau_{\theta z}}{2k_e \sqrt{\sigma_{zz}^2 + 3k_s^2 \tau_{\theta z}^2}} \xi_{fwd},
\]

(2.30)

\[
\epsilon_{zz} = \frac{1}{E_A + \xi(E_M - E_A)} \sigma_{zz} + \frac{H \sigma_{zz}}{\sqrt{\sigma_{zz}^2 + 3k_s^2 \tau_{\theta z}^2}} \xi_{fwd} + \alpha(T - T_0),
\]

(2.31)

\[
- \frac{1}{D_{fwd}}(-Y + \rho \Delta s_0 T) \left\{ \left[ \frac{3Hk_s^2}{\sqrt{\sigma_{zz}^2 + 3k_s^2 \tau_{\theta z}^2}} + \Delta S_{44} \right] \tau_{\theta z} + \frac{H}{\sqrt{\sigma_{zz}^2 + 3k_s^2 \tau_{\theta z}^2}} \xi_{fwd} \right\} \dot{\tau}_{\theta z} + \left[ \Delta S_{33} \sigma_{zz} \dot{\sigma}_{zz} \right] \dot{\sigma}_{zz} = -\text{div}(q) + \rho \dot{g},
\]

(2.32)

and for the reverse transformation, the constitutive equations are:

\[
\epsilon_{\theta z} = \frac{1 + \nu}{E_A + \xi_{rev}(E_M - E_A)} \tau_{\theta z} + \frac{\epsilon_{\theta z}^{t-r}}{\xi_{t-r} \xi_{rev}},
\]

(2.33)

\[
\epsilon_{zz} = \frac{1}{E_A + \xi_{rev}(E_M - E_A)} \sigma_{zz} + \frac{\epsilon_{zz}^{t-r}}{\xi_{t-r} \xi_{rev}} + \alpha(T - T_0).
\]

(2.34)

\[
- \frac{1}{D_{rev}}(Y + \rho \Delta s_0 T) \left\{ \left[ 2k_s k_e \epsilon_{\theta z}^{t-r} \xi_{t-r} + \Delta S_{44} \tau_{\theta z} \right] \dot{\tau}_{\theta z} + \left[ \epsilon_{zz}^{t-r} \xi_{t-r} + \Delta S_{33} \sigma_{zz} \right] \dot{\sigma}_{zz} \right\} + \left[ \rho c - \frac{\rho \Delta s_0}{D_{fwd}} (Y + \rho \Delta s_0 T) \right] \dot{T} = -\text{div}(q) + \rho \dot{g},
\]

(2.35)

where \( \nu \) is Poisson's ratio and is assumed to be the same for both phases. Since there is no internal heat generation source like Joule heating, assuming \( \dot{g} = 0 \) is acceptable. Also due to Fourier’s law of thermal conduction and for a cylindrical element, we can take \( \text{div}(q) = -k \left( \frac{\partial T}{\partial r} + \frac{1}{r} \frac{\partial T}{\partial r} \right) \), where \( r \) is the radius of the annular element in which the constitutive equations are studied. As shown in Equations (2.32) and (2.35), both temperature and stress components are functions of time and radius. Thus, it is necessary to define initial and boundary conditions for the problem. As initial
conditions we prescribe temperature and stress distribution at $t = 0$ as:

$$T(r, 0) = T_{\infty}, \tau_{\theta z}(r, 0) = 0, \sigma_{zz}(r, 0) = 0, \quad (2.36)$$

where $T_{\infty}$ is the ambient temperature. Due to convection at the surface of the rod and axi-symmetric distribution of the temperature throughout the cross section, the boundary conditions at the surface and the center of the rod can be defined as:

$$k \frac{\partial T(r, t)}{\partial r}|_{r=R_o} = h[T_{\infty} - T(R_o, t)], \quad k \frac{\partial T(r, t)}{\partial r}|_{r=0} = 0, \quad (2.37)$$

where $h$ is the heat convection coefficient and $R_o$ is the rod radius.

**Model parameters identification**

Given these constitutive relations, the following model parameters must be calibrated: (i) the thermoelastic parameters of martensite and austenite ($E_M, E_A, G_M, G_A, \nu, \alpha$), (ii) the maximum transformation strain $H$, (iii) the material thermal parameters ($\rho c, k$) and (iv) five additional model parameters ($\rho \Delta s_0, \rho \Delta u_0, \mu_1, \mu_2, Y$) that are characteristic of the martensitic transformation. These are listed in Table 2.1. Also listed are the common material properties that should be used to calibrate the model. The elastic constants can be calculated directly from isothermal stress-strain curves where loads are applied at temperatures below the transformation regions. The parameter $H$ is calibrated from a stress-strain curve of a uniaxial test in which the forward transformation has completed. The remaining parameters are calibrated by considering the conditions under which the two transformations (forward and reverse) begin and end in a stress-temperature space which results in the relations presented in Equation (2.25).
Table 2.1: Required model parameters and associated material parameters

<table>
<thead>
<tr>
<th>Model parameters</th>
<th>Common SMA material properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_A, E_M, G_A, G_M, \nu, \alpha$</td>
<td>$E_A, E_M, \nu, \alpha$</td>
</tr>
<tr>
<td>$H$</td>
<td>$H$</td>
</tr>
<tr>
<td>$\rho \Delta s_0, \rho \Delta u_0, \mu_1, \mu_2, Y$</td>
<td>$M_s, M_f, A_s, A_f, C^M, C^A$</td>
</tr>
<tr>
<td>$k_s, k_c$</td>
<td>-</td>
</tr>
</tbody>
</table>

2.3 Implementation: time-discretization and solution algorithms

Constitutive Equations (2.30), (2.31) and (2.32) for the forward transformation and Equations (2.33), (2.34) and (2.35) for the reverse transformation along with the initial and boundary conditions of (2.36) and (2.37) must be solved simultaneously when transformation is occurring in the material. Solving such equations is computationally expensive using implicit schemes. Instead, an iterative approach based on the finite difference method is implemented as a MATLAB code for solving the highly nonlinear governing equations. The radius of the rod (or tube) is divided into $M$ equal segments of size $\Delta r$ as shown in Figure 2-1.

