Finite element analysis of shape memory alloy biomedical devices

Majid Tabesh

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A Thesis

entitled

Finite Element Analysis of Shape Memory Alloy Biomedical Devices

By

Majid Tabesh

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

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Dr. Mohammad H. Elahinia, Committee Chair

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Dr. Patricia Komuniecki, Dean
College of Graduate Studies

The University of Toledo

May 2010
Degradation of the bone, mainly as a result of osteoporosis, causes loosening of the screw-bone interface. This problem exists, for example, in pedicle screws that are widely used for the treatment of certain spine-related illnesses. As a result of bone degradation, the pull-out strength of pedicle screws hazardously diminishes. The conventional remedies such as using bone cement add their own problematic issues. This thesis is about developing a pedicle screw that mitigates these unwanted effects. The design and development of the so-called $SMArt^\text{TM}$ pedicle screw was described which utilizes the shape memory and superelasticity properties of NiTi alloys to expand itself in case its surrounding bone goes through osteoporosis.

The $SMArt^\text{TM}$ pedicle screw makes use of Niti wire-tube inserts wrapped around its body. The wire is inserted into the tube. The screw is implanted in the pedicle in a collapsed form. However, the tube extends the assembly while reaching to body temperature; therefore enhancing the purchase of the screw in the bone. Another feature of such a design is removability. The wire can be activated at a safe higher temperature to retract the assembly so that the screw can be easily removed.
A finite element (FE) model was developed to predict and evaluate the performance of the NiTi elements. This general model was implemented in COMSOL Multiphysics®. It was shown that this model can predict the thermomechanical behavior of shape memory alloys. The model can capture superelasticity, shape memory effect, partial transformation, and tension-compression asymmetry in SMAs and was validated against experimental results taken from the literature.

The FE model was consequently used to simulate the performance of shape memory NiTi inserts on the SMArt™ pedicle screw. The outcomes of the simulation suggest that the assembly can achieve the desired functionality of expansion and retraction. Consequently, a parametric analysis was conducted over the effect of different sizes of the wire and the tube. The geometry sizes for the first sample of this innovative pedicle screw were determined based on the results of this analysis.
Acknowledgements

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Besides my advisor, I would like to express my thanks to the rest of my thesis committee: Professor Vijay Goel, Dr. Ashok Biyani, and Professor Mehdi Pourazady, for their encouragement, insightful comments, and guidelines, upon whom the realization of the SMArt pedicle screw and the SMA model in COMSOL relies. I would also like to express my thanks to the faculty and staff of the M.I.M.E. department.

I thank my present and past fellow lab-mates in the Dynamic and Smart Systems Laboratory for all the learning, fun, and wonderful times we have had in the last two years. I offer my regards and blessings to all my Iranian friends at the University of Toledo, with whom I passed a memorable time. Their company was a remedy to my difficult times.

I would like to thank my family, whom I miss so much, my parents for their spiritual support and their long-distance love.
Last but not the least; thanks be to the Lord (S.W.T), the most companionate and the most merciful, for his bountiful Providence and perpetual mercy.
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Nomenclature

$E_{zz}^{tr}$ The component of the transformation strain in the axial (z) direction

$\dot{q}$ Heat generation per unit volume

$\dot{T}$ Rate of the change of temperature with respect to pseudo-time

$\Delta_H$ The overall deflection of the SM-SE assembly at high temperature.

$\Delta_L$ The overall deflection of the SM-SE assembly at low temperature.

$\varepsilon_{Ln}$ Maximum transformation strains in compression

$\varepsilon_{Lp}$ Maximum transformation strains in tension

$\sigma_{fn}^{cr}$ Critical stress for the finish of forward transformation in compression

$\sigma_{fp}^{cr}$ Critical stress for the finish of forward transformation in compression

$\sigma_{sn}^{cr}$ Critical stress for the stat of forward transformation in compression

$\sigma_{sp}^{cr}$ Critical stress for the stat of forward transformation in tension

$A$ Matrix containing the rate of change of different Martensite phases

ADE Algebraic-differential equation(s)

$Af$ Temperature for the finish of Martensite transformation

$Ap$ The peak temperature on the DSC plot for Austenite transformation

$As$ Temperature for the start of Austenite transformation

B.C. Boundary condition
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>Elastic stiffness tensor</td>
</tr>
<tr>
<td>C_A</td>
<td>Elastic stiffness tensor for the fully Austenitic material</td>
</tr>
<tr>
<td>C_AN</td>
<td>Stress influence factor for the reverse transformation in compression</td>
</tr>
<tr>
<td>C_AP</td>
<td>Stress influence factor for the reverse transformation in tension</td>
</tr>
<tr>
<td>C_d</td>
<td>Vector containing the conditions of transformation for (\sigma)-T paths</td>
</tr>
<tr>
<td>C_M</td>
<td>Elastic stiffness tensor for the fully Martensitic material</td>
</tr>
<tr>
<td>C_MN</td>
<td>Stress influence factor for the forward transformation in compression</td>
</tr>
<tr>
<td>C_MP</td>
<td>Stress influence factor for the forward transformation in tension</td>
</tr>
<tr>
<td>Cp</td>
<td>Specific heat</td>
</tr>
<tr>
<td>D</td>
<td>Modulus of elasticity</td>
</tr>
<tr>
<td>D_a</td>
<td>Modulus of elasticity for the fully Austenitic material</td>
</tr>
<tr>
<td>D_m</td>
<td>Modulus of elasticity for the fully Martensitic material</td>
</tr>
<tr>
<td>DSC</td>
<td>Differential scanning calorimetry</td>
</tr>
<tr>
<td>E</td>
<td>Green-Lagrange strain in the axial direction</td>
</tr>
<tr>
<td>E_el</td>
<td>Elastic Green-Lagrange strain tensor</td>
</tr>
<tr>
<td>E_th</td>
<td>Thermal Green-Lagrange strain tensor</td>
</tr>
<tr>
<td>E_tr</td>
<td>Transformation Green-Lagrange strain tensor</td>
</tr>
<tr>
<td>F</td>
<td>Deformation gradient tensor</td>
</tr>
<tr>
<td>f</td>
<td>Density of the external body forces per unit mass</td>
</tr>
<tr>
<td>I</td>
<td>Second order identity tensor</td>
</tr>
<tr>
<td>J</td>
<td>Jacobean</td>
</tr>
<tr>
<td>k</td>
<td>thermal conductivity</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>Mf</td>
<td>Temperature for the finish of Martensite transformation</td>
</tr>
<tr>
<td>Ms</td>
<td>Temperature for the start of Martensite transformation</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial differential equation</td>
</tr>
<tr>
<td>S</td>
<td>Second Piola-Kirchoff stress in the axial direction</td>
</tr>
<tr>
<td>SE</td>
<td>Superelasticity (Pseudo-elasticity)</td>
</tr>
<tr>
<td>SM</td>
<td>Shape memory effect</td>
</tr>
<tr>
<td>SMA</td>
<td>Shape memory alloy</td>
</tr>
<tr>
<td>T</td>
<td>Temperature</td>
</tr>
<tr>
<td>T</td>
<td>Field of tractions</td>
</tr>
<tr>
<td>V</td>
<td>Deformed body</td>
</tr>
<tr>
<td>V₀</td>
<td>Undeformed (reference) body</td>
</tr>
<tr>
<td>δE</td>
<td>Variation of the strain</td>
</tr>
<tr>
<td>δu</td>
<td>Variation of the displacement field</td>
</tr>
<tr>
<td>ζ</td>
<td>Volumetric fraction of Martensite</td>
</tr>
<tr>
<td>ζ₈₅</td>
<td>Volumetric fraction of detwinned (or temperature-induced) Martensite</td>
</tr>
<tr>
<td>ζ₆₅</td>
<td>Volumetric fraction of twinned (or stress-induced) Martensite</td>
</tr>
<tr>
<td>ζₛₘₙ</td>
<td>Volumetric fraction of stress-induced Martensite in the negative direction</td>
</tr>
<tr>
<td>ζₛₚ⁺</td>
<td>Volumetric fraction of stress-induced Martensite in the positive direction</td>
</tr>
<tr>
<td>Θ</td>
<td>Coefficient of thermal expansion for SMA</td>
</tr>
<tr>
<td>ν</td>
<td>Poisson ratio</td>
</tr>
<tr>
<td>ρ</td>
<td>Material density in the deformed state</td>
</tr>
<tr>
<td>ρ₀</td>
<td>Material density in the undeformed state</td>
</tr>
<tr>
<td>σ</td>
<td>Cauchy stress tensor</td>
</tr>
</tbody>
</table>
τ  Tension-compression coefficient of asymmetry

Ω  Transformation coefficient
Chapter One

Introduction

1.1. Shape Memory Alloys:

NiTi belongs to a group of smart materials with the general name of shape memory alloys (SMA). Among different SMAs, NiTi is the most commonly studied and implemented one. This alloy, in addition to the distinctive properties of shape memory (SM) and superelasticity (SE), is biocompatible (with mechanical properties more comparable to bone than Ti-based compounds or Stainless Steel) and has a good resistance to wear and corrosion.