The total twist angle $\theta$ and axial displacement $\Delta L$ are considered as inputs. These inputs as loading parameters are discritized in a way to be applied during $N$ identical steps. Thus, the shear and axial strain components for the $ith$ annular region at the $jth$ time increment can be expressed as:

$$\epsilon_{\theta z i}^j = \frac{r_i \theta_j}{2L},$$  \hspace{1cm} (2.38)
Figure 2-1: Partitioning the rod cross section into a finite number of narrow annular regions

\[ \epsilon_{zz}^j = \frac{\Delta L_j}{L}, \]

where \(1 \leq i \leq M\) and \(1 \leq j \leq N\).

In Equations (2.38) and (2.39), \(L\), \(r_i\), \(\Delta L_j\) and \(\theta_j\) are length of the rod, the distance of the \(i\)th annular region from the axis of the rod, axial displacement and angle of twist in the \(j\)th time increment, respectively. During loading, after the strain components are calculated at each radial element, the material is first considered to be in austenitic elastic regime and temperature is held constant since no transformation has occurred yet. Thus, stress components are found as:

\[ \tau_{\theta z}^j = 2G_A \epsilon_{\theta z}^j, \]

\[ \sigma_{zz}^j = E_A \epsilon_{zz}^j. \]

Then, the martensitic volume fraction \(\xi_{\text{fwd}}^j\) is computed at the element using equation (2.26). If the transformation has started \((0 < \xi_{\text{fwd}}^{ij} < 1)\) the Equations
(2.30), (2.31) and (2.32) would be valid. The finite difference form of the Equation (2.32) is: (see [52] for details)

\[
-\frac{1}{D_{wd}}(Y + \rho \Delta s_0 T_i^{j-1})\{[\frac{3k_s^2 H}{\sqrt{(\sigma_{zz_i} j-1)^2 + 3k_s^2(\tau_{\theta z_i} j-1)^2}}] + \Delta S_{44}\tau_{\theta z_i} j-1 \tau_{\theta z_i} j-1 \Delta t \nonumber
\]

\[+ \frac{H}{\sqrt{(\sigma_{zz_i} j-1)^2 + 3k_s^2(\tau_{\theta z_i} j-1)^2}} + \Delta S_{33}\sigma_{zz_i} j-1 \sigma_{zz_i} j-1 \Delta t\}\} + [\rho c - \frac{\rho \Delta s_0}{D_{wd}}(Y + \nonumber
\]

\[\rho \Delta s_0 T_i^{j-1})] \frac{T_i^j - T_i^{j-1}}{\Delta t} = k[(r_i + \frac{\Delta r}{2}) T_i^{j-1} - T_{i+1}^{j-1} - \nonumber
\]

\[r_i (\Delta r)^2] \nonumber \]

where \(1 < i < M\) and \(\Delta t\) is the time increment. For calculating the finite difference approximation of the boundary conditions (central and outer nodes) the heat balance for the associated control volumes should be considered. For the central node \(i = 1\), consider a control volume with radius \(\Delta r/2\). The finite difference approximation of the boundary condition in this node is obtained as [52]:

\[
kT_i^{j-1} - T_i^{j-1} = \frac{1}{8}(\Delta r)^2 \kappa_i^{j-1} = \frac{1}{8}(\Delta r)\rho c \frac{T_i^j - T_i^{j-1}}{\Delta t}, \tag{2.43}
\]

and for the outer node \(i = M\) with the convection boundary condition, assuming a cylindrical volume with the inner radius \(R_o - \Delta r/2\) and outer radius \(R_o\) results in:

\[
R_o h(T_{\infty} - T_M^{j-1}) + k(R_o - \frac{\Delta r}{2}) T_M^{j-1} - T_M^{j-1} \frac{\Delta r}{2} + [R_o \Delta r - \frac{(\Delta r)^2}{4}] \kappa_M^{j-1}
\]

\[= \frac{R_o \Delta r}{2} - \frac{(\Delta r)^2}{4} \rho c \frac{T_M^j - T_M^{j-1}}{\Delta t}, \tag{2.44}
\]

where \(\kappa_i^{j-1}\) and \(\kappa_M^{j-1}\) are the equivalent internal heat generation due to phase trans-
formation calculated at the central and outer nodes as [52]:

\[
\kappa^j_i = -\frac{1}{D^\text{fwd}}(-Y + \rho\Delta s_0 T_i^{j-1})\left\{\frac{3k_h^2 H}{\sqrt{(\sigma_{zz}^{j-1})^2 + 3k_h^2(\tau_{zz}^{j-1})^2}} + \Delta S_{44}\right\}
\]

\[
\tau_{\theta z_i}^{j-1} = \frac{\tau_{\theta z_i}^j - \tau_{\theta z_i}^{j-1}}{\Delta t} + \left[\frac{H}{\sqrt{(\sigma_{zz}^{j-1})^2 + 3k_h^2(\tau_{zz}^{j-1})^2}} + \Delta S_{33}\right] \sigma_{zz}^{j-1} - \sigma_{zz}^{j-1} \frac{\Delta S_{44}}{\Delta t}
\]

\[
+ \left[-\rho\Delta s_0 D^\text{fwd}(-Y + \rho\Delta s_0 T_i^{j-1})\right] \frac{T_i^j - T_i^{j-1}}{\Delta t}.
\]