Shape memory alloys undergo a phase transformation in their crystal structure when cooled from the stronger, high temperature form (Austenite) to the weaker, low temperature form (Martensite). This inherent phase transformation, which can be either stress or temperature induced, is the basis for the unique properties of these alloys.

Shape memory effect, as shown in Figure 1-a, is the recovery of large strains (up to 8%) created in the material while in the low temperature range by raising the temperature to a specific level (high temperature range). That specific temperature level (called Austenite finish Af) can be manipulated via changing the composition of the
material or thermo-mechanical treatment to a value around body temperature. In other words, apparent plastic deformation and subsequent full recovery is the shape memory effect (SME); also called one-way shape memory effect. In two-way shape memory effect, a properly processed sample can exhibit one shape when cold, change to a second shape when heated, and return to its original shape when cooled again; all without mechanical intervention. Shape change occurs in two directions, during both heating and cooling, although no appreciable force in the SMA structure is developed during the transition from a high to a low-temperature shape.

Figure 1 Schematic representation of (a) the shape memory effect and (b) superelasticity.

Superelasticity (or pseudoelasticity), as shown in Figure 1-b, allows the formation of an elastic behavior but with strain values more significant than those of the classic metals or alloys (the recoverable strain for a mono crystalline sample of SMA can reach 10% [1]). Superelasticity describes the nonlinear recoverable deformation behavior of
NiTi alloys at temperatures above the Af temperature, which arises from the stress-induced Martensitic transformation in loading and the spontaneous reversion of the transformation upon unloading.

High-damping effect, as another property of these alloys, is the ability of the material to transform mechanical energy (e.g. provided by an applied force) into thermal energy (in the form of heat dissipation). This irreversible energy transformation allows the material to resist shocks and absorb vibrations. The internal friction, by which energy in the form of heat is dissipated, results in an increased high-damping effect through the movement of interfaces between Austenite and Martensite for when both phases exist in the material (dual phase domain).

SMAs have been used in medical applications. Shape memory effect and superelasticity can be employed to activate the medical devices into operation through body heat or external sources of heat. Such designs could not be realized with conventional alloys (See Table 1). In many cases, NiTi is substituted in an application which has traditionally used stainless steel.

Due to superior thermo-mechanical properties and biocompatibility, NiTi has gained researchers’ attention for implementation in biomedical fields such as orthopedics, orthodontics, cardiovascular, minimally invasive surgical instruments, etc. (Refer to the next chapter “

SMArt™ Pedicle Screw” for more detailed description of such applications).
Table 1 Physical and mechanical properties of NiTi vs. Stainless Steel [2].

<table>
<thead>
<tr>
<th>Property</th>
<th>NiTi</th>
<th>Stainless Steel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Recovered Elongation</td>
<td>8%</td>
<td>0.8%</td>
</tr>
<tr>
<td>Biocompatibility</td>
<td>Excellent</td>
<td>Fair</td>
</tr>
<tr>
<td>Effective Modulus</td>
<td>approx. 48 (GPa)</td>
<td>193 GPa</td>
</tr>
<tr>
<td>Torqueability</td>
<td>Excellent</td>
<td>Poor</td>
</tr>
<tr>
<td>Density</td>
<td>6.45 (g/cm³)</td>
<td>8.03 (g/cm³)</td>
</tr>
<tr>
<td>Magnetic</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Ultimate Tensile Strength (UTS)</td>
<td>approx. 1,240 (MPa)</td>
<td>approx. 760 (MPa)</td>
</tr>
<tr>
<td>Coefficient of Thermal Expansion (CTE)</td>
<td>Martensite - 6.6 x 10⁻⁶ (cm/cm/°C)</td>
<td>17.3 x 10⁻⁶ (cm/cm/°C)</td>
</tr>
<tr>
<td></td>
<td>Austenite - 11.0 x 10⁻⁶ (cm/cm/°C)</td>
<td></td>
</tr>
<tr>
<td>Resistivity</td>
<td>80 to 100 (µΩ*cm)</td>
<td>72 µΩ*cm</td>
</tr>
</tbody>
</table>
1.2. Manufacturing and processing aspects of Nitinol shape memory alloy components:

A durable, compact, and reproducible structure is the requirement for any engineering and bioengineering application component. In the light of the properties and characteristics mentioned in the previous section, NiTi shape memory alloys are gaining attention as a multifunctional material in many engineering and biomedical applications.

The shape memory effect, superelasticity, damping and impact absorbing as well as thermo-mechanical properties of near equiatomic composition of Ni and Ti is strongly dependant on the stoichiometry and thermal/mechanical treatments rendered to the composition. 0.1 atomic % variation of the Ni content is shown to shift the transformation temperatures by nearly 10 °C. Impurities such as Oxygen, Nitrogen and Carbon should also be avoided from the NiTi alloy matrix since the transformation temperatures, hysteresis, strength, and ductility of the material are very sensitive to these impurities.

Figure 2 illustrates the NiTi binary phase diagram according to which additional stable phases exist in the proximity of near equiatomic composition. Thus annealing, solution treatment, and aging of the material in different temperatures can have significant effects on the thermo-mechanical properties of NiTi shape memory alloys.
The precipitation reaction of Ti11Ni14, in the aging temperature range of 300-500°C, results in the Ni atoms to congregate in the precipitate and the Ti atoms to diffuse to the TiNi matrix. This ultimately leads to the increase of transformation temperatures. However, at temperatures above 500°C the Ti11Ni14 precipitates dissolve and as the Ni atoms diffuse back to the matrix, the transformation temperatures decrease correspondingly [10] [10]. Figure 3 depicts the effect of ageing temperature and time on the transformation temperature of Ti-50.8% Nitinol wire with an initial Af temperature of 11°C. The maximum precipitation rate is about 400°C. Nevertheless, between 500°C and
550°C the precipitates dissolve and tend to lower the Af asserting the importance of controlling NiTi thermal treatments.

![Figure 3 Conventional time–temperature–transformation (TTT) diagram for NiTiNol wire with initial Af=11°C [10].](image)

More so than other materials, properties of Nitinol are significantly affected by its manufacturing processes. There are abundant amounts of processing data available in the industry to process the material. However, they are often kept proprietary and not released in the public domain.

1.2.1. Conventional manufacturing processes:

Production of SMA components conventionally entail arc or induction melting followed by a hot working process and machining to the final shape.
Meling of Nitinol prevents contamination because of the inert working atmosphere and pure raw materials and also makes it possible to achieve good mixing of the constituent elements resulting in material homogeneity and uniformity of the properties [11] [12] [15].

Two major methods of melting commonly used are Vacuum Induction Melting (VIM) and Vacuum Arc Remelting (VAR). The cost of production by either method is similar and they both provide suitable material for current medical device requirements (ASTM F2063).

A graphite crucible is used in VIM in which all raw materials are melted at once. Graphite crucibles are generally preferred for this process due to their easy handling, inexpensiveness compared to other crucibles, and chemical homogeneity of the melt product. On the other hand, their use results in increased carbon contents in the alloy in the form of TiC. This increases the Ni concentration in the NiTi alloy which in turn depresses the phase transformation temperatures. Other crucible materials failed to substitute for graphite in VIM owing to a number of problems such as sensitivity to thermal cracking, higher prices, and thermodynamic instability as for Oxygen evolution. Good mixing and uniformity is achieved with the graphite crucibles in VIM. This process is often followed by VAR to get further refining.

VIM involves melting of a metal under a vacuum or inert gas atmosphere. Electrical eddy currents induced in the graphite crucible and in the metal heat and melt the charge. The alternating magnetic field produced by an induction coil is the source for the eddy current. Also, electrodynamics forces result in stirring and mixing of the melt.
Figure 4 illustrates a laboratory setup for VIM processing of binary NiTi shape memory alloys by ingot metallurgy in a graphite crucible and starting with pure elemental Ni pellets and Ti rods. The researchers could yield 1 Kg of high quality low carbon and chemically homogeneous SMA ingots. They could achieve a significant reduction in the carbon contact by deterring the direct contact between Ni and graphite utilizing Ti disk cladding. The protective TiC layer on the inside surface of the crucible could partially but not completely diminish the transfer of C from the crucible to the melt [12].

SAES Smart Materials and FURUKAWA, two major suppliers of NiTi, utilize this method.
VAR procedure does not need any crucible. It gives very high purity yields and multiple melting cycles are used to obtain high homogeneity. Small amounts of inclusions could find their way into the product but they are not evenly distributed. Wah Chang, another supplier of NiTi, uses the VAR method.

Double melting process using VIM primary melting followed by VAR re-melting is successfully used in production. Ingots of 1,000 Kg and 35.5 cm diameter are normally produced using the VIM/VAR double melt process.

The raw materials used for the above procedures comprise 99.99% pure Titanium sponge along with Electrolytic Nickel with 99.94% purity. Inclusions and impurities can affect the Martensitic transformation characteristics such as transformation temperatures and hysteresis. For instance, ceramic-like inclusions could depress the transformation temperatures.

The above processes have major drawbacks including extreme reactivity of the melt and going under segregation due to the density difference of the reacting melts. Also, rapid grain growth occurs as a result of subsequent high-temperature working which leads to poor fatigue properties.

Despite the fundamental differences between the VIR and VIM melting processes, VAR and VIM/VAR double melt products appear to have similar mechanical and fatigue properties [13].