When the transformation is completed \((\xi_{ij}^{\text{fwd}} = 1)\), stresses would be expressed as:

\[
\tau_{\theta z_i}^j = \tau_{\theta z_i}^f + \frac{G_MT_i(\theta^j - \theta^f)}{L},
\]

\[
\sigma_{zz}^{j} = \sigma_{zz}^f + \frac{E_M(\Delta L^j - \Delta L^f)}{L},
\]

where, \(\tau_{\theta z_i}^f, \sigma_{zz}^f, \theta^f\) and \(\Delta L^f\) are the shear stress, normal stress, angle of twist and axial displacement at the \(i\)th annular region when the forward phase transformation is completed. At each step of loading, the cross section is divided into three regions based on the transformation status: Region I, in which the material is completely in the austenite phase, Region II where the transformation is occurring and Region III, in which the phase transformation is completed and the material is in martensite phase. The martensitic volume fraction at the end of loading for the \(i\)th annular element \(\xi_{iN}^{\text{fwd}}\) would be considered as the martensitic volume fraction at the reversal \(\xi_i^{r} \) and will consequently be used in the unloading of the element. One of the main benefits of the present method is the ability to capture different transformation reversal status at various radial points. This results in the accuracy of the model in predicting the unloading behavior of the material, as well as the loading.

In the unloading of the rod, all the points inside the elastic region of the final loading step will unload elastically. For any point outside the elastic core with a
reversal martensitic volume fraction of 0 < ξ_{i}^{t-r} < 1, an elastic unloading with rates of \( G_{eff} = G_{A} + \xi_{i}^{t-r}(G_{M} - G_{A}) \) and \( E_{eff} = E_{A} + \xi_{i}^{t-r}(E_{M} - E_{A}) \) is first assumed. Then, the martensitic volume fraction \( \xi_{i}^{rev} \) is computed at the element using Equation (2.27). If the reverse transformation has started \( \xi_{i}^{rev} < \xi_{i}^{t-r} \), the stress components and temperature must be updated using Equations (2.33), (2.34) and (2.35). The finite difference form of Equation (2.35) is given by:

\[
\frac{1}{D^{rev}}(Y + \rho \Delta s_{0}T_{i}^{j-1})\{[2k_{s}k_{e}^{t-r} \xi_{i}^{t-r} + \Delta S_{44}\tau_{\theta z_{i}}j-1] \frac{\tau_{\theta z_{i}}j - \tau_{\theta z_{i}}j-1}{\Delta t} + [\frac{\xi_{i}^{t-r}}{\xi_{i}^{t-r}} \\
+ \Delta S_{33}\sigma_{zz_{i}}j-1] \frac{\sigma_{zz_{i}}j - \sigma_{zz_{i}}j-1}{\Delta t} \} + \rho c - \frac{\rho \Delta s_{0}}{D^{rev}}(Y + \rho \Delta s_{0}T_{i}^{j-1})\frac{T_{i}^{j} - T_{i}^{j-1}}{\Delta t} = k_{i}(r_{i} + \frac{\Delta r}{2}) \frac{T_{i+1}^{j-1} - T_{i}^{j-1}}{r_{i}(\Delta r)^{2}} - (r_{i} - \frac{\Delta r}{2}) \frac{T_{i}^{j-1} - T_{i-1}^{j-1}}{r_{i}(\Delta r)^{2}}, \tag{2.48}
\]

where 1 < i < M. For the central and outer nodes (i = 1 and i = M), Equations (2.43) and (2.44) can be used. The equivalent internal heat generation \( \kappa_{i}^{j} \), instead of Equation (2.45) should be calculated as:

\[
\kappa_{i}^{j} = -\frac{1}{D^{rev}}(Y + \rho \Delta s_{0}T_{i}^{j-1})\{[2k_{s}k_{e}^{t-r} \xi_{i}^{t-r} + \Delta S_{44}\tau_{\theta z_{i}}j-1] \frac{\tau_{\theta z_{i}}j - \tau_{\theta z_{i}}j-1}{\Delta t} + [\frac{\xi_{i}^{t-r}}{\xi_{i}^{t-r}} \\
+ \Delta S_{33}\sigma_{zz_{i}}j-1] \frac{\sigma_{zz_{i}}j - \sigma_{zz_{i}}j-1}{\Delta t} \} + \rho c - \frac{\rho \Delta s_{0}}{D^{rev}}(Y + \rho \Delta s_{0}T_{i}^{j-1})\frac{T_{i}^{j} - T_{i}^{j-1}}{\Delta t}. \tag{2.49}
\]

When the reverse transformation is completed (\( \xi_{i}^{rev} = 0 \)), shear and axial stresses are calculated from Equations (2.40) and (2.41).