Notably, general requirements on Nitinol chemistry and trace elements are defined in the ASTM standard, F2063-00 [14].

As-cast microstructure of Nitinol, however, is not acceptable for medical applications and further processing is required; commonly hot working, cold working,
and heat treatment. Hot working procedures include press forging, hot rolling, rotary forging, etc. Final product shapes such as wire, tubing, and sheet can be achieved via cold working. The average ductility of NiTi allows 30 to 50% of cold work.

Nitinol wires, the most widely available form of this material, are produced via drawing. Drawn seamless tubing is also possible to produce (mostly available in superelastic form). Rolled sheets and strips of NiTi can be used for photochemically etched or stamped devices.

Machining of Nitinol is difficult due to its specific properties and resistance to deformation. It causes severe tool wear but abrasive methods such as grinding and abrasive saws are preferred to cutting methods for this material (See Figure 5).

The machinability of Nitinol significantly depends on the cutting speed and feed rate which should be chosen high enough. Poor chip breaking and the formation of burrs is another problem which is attributed to the high ductility as well as unconventional stress-strain behavior of SMAs. Despite the optimization of machining parameters, tool wear still remains a problem in machining shape memory alloys. Drilling Nitinol components with high cutting feeds and speeds will help to extend the tool life and improve work piece quality although it results in an increased micro hardness in the subsurface zones of the part [16].
Figure 5 Major drawbacks in machining NiTi shape memory alloys: (a) high tool wear; (b) undesirable chip formation; (c) formation of burrs after turning (d) and grinding [16].

Laser cutting, Electro discharge machining (EDM), Photo-chemical etching and water jet cutting proved to be better alternative processes to manufacture final products.

Laser cutting has the advantage of causing no mechanical stresses, no significant heat dissipation, no tool wear, and high lateral resolution. However, laser-cut parts must undergo further processing to remove the heat affected zone (HAZ). Modern laser cutting machines, using a pulsed Nd:YAG laser and equipped with a CNC motion control system, offer high speed, high accuracy, and the capability for rapid prototyping [17].

EDM works well with most Nitinol compositions. A recast surface layer consisting of oxides and contaminants from Cu electrode and dissolved dielectric medium will be present and may need to be removed depending on the application [18].
The surface oxide of Nitinol makes adhesion difficult for many joining methods. Welding, brazing, and soldering could be effective if done properly.

Nitinol, with removed surface oxide through aggressive acid-based flux, can be soldered effectively to other Nitinol parts and also to stainless steel. Laser welding of Nitinol parts can be successful under controlled conditions.

1.2.2. Powder Metallurgy:

Considering production of NiTi components for industrial purposes, near net shape fabrication processes are preferred due to the limited machinability of shape memory alloys. Powder Metallurgy (PM) is a well known process for its ability of providing semi-finished and net-shaped products. Furthermore, material savings and process automation as well as precise control of the chemical compositions can be achieved by PM while avoiding problems associated with the melting procedures like segregation.

On the other hand, porous NiTi SMA has gained the researchers attention for biomedical applications as for bone implants. Porous NiTi has excellent mechanical properties that can be adjusted via manipulating the production procedure to that of the bone or tissue where it is going to be implanted. It has also good corrosion resistance and biocompatibility and can exhibit partial superelasticity and shape memory effect. The porous structure provides a fine ground for reduced density and permeability that permits the ingrowth of new bone tissue as well as the transport of body fluids.
Various powder metallurgy (PM) processes have been experimentally developed for Nitinol in which both pre-alloyed powders and elemental powders can be used as starting materials.

Three methods are commonly used for the production of porous NiTi shape memory alloys (SMAs) from elemental powders. These include conventional sintering [19], Self-propagating High temperature Synthesis (SHS) [20][21][20], and sintering at elevated pressure via a Hot Isostatic Pressing (HIP) [9].

In **conventional sintering** (CS), a green compact of elemental Ni and Ti powders is prepared and further sintered at near melting temperatures to yield in binary NiTi from diffusion of Ni and Ti elements. Conventional sintering requires long heating times and samples are limited in shape and pore size. The porous structure in the product of conventional sintering is shown to be of small size and irregular shape. Maximum porosity of 40% can be achieved with this procedure. [19] [23].

**Self-propagating High temperature Synthesis** (SHS) is initiated by a thermal explosion ignited at one end of the specimen which then propagates through the specimen in a self-sustaining manner (due to the exothermic reaction between Ni and Ti). One of the difficulties with SHS is the inability to control the intermetallic phases. A schematic representation of the SHS process is shown in Figure 6.
Figure 6 Schematic representation of the SHS process: Ni+Ti → NiTi + 67 KJ/mol [21].

The porosity of the SHS product is dependent on the original porosity of the green compact and synthesis parameters such as the change in the molar volume, the combustion front thermal gradients, and the gas evolution as a result of volatile impurity expulsion. The porosity and the mean pore size and the distribution of that can be to some extent controlled in SHS. Performing the reaction under a reduced pressure or adding a gasifying agent will increase the porosity. Manipulating the reaction temperature by adding diluents to the initial mixture can be a way to control the pore size. Uniformity of the temperature profile within the sample greatly affects the homogeneity of the product. Nevertheless, Ti₂Ni, Ni₃Ti, and Ni₄Ti₃ stable phases are usually present in the SHS product matrix that will lead to a corresponding embrittlement effect [26][27].

The SHS reaction can be performed in two different approaches; first by locally initiating the reaction which will further propagate along the sample [21][28] and second by volume combustion [29] i.e. heating the entire sample up to the reaction temperature which will let the reaction to take place simultaneously throughout the whole sample.
Porosities above 50% can be achieved by SHS. The synthesis of NiTi with this method requires preheating of the sample to achieve self-sustained combustion since the exothermicity of the reaction is relatively low. The preheating temperature affects the amount of transient liquid phase present at the combustion front. Excessive pre-heating has been shown to have detrimental effects such as anisotropy in the pore structure [28].

Unlike the conventional metallic SHS reactions, the ignition temperature is not around the lowest melting point of the constituents and is shown to be in the range of 870–1070 °C; well below the melting point of both Ni and Ti. Ignition temperatures, times, and energies for different NiTi compositions was established to be significantly affected by the heating cycle of the sample and less affected by the reactant particle’s size and composition. Moreover, it was shown that controlling the preheating phase in the SHS sample via an external furnace while instigating the ignition in a very short period of time (in this case via laser power) would alleviate the temperature gradients inside the sample leading to a much more homogeneous product [20].

A bulk porous NiTi SMA has been produced via SHS from Ni and Ti green compact with a pre-heating temperature of 550 °C. The porosity of the green compact, the transient liquid phase, and the volatilization of the impurities followed by the escape of absorbed gases left three dimensionally interconnected pores in the product which formed banded channel structures along the propagation direction of the reaction (See Figure 7). The product contained 100% intermetallic NiTi compounds [21][21].
**Hot Isostatic Pressing** (HIP) is a pressure enhanced sintering technique that can be utilized to manufacture almost theoretically dense products (0.0% porosity). The powder mixture is encapsulated in an evacuated gastight welded canister and undergoes simultaneous isostatic pressure and elevated temperature. Other than that, Argon gas can be used as an inert environment without the need for the air tight canister of elemental compact. In this case, HIP can be used to compress and trap Ar gas bubbles in between the elemental powders. A subsequent high pressure diffusion stage will lead to Ar-filled pores. Sintering the product of this stage at reduced pressures will cause the gas to expand and bring about near-spherical pores in the final product. Elemental powders can be used in this technique leading to relatively homogenous test specimens except for NiTi2/Ni3Ti precipitates in the matrix (See Figure 8). On the other hand, the HIP process
has some advantages such as shorter solid state diffusion time, good control over the pore size, ability to manipulate various geometries, and finally having a more stable and manageable reaction compared to SHS process. A typical heating and pressurizing procedure for HIP is shown in Figure 9 [19].

The capsule-free HIP process was shown to produce homogenous porous NiTi (30~40% Vol.) with near-spherical pores. Due to the alleviation of stress concentration in near-spherical pores, the structure could show acceptable superelasticity. Controlling the porosity characteristics in porous SMA has a great influence on the mechanical properties of products [23].

Figure 8 Formation of non-binary phases in HIP process as a result of non complete diffusion [24].
Metal Injection molding (MIM) is another powder procedure for manufacturing near-net-shape NiTi products. MIM operates on the basis of the injection molding of plastics. This process was developed for long production runs of small sized (normally below 400 gm) complex shaped parts in a cost-effective manner. Furthermore, the process can also be used for high density metallic, intermetallic, or ceramic components by increasing the metal or ceramic particle content. Advantages of this technique include near net shape fabrication, geometrical precision of the parts, and low costs, for high production volumes.

Figure 10 demonstrates the region in which following the MIM process is cost effective; i.e. high complexity in geometry and shape as well as a production rate of 104 to 106 pieces per year.
According to Figure 11, MIM can achieve savings of up to 50% as compared to other manufacturing methods especially the ones that involve extensive machining.
The advantages that MIM provides in relation to the conventional manufacturing processes are tabulated in Figure 12. The global market for metals produced via MIM has grown at a double-digit rate annually.