In many applications, it is necessary to calculate the response of the rod (or tube) with respect to the applied torque and force. For this purpose the following expressions can be used for calculating the required torque (M) and force (F) for producing a specific twist angle and axial displacement as:

\[
M(j) = 2\pi \int_{R_{i}}^{R_{o}} \tau_{\theta z}r^{2}dr = 2\pi \Delta r \sum_{i=1}^{M} \tau_{\theta z_{i}}r_{i}^{2}, \tag{2.50}
\]

41
\[
F(j) = 2\pi \int_{R_i}^{R_o} \sigma_{zz} r dr = 2\pi \Delta r \sum_{i=1}^{M} \sigma_{zzj} r_i,
\] (2.51)

where \( R_i \) and \( R_o \) are the inner and outer radii of the tube.
Chapter 3

Results: Evaluation and discussion

Two sets of experiments are conducted on NiTi tubular specimens to evaluate the performance of the presented modeling approach in predicting the SMA behavior. The aim of the first set is to investigate the isothermal quasi-static loading conditions and the second set is carried out under dynamic loading states. As will be discussed later, the dynamic tests are done on smaller samples due to limitations with the experimental setup. Tests were done using an electro-mechanical testing machine (BOSE ElectroForce 3330) equipped with temperature-controlled environmental chamber (Applied Test Systems). An infrared camera (Micro Epsilon model #2) recorded the evolution of the specimen surface temperature during the dynamic tests. The NiTi samples were provided by Johnson Matthey and they were fixed in a custom grip setup with ER-11 collets to hold the specimens in place.

3.1 Tests with isothermal loading conditions

The diameter, thickness and length of the specimen I used for the isothermal tests are $d_{ext} = 4.5$ mm, $t = 0.3$ mm and $L = 14$ mm, respectively. In order to stabilize the stress-strain behavior of the SMA tube, a series of 20 load/unload tension cycles was conducted at a strain rate of $\dot{\varepsilon} = 0.00023/s$ and at a constant temperature of $45^\circ C$. The strain rate was slow enough to prevent self-heating of the specimen and
thus guarantee the isothermal condition. Three uni-axial characterization tests were then performed at $T = 20^\circ C$, $T = 35^\circ C$ and $T = 45^\circ C$ and results were used for calibration of the phase diagram properties based on tangent intersection method (see [51] for the details of this method). The material parameters calibrated from these experiments are listed in Table 3.1. Figures 3-1(a), (b) and (c) compare the model prediction with experimental data at the temperatures $T = 20^\circ C$, $T = 35^\circ C$ and $T = 45^\circ C$, respectively (see [53] for details about the material properties calibration of NiTi).

Table 3.1: Material properties for the NiTi tube specimen I calibrated from the pure tension tests.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_A$</td>
<td>$20.0 \times 10^3$</td>
<td>MPa</td>
</tr>
<tr>
<td>$E_M$</td>
<td>$10.0 \times 10^3$</td>
<td>MPa</td>
</tr>
<tr>
<td>$M_f$</td>
<td>$-32.0$</td>
<td>$^\circ C$</td>
</tr>
<tr>
<td>$M_s$</td>
<td>$-15.0$</td>
<td>$^\circ C$</td>
</tr>
<tr>
<td>$A_s$</td>
<td>$0$</td>
<td>$^\circ C$</td>
</tr>
<tr>
<td>$A_f$</td>
<td>$10.0$</td>
<td>$^\circ C$</td>
</tr>
<tr>
<td>$C_M$</td>
<td>$8.3$</td>
<td>Mpa/$^\circ C$</td>
</tr>
<tr>
<td>$C_A$</td>
<td>$7.5$</td>
<td>Mpa/$^\circ C$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>$0.33$</td>
<td>-</td>
</tr>
<tr>
<td>$H$</td>
<td>$0.03$</td>
<td>-</td>
</tr>
</tbody>
</table>
Figure 3-1: Comparison of the model’s prediction with the experimental data. Isothermal uniaxial stress-strain responses of specimen I at temperatures $T = 20^\circ C$, $T = 35^\circ C$ and $T = 45^\circ C$. These uniaxial tension tests are used to calibrate the model parameters.

**Isothermal pure torsion:**

Pure torsion tests were conducted on the same specimen without any additional training and at three different temperatures to evaluate the capability of the approach in capturing the shear response of an SMA tube. The strain rate was $\dot{\gamma} = 0.0001/\text{s}$ to simulate an isothermal loading condition. The torsion was applied to the tube
while one end of the specimen was axially fixed and the other end was free. The experimental shear stress-strain response of the tube along with the corresponding uniaxial data at $T = 20^\circ$C was first used to find the effective coefficients of $k_s$ and $k_e$. These coefficients are found through equations 2.6 and 2.7 as $k_s = 0.52$ and $k_e = 1.44$. Figure 3-2 shows the comparison between the model’s prediction and experiment for the pure torsion response at $T = 20^\circ$C after calibration of $k_s = 0.52$ and $k_e = 1.44$.

![Figure 3-2: Comparison of the model’s prediction with the experimental data for the isothermal pure torsion of specimen I at $T = 20^\circ$C with $k_s = 0.52$ and $k_e = 1.44$. Calibration has been done at this temperature.](image)

The model was then used to predict the shear response of the tube at two higher temperatures of $T = 35^\circ$C and $T = 45^\circ$C. Figures 3-3(a) and 3-3(b) compare the model’s prediction with the experimental response at these two temperatures.
In order to see how implementation of the stress/strain effective coefficients of \( k_s \) and \( k_e \) can improve the performance of the model, a comparison is made between the shear response of the proposed modified model, original Mises based model and experiment at \( T = 35^\circ C \). As depicted in figure 3-4, the modification proposed in this work has significantly improved the functionality of the model. It is worth noting that the calibration of \( k_s \) and \( k_e \) has been done at a different temperature (20°C).
Figure 3-4: Comparison of the modified model, original Mises model and experiment for the pure torsion of specimen I at $T = 35^\circ C$.

**Isothermal combined loading paths in the tension-torsion subspace:**

In the following, the material response to different combined tension-torsion tests is reviewed. Here, special attention is made to the loading sequence and the path dependence of the specimen material. All experiments are carried out under macroscopically isothermal conditions with a testing temperature of $T = 20^\circ C$.

The strain history imposed on the specimen during a proportional tension-torsion experiment is shown in figure 3-5(a). The axial strain $\varepsilon$ is increased at a constant rate from 0 to 3.5% in 100 s, while the shear strain $\gamma$ is increased at a constant rate from 0 to 4.2 % in the same time period. These strains are then linearly reduced to zero, in another 100 s. Predictions of the axial stress vs. axial strain, and shear stress versus shear strain from the proposed model are compared against corresponding experimental measurements in figures 3-5(b) and 3-5(c), respectively. The measured stress-strain response in the tension-torsion experiment is well-approximated by the model. A comparison is made between the shear response of the modified model and the original Mises based model in figure 3-6 to better demonstrate the importance of
the applied modifications.

Figure 3-5: Comparison of the model’s prediction with the experimental data. Isothermal proportional tension-torsion response at temperature of $T = 20^\circ C$ for specimen I.
Figure 3-6: Comparison of the modified model, original Mises model and experiment for the shear response of specimen I under proportional tension-torsion loading at $T = 35^\circ C$.

The strain pattern imposed on the specimen I during a non-proportional box shape tension-torsion experiment is depicted in figure 3-7(a). As indicated by arrows, first the axial strain is increased at a constant rate from 0 to 3.6% in 100 s, while the shear strain is maintained at zero. After this, the shear strain is linearly increased from zero to 4.2% in 100 s, while the axial strain is held at 3.6%. Then, axial strain is unloaded in 100 s, while the shear strain is maintained constant. Finally, the shear strain is reduced to zero in another 100 s, while the axial strain is zero. Stress-strain response of the tube in the axial and shear directions are shown in figures 3-7(b) and 3-7(c), respectively.
Figure 3-7: Comparison of the model’s prediction with the experimental data. Isothermal non-proportional box tension-torsion response at temperature of $T = 20^\circ C$ for the specimen I.

A triangular non-proportional strain path is imposed on specimen I as depicted in figure 3-8(a). First, axial strain is increased at a constant rate from zero to 3.6% in 100 s, while the shear strain is maintained at zero. After this, the shear strain is linearly increased from 0 to 4.2% in 100 s, while the tensile strain is maintained at
3.6%. Next, the shear strain is linearly reduced from to zero again in 100 s, while maintaining the tensile strain. Finally, the tensile strain is linearly reduced to zero in another 100 s, while maintaining the shear strain at zero. Stress-strain response of the sample are shown in figures 3-8(b) and 3-8(c) for the axial and shear directions, respectively.

For a better understanding of the effective response of the material, the measured equivalent stress-strain response of the tube is compared against the model’s prediction in figure 3-9 for the triangular loading history depicted in 3-8(a). The equivalent stress and strain are defined by:

\[
\sigma_{eq} = \sqrt{\sigma^2 + 3k_s^2 \tau^2}, \quad \varepsilon_{eq} = \sqrt{\varepsilon^2 + \frac{k_s^2}{3} \gamma^2}
\] (3.1)

Significant variations in the equivalent stress-strain curve is observed when the loading path changes. The model is shown to be able to predict this phenomenon.
Figure 3-8: Comparison of the model’s prediction with the experimental data. Isothermal non-proportional triangular tension-torsion loading at temperature of $T = 20^\circ C$ for specimen I.
3.2 Tests with dynamic loading conditions

Specimen II with the external diameter of \( d_{\text{ext}} = 1.5 \text{ mm} \), wall thickness of \( t = 0.085 \text{ mm} \) and length of \( L = 33.5 \text{ mm} \) was selected for the second set of experiments which are designed to study the performance of the model in dynamic simulations. In order to stabilize the stress-strain behavior of the SMA tube, a series of 20 axial load-unload cycles were conducted at a strain rate of 0.0001/s and at a constant temperature of \( T = 23.5 \degree \text{C} \).

A set of isothermal uniaxial data was used to calibrate the model parameters for the specimen II from the same method used for specimen I. The adopted material parameters for this sample are listed in Table 3.2. Figure 3-10 displays the model prediction against the experimental response of a uniaxial loading case at \( T = 24\degree \text{C} \) with a very slow loading rate which implies an isothermal condition.
Table 3.2: Material properties for the NiTi tube specimen II calibrated in the isothermal condition and used for the dynamic simulations.

<table>
<thead>
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</tr>
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<td>Mpa/°C</td>
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<td>-</td>
</tr>
<tr>
<td>$H$</td>
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</tr>
</tbody>
</table>

Figure 3-10: Comparison of the model’s prediction with the experimental data for the isothermal uniaxial stress-strain response at $T = 24$°C conducted on specimen II.

For the specific heat and thermal conductivity, we use the following values: $\rho c =$
2.6 \times 10^6 \text{ J/m}^3\text{K} \text{ and } k = 18 \text{ W/(mK)}. These adopted values are for a general NiTi recently reported in [52]. Both the inner and outer surfaces of the tube are subjected to free convection by air. In the numerical simulations, both the inner and outer nodes are considered as the boundary nodes and the convection boundary condition 2.37 is imposed for both these nodes. The free convection coefficient for both surfaces is \( h = 10 \text{ W/m}^2\text{K} \) (see [48, 52] for calculation details).