<table>
<thead>
<tr>
<th>Method</th>
<th>Limitations</th>
<th>MIM Advantage</th>
</tr>
</thead>
</table>
| Investment casting | • Slow, labour intensive  
                     • Tolerances hard to control  
                     • Many secondary operations  
                     • Expensive               | • Lower cost  
                     • Short production cycles  
                     • High repeatability  
                     • Excellent surface finish  
                     • Minimal secondary operations |
| Die casting     | • Poor mechanical properties  
                     • Rough finishes  
                     • Limited range of materials | • Excellent mechanical properties  
                     • Wide range of materials |
| Machining       | • High level of wastage  
                     • High tooling costs  
                     • Design limitations  
                     • Not good for intricate shapes | • Virtually no material waste  
                     • Excellent for intricate parts |
| Conventional PM | • Lower densities  
                     • No complex shapes  
                     • Many secondary operations | • Very high densities (93-99%) |

**Figure 12** Comparison of MIM with conventional manufacturing methods [36].

The MIM process entails four major steps of feedstock fabrication, injection molding, debinding, and sintering (See Figure 13).

**Figure 13** Schematic process of the metal injection molding [22].

To reach the ideal results, each step must be optimized based on its effective parameters. In the feedstock preparation, the alloy powder is mixed with a binder whose composition and volume percentage is critical. The feedstock is later injected into the
mold; here the pressure and temperature of the feed as well as the mold are the playing parameters. It is worth mentioning that special attention should be directed to the design of the mold such that it gives proper pressure and temperature distribution of the melting front and ensures damage free removal of the green product out of the mold. Debinding is performed in a chemical bath and also under a vacuum with an elevated temperature environment to vaporize the binder from the product. Finally, the sintering stage is performed at high temperature levels (~1200 °C) which is sought to yield a product with a density close to the theoretical density of the material. Due to the low sintering activity of the NiTi powders and the lack of pre-compaction, high sintering temperatures are needed in MIM process [9]. Furthermore, preparing the suitable powder in terms of size and composition as well as protecting the process from external contamination, especially when working with Ti alloys, guarantees a successful MIM process.

The structural aerospace and medical implant parts, according to ASTM F 167, require Oxygen impurity levels below 300 ppm; hence the above mentioned procedures should be performed under a protective environment and with minimal interaction with external contaminants.

Titanium parts of up to a foot in length can be produced via MIM, however sizes over three or four inches (about 50 gm in weight) are not common [38].

Aust et al. [35] applied Metal Injection Molding to manufacture a geometrically complex (cannulated double threaded) bone screw implant from TiAl6Nb7. The screw, as depicted in Figure 14, had a length of 41 mm, an OD of 2.6 mm, and had a cylindrical bore with a wall thickness of 0.5 mm. The powder necessary for their process was made by argon gas atomization with a diameter of < 45 μm. The chemical analysis on the
manufactured part showed limited increase in the Oxygen, Nitrogen and Carbon impurities. Also, the average porosity (closed pores) achieved was measured to be 2.4%. The mechanical tensile tests on the screw samples and tension test specimens produced by the same procedure demonstrated that porosity level have minor influence on the tensile properties while the impurity level pressed the ductility and decreased the plastic elongation. It was concluded that the innovative MIM procedure is capable of producing products with fine details such as self-cutting threads and internal hexagonal bores. The strict protection of the MIM process from contaminants would result in good mechanical properties including tensile/torsional strength and ductility.

Figure 14 The MIM bone screw prototype and a typical implant positioned into the cervical vertebrae [34].
Nitinol implants are typically prepared by casting and formed to the semi-finished parts by rolling, drawing, or forging [39]. In an attempt to manufacture medical devices from NiTi, Krone et al. [37] utilized MIM to produce a staple implant (See Figure 15). The powder metallurgy of NiTi is more intricate relative to the conventional materials due to its high sensitivity to impurity content and influential procedure parameters. To avoid the exothermic reaction problems with elemental Ni and Ti powders, NiTi pre-alloyed powders (dia. < 21 μm) were used. It was previously established [9] that pre-alloyed powders are required for NiTi MIM process because of the anisotropic swelling of the compounds made of elemental powders in the sintering stage [9]. An Arburg Allrounder 270 CMD 400-100 injection molding machine (See Figure 16) was used in this experiment [40].