In addition to the above parameters, the effective coefficients of \( k_s \) and \( k_e \) should be calibrated for the forward and reverse phase transformations. To this end, experimental shear stress-strain response of the tube along with the corresponding uniaxial data at \( T = 24^\circ \text{C} \) was used. Considering \( k_{sl} = 0.58 \) and \( k_{el} = 1.57 \) for the forward transformation and \( k_{su} = 0.58 \) and \( k_{eu} = 1.44 \) for the reverse transformation produce acceptable agreement between the experiment and model’s prediction in torsion. Figure 3-11 shows the comparison between model’s prediction and experiment for the pure torsion response at \( T = 24^\circ \text{C} \) after employing these parameters.

![Figure 3-11: Comparison of the model’s prediction with the experimental data for the isothermal pure torsion stress-strain response at \( T = 24^\circ \text{C} \) for specimen II.](image-url)
Dynamic uniaxial tensile test:

Two loading rates were considered corresponding to strain rates of $\dot{\varepsilon} = 3 \times 10^{-3}/s$ (fast) and $\dot{\varepsilon} = 9 \times 10^{-5}/s$ (slow) to experimentally observe the effect of loading rate on the mechanical response of the superelastic tube. As shown in figure 3-12, the transformation finish stresses and the slopes of the phase transformation plateaus increase with increasing strain rate. The model’s prediction for the stress-strain, temperature-strain and temperature-time responses are compared with the experimental data corresponding to the high strain rate of $\dot{\varepsilon} = 3 \times 10^{-3}/s$ in figures 3-13(a), 3-13(b) and 3-13(c), respectively. As the model predicts, the temperature of the material begins to increase at the beginning of the forward phase transformation. At the beginning of the unloading and before the beginning of reverse transformation, the temperature decreases because of free convection. During reverse phase change, temperature rapidly decreases, sometimes below ambient depending on the loading rate and condition. Finally, during the last unloading elastic region, the temperature tends to equalize the surrounding environment.

Figure 3-12: Evolution of the mechanical response at different loading rates. Experiments are conducted on specimen II.
Figure 3-13: Comparison of the model’s prediction with the experimental data. Uniaxial response at room temperature with $\dot{\varepsilon} = 3 \times 10^{-3}/s$ for specimen II.
Dynamic pure torsion test:

A high-speed pure torsion test was conducted to study the capability of the approach in capturing the torsional response of the SMA tube. A 90 degree rotation with the rate of 10 degree/s was applied to the tube while one end of the specimen was fixed. This loading rate corresponds to the strain rate of $\dot{\gamma} = 4 \times 10^{-3} / s$. Figures 3-14(a) and 4-5(a) display the comparison between the shear stress-strain and temperature-time responses of the experiment and the model. The relatively large deviation observed in Figure 3-13(c) is thought to be due to the uncertain assumptions made to model the heat transfer between the specimen and environment.

![Shear stress-strain response](image1)

(a) Shear stress-strain response

![Temperature evolution](image2)

(b) Temperature evolution

Figure 3-14: Comparison of the model’s prediction with the experimental data. Pure torsion response at room temperature with $\dot{\gamma} = 4 \times 10^{-3} / s$ for specimen II.

Dynamic combined loading paths in the tension-torsion subspace:

In the following, the material response to different dynamic combined tension-torsion loading patterns is investigated and the capability of the model in capturing the thermomechanical coupled behavior of an SMA tube undergoing multi-axial loading conditions is evaluated. Here, special attention is paid to the loading sequence
and the path dependence of the specimen material.

The strain history applied on specimen II during a proportional tension-torsion loading is shown in figure 3-15(a). Temperature evolution of the tube due to this loading pattern is depicted in figure 3-15(b). Predictions of the axial stress-strain, and shear stress-strain from the proposed model are also compared against corresponding experimental measurements in figures 3-15(c) and 3-15(d), respectively. The measured stress-strain response in the tension-torsion experiment is well-approximated by the model.
Figure 3-15: Comparison between model’s predictions and experimental data for a proportional loading pattern ($\dot{\varepsilon} = 3 \times 10^{-3}/s$ and $\dot{\gamma} = 2.4 \times 10^{-3}/s$) conducted on specimen II.

A box shape non-proportional strain path as shown in figure 3-16(a) is imposed in a strain control test. As indicated by arrows, first the axial strain is increased, while the shear strain is maintained at zero. After this, the shear strain is linearly increased while the axial strain is held constant. Then axial strain is unloaded, while the shear strain is maintained constant. Finally, the shear strain is reduced to zero, while the axial strain is zero. Experimental results and model simulations are then compared.
Specifically, comparisons are provided for the temperature evolution in figure 3-16(b), axial stress-strain response in figure 3-16(c) and shear stress-strain response in figure 3-16(d).

![Proposed non-proportional strain path](image1) ![Temperature evolution](image2)

![Axial stress-strain response](image3) ![Shear stress-strain response](image4)

Figure 3-16: Comparison between model’s predictions and experimental data for a non-proportional box shape loading pattern ($\dot{\varepsilon} = 2.7 \times 10^{-3}/s$ and $\dot{\gamma} = 2.1 \times 10^{-3}/s$) conducted on specimen II.

The last simulated strain pattern is depicted in figure 3-17(a). First, axial strain is increased while the shear strain is maintained at zero. After this, the shear strain is linearly increased, while the tensile strain is kept constant. Next, the shear strain is linearly reduced to zero again, while still maintaining the tensile strain. Finally, the tensile strain is linearly reduced zero in another, while maintaining the shear strain at zero. The temperature evolution as well as the stress-strain responses of the sample
are shown in figures 3-17(b) to 3-17(d).

Figure 3-17: Comparison between model’s predictions and experimental data for a non-proportional triangular shape strain pattern ($\dot{\varepsilon} = 2.7 \times 10^{-3}/s$ and $\dot{\gamma} = 2.1 \times 10^{-3}/s$) conducted on specimen II.
Chapter 4

Numerical example; a combined tension-torsion SMA application

4.1 Introduction

In many of the current SMA based actuators, SMA wire or tube is subjected to simple uni-axial tension or pure torsion loading/unloading conditions. In these simple cases, the SMA element would provide a unique stress-strain hysteresis like profile which is associated with the force/torque requirement of the device at a constant temperature. There are however potential applications, in which the required force/torque profiles are more complex than simple hysteresis loops resulted from simple tension or torsion loading/unloading. In such actuators, using combined tension-torsion loading paths might be a solution to achieve and control a complicated pre-defined response. An ankle foot orthosis (AFO) is selected and further discussed in this chapter to show the capability of the proposed actuation technique.
4.2 Anke foot orthosis

Patients suffering from a certain neuromuscular disorder have a problem lifting their feet during walking. This condition is called “drop foot” and the AFO is the device usually used to address this irregularity. Currently, passive plastic AFOs are widely used to prevent the drop foot by inhibiting the ankle movement. Although these light orthoses prevent drop foot, walking is still difficult with them since they do not allow for ankle rotation, which is necessary for normal walking. In order to address this issue, researchers have developed active AFOs in which the impedance (stiffness) of the orthotic joint can be modulated throughout the walking cycle. Blaya et al. [54], developed a powered ankle-foot orthosis based on a series of elastic actuators. The basic idea of this device is to change the orthosis impedance (stiffness) actively. As a result, the AFO mimics the walking kinematic of a normal gait. This device includes a DC motor, mechanical links and springs and although it shows promising results in a lab environment, the actuator weighs 2.6 kg and requires bulky batteries and electronics for operation. Another active AFO which uses pneumatically powered lower limb exoskeleton was developed in the Human Neuromechanics Laboratory at the University of Michigan [55]. This AFO is actuated by McKibben muscles which are pneumatic actuators. One pneumatic actuator provides plantar flexion torque and a second actuator provides dorsiflexion torque. A control algorithm adjusts air pressure in each actuator independently. The study has shown promising results in gait rehabilitation, human motor adaptation and muscle activation. However, the applicability of these orthoses is limited to laboratory studies since on board power supplies and computers are required for their operation. SMA based active AFOs have been also studied in recent years by several research groups [56, 57, 58]. Although, these designs could provide the required motion during a gait cycle and prevent the drop foot, they practically failed due to several issues. The main problem reported was
dealing with lengthy and hardly controllable cooling of the embedded SMA elements.

### 4.3 Biaxial SMA actuator for AFO

A proposed active AFO currently under study, deploys a superelastic SMA hinge which its torsional stiffness could be controlled by applying an axial load via a linear actuator connected to the superelastic rotary rod. Due to the complex torque profile needed during the walking cycle, the hinge should undergo non-proportional combined tension-torsion loading/unloading patterns. Superelastic SMA is employed so that the AFO would capture energy during the powered plantarflexion (in stance phase) and then raise the foot in the dorsiflexion portion of swing phase as depicted in Figure 4-1. Figure 4-2 illustrates the overall mechanism of the design. SMA is loaded during the powered plantarfexion, storing the mechanical energy of the ankle. It will then raise the foot while releasing energy and recovery in dorsiflexion. The unloading may be either passive, relying on the superelastic behavior of a proper material, or active, relying on an external actuation.

![Biomechanics of ankle during a gait cycle](image)

**Figure 4-1:** Biomechanics of ankle during a gait cycle.
A typical passive AFO is a brace which constraints the motion of ankle during walking. Figure 4-3 depicts a passive SMA AFO. In this embodiment the SMA is a superelastic torsion hinge which connects the back brace to the foot brace. The SMA torsional hinge will load in torsion during the powered plantarflexion portion of the stance phase when the patient has the ability to move his/her ankle. The passive SMA AFO will then restore this energy during the swing dorsiflexion when the patient is unable to raise their foot by lifting foot brace.

A shortcoming of the passive SMA AFO is that the SMA stiffness in plantarflexion is higher than that in dorsiflexion. This means the foot has to apply more force/torque to load the SMA and also SMA is weaker in unloading when it should cause the foot to swing.
A novel idea to overcome this issue is to have an actuator undergoing both axial and torsion loading modes; one as the primary mode and the other as the secondary mode. While the primary state supplies the required force/torque of the device, the secondary mode controls the stiffness of the motion in the primary direction. In order to show this concept, a qualitative comparison is made between the torque response of a torsion mode SMA actuator and a coupled mode SMA actuator with the same size and material. The torsion actuator undergoes a simple pure torsion loading/unloading. But the coupled actuator undergoes a combined out of phase axial and torsional loading/unloading blocks. An axial loading is first applied to the SMA, causes the material to start transforming from the stiff austenite phase to the soft martensite phase prior to rotation. Thus the torsional stiffness is lower than a pure torsion mode, reducing the amount of torque required to rotate the actuator. When the axial load is removed in the next block, the SMA partially transforms backs to austenite, raises the torsional stiffness for the next unloading block in torsion. The torque angle responses of the two actuators are compared against each other in Figure 68.
4-4. Arrows in the plots show the direction of loading/unloading. In the torsion mode actuator, as expected from a normal SMA, the torque of the loading plateau is higher than the torque in unloading. But in the coupled mode actuator, the torsional loading occurs at a lower torque than unloading. This enables a robust control of the torsional response of the actuator and be employed for numerous applications.

Figure 4-4: Comparison of a passive torsion mode actuator and an active coupled mode actuator.

A proposed design for the combined mode AFO actuator is shown in Figure 4.3. The SMA rod is fixed to the actuator base at one end and is coupled with a linear actuator at the other end. The linear actuator rotates with the rotation of the arm connected to the bottom of the device, while it can apply axial displacement to the SMA rod when necessary. Figure 4-5(b) schematically shows the AFO when the SMA combined actuator is mounted.
Figure 4-5: An active SMA AFO in combined axial-torsional mode

Hansen et al. [59] studied the torque angle curves of the human ankle joint by doing motion lab analysis on able-bodied subjects. They reported that the torque angle response changes as the walking speed increases. The loading and unloading
portions of the moment versus angle curves show clockwise loop (hysteresis) at slow speeds that reduces to zero as the speed increases to normal speeds. Above the normal speeds, the loops start to traverse a counter-clockwise path. To mimic this behavior, a system with active components would be necessary.

A preliminary analytical study is conducted to investigate the capability of the proposed coupled actuation method in mimicking the real moment response of the ankle. The analytical platform discussed in Section 2 is employed to simulate a circular SMA rod subjected to combined axial-torsional loads. The rod has the diameter of 3.5 mm and length of 10 mm and all simulations are supposed to be done at the temperature of 20°C in which the SMA is initially in its austenitic phase. For the material properties, parameters listed in Table 3.1 are employed.

The moment versus angle curve of an SMA shows a clock-wise hysteresis loop when it is subjected to a pure torsion (Figure 4-6(a)). This response corresponds to the slow walking speeds (Figure 4-6(b)). As an extra axial load is being applied to the SMA (Figure 4-7(a), the stiffness of the component changes such that the hysteresis loop disappears. This kind of behavior would be correlated to the normal walking speed (Figure 4-7(b)). Finally, at high axial loads (Figure 4-8(a)), the hysteresis loop of the moment versus angle curve approaches to a counter-clockwise loop, which is identical to the ankle behavior at high walking speeds (Figure 4-8(b)).
(a) Strain history applied to the SMA: the SMA component is subject to a pure torsion

(b) Comparison of the experimental data against the modeling results of the coupled mode actuator for the ankle moment versus angle curves at slow walking speed (1.2m/sec)

Figure 4-6: An active SMA AFO in combined axial-torsional mode at the slow walking speed
(a) Strain history applied to the SMA; the SMA component is subject to torsion and a small axial strain of 1.5%

(b) Comparison of the experimental data against the modeling results of the coupled mode actuator for the ankle moment versus angle curves at normal walking speed (1.5m/sec)

Figure 4-7: An active SMA AFO in combined axial-torsional mode at the normal walking speed
(a) Strain history applied to the SMA; the SMA component is subject to torsion and the axial strain of 5%.

(b) Comparison of the experimental data against the modeling results of the coupled mode actuator for the ankle moment versus angle curves at fast walking speed (1.9m/sec).

Figure 4-8: An active SMA AFO in combined axial-torsional mode at the fast walking speed.
Chapter 5

Conclusions and future work

5.1 Conclusions

Shape memory alloys (SMAs) exhibit specific thermomechanical behaviors due to their ability to undergo martensitic transformation. Depending on working temperature and stress, SMAs exhibit various responses such as superelasticity, one way shape memory effect and two way shape memory effect. Among these properties, superelasticity which is the featured ability of SMAs to recover large amount of deformations and is widely used in biomedical devices, is studied in this work.

A 3-D constitutive model was developed for superelastic NiTi to capture the rate dependent non-Mises behavior of this material. General definitions for effective stress and strain are provided and modified flow rule and transformation tensor are subsequently introduced. The 3-D constitutive equations are derived for quasi-static isothermal loading conditions as well as dynamic loading states.

A semi-analytic approach and its implementation method are presented for the analysis of shape memory alloy tubes and rods with circular cross section subjected to simultaneous tension and torsion. A 2-D reduction of the developed polynomial SMA constitutive model is first obtained. Then, the cross section is divided into a finite number of narrow annular regions, and the loading is partitioned into a finite
number of increments. Appropriate assumptions are made in each region in order to find the equilibrium equations in terms of radial and axial displacements within the regions before, during and after the phase transformation. Considering the history of loading and the final values of transformation strain components, the unloading behavior of the material is also properly modeled.

Several set of mechanical tests were conducted to evaluate the developed platform. Comparing the model’s predictions against the experimental observations in pure torsion tests showed the capability of the formulation. The model is calibrated at one temperature and is used to predict the shear response at other temperatures. The model is also capable of predicting the SMA response under various proportional and non-proportional tension-torsion loading histories. The proposed method provides an efficient tool to design SMA elements subjected to complex loading cases.

Multiaxial loading is not only the real loading case in many applications, but it can also be used to design active SMA devices with adjustable stiffness. A novel SMA ankle foot orthosis was introduced and analytically studied by the developed model, in which the torsional stiffness could be adjusted by applying an external axial load in a non-proportional manner. The proposed orthosis is shown to be able to mimic the requisite complex shear response.

5.2 Future work

This work can be continued in different aspects. First, since the developed equations are appropriate for any geometry and loading case the model can be implemented in a finite element platform, more likely through a UMAT subroutine, in order to model general geometries and structures.

The focus of this work was on superelastic SMAs. However, the model can be extended to include the shape memory effect by defining an extra internal variable to
record the stress induced martensite. Furthermore, experiments could be conducted for the multiaxial behavior of SMAs in the shape memory regime.

Moreover, the introduced general platform can be further completed by including secondary effects of SMAs such as tension-compression asymmetry and cyclic response (ratcheting effect).
References