Figure 15 Dimensions of the manufactured staples as well as sintered green and sintered specimens [37].
The increase in the impurity level after processing was mainly in terms of the Oxygen content which changed from 0.11 to 0.23 wt%. The density of the MIM product was 95% of the NiTi’s theoretical density. In the course of the MIM procedure, Ti rich impurity phases (TiC or TiO$_2$) appeared in the binary NiTi matrix that changed the composition in favor of a Ni-rich phase. This shifted the phase transformation properties compared to the initial alloyed NiTi powders. Hence, this aspect should be considered in the design of medical devices that utilize the shape memory and superelasticity of Nitinol. The mechanical properties of a Nitinol tension test sample, prepared via MIM, were investigated. The material can be elongated up to 7.3% of strain prior to its brittle fracture and can undergo a level of stress around 780 MPa. With increasing the number of cycles in a fatigue test, the critical stress for the start of the transformation reduced, the residual strain increased, and the hysteresis diminished; a fatigue behavior typical to NiTi shape memory alloys. Furthermore, the thermal cycling was shown to have negligible effects on the transformational properties of the material.
The material showed no loss of structural integrity after $1.2 \times 10^6$ loading/unloading cycles in the air or saline solution. Additionally, the biocompatibility testing of the product in contact with osteoblast-like cells demonstrated excellent results. The authors concluded that the NiTi part produced with MIM process showed stable behavior in terms of cyclic mechanical loading and was suitable for the application in medical devices.

**Spark plasma sintering** method (SPS) was used to produce porous NiTi SMA components starting with pre-alloyed powders. In this procedure, pre-alloyed powders are loaded and pressed in a graphite die. A strong step current is further applied to the compact. The pulsed current introduces high energy to the compact which causes a joint formation in the particles at relatively low temperatures and in a very short period of time compared to sintering processes such as CS, HIP, or SHS. The spark discharge also results in the purification of the particles’ surface leading to a quality sintered product [30].

Inert gas atomization [31], hydriding and pulverization [32], or mechanical alloying can be used to produce pre-alloyed Nitinol powders [33].

SMAs are an excellent candidate for high efficiency damping and impact absorbing components thanks to their ability to sustain repeated large recoverable strains with a hysteresis response and variable stiffness. Porous SMAs have the additional advantages of higher dynamic energy damping capacity and possibility of wave scattering; moreover, their mechanical impedance can be adjusted to the working structure.
1.2.3. Electron beam melting (EBM) Processing:

Additive manufacturing (AM) is the process of making a part by adding successive layers of the material, rather than removing the material, such that there is little or no waste. Each layer is melted according to an exact geometry defined by a 3D CAD model. Additive Manufacturing has advantages of building parts with very complex geometries, such as one depicted in Figure 17, without any sort of tools or fixtures. Also, it is a fast production route from CAD to physical part with a very high material utilization and without requiring expensive castings or forgings on stock. Therefore, it is a very cost-effective, energy efficient, and environmentally friendly manufacturing process.

EBM is a type of Additive Manufacturing of metals that is sometime categorized as rapid manufacturing method. In this process, the part is manufactured by melting metal powders layer by layer using an electron beam in a high vacuum. This makes EBM suitable for materials with a very high Oxygen affinity.
In comparison to Selective Laser Sintering (SLS), the electron beam fully melts the metal particles to produce a void-free part. With laser-based systems, 95 percent of the light energy is reflected by the powder rather than being absorbed which significantly reduces the efficiency. The higher efficiency of EBM results in the creation of parts 3 to 5 times faster than other metal AM methods.

Since the parts are built in vacuum (base pressure of $1 \times 10^{-4}$ or better) at elevated temperatures, the result will be stress-relieved parts with material properties better than cast and comparable to wrought product. The electron beam heats up the powder bed to an optimal temperature therefore the parts are free from residual stresses and do not suffer from distortion.

It can also produce 100% solid parts as well as porous structures with controlled pore geometry and size.
As mentioned in Time Compression magazine [41], Arcam AB, a company from Sweden, developed the Electron Beam Melting (EBM) approach.

The Arcam A1 machine, shown in Figure 18, is designated for additive manufacturing of orthopedic implants. It offers a beam power of 5-3000 W with a scan speed of up to 8000 m/s and a maximum part size of 200×200×180 mm.

The device uses a thermionic emission gun that utilizes a Tungsten filament to make an electron beam which selectively melts the metal powders with a thickness of 0.07 to 0.25 mm.

![Figure 18 Different units of the EBM machine.](image)

Parts made of Titanium alloys are widely fabricated with this technology which makes it a suitable choice for the medical implant market.

The processed part from Ti6Al4V can be heat treated via Hot Isostatic Pressing (HIP) to achieve better fatigue properties and also can be used as a machining or welding stock. Because of the rapid cooling of the melt pool, the Ti6Al4V microstructure has
higher density and finer grains with lamellar $\alpha$-phase and larger $\beta$-grains; properties that are better than cast Ti6Al4V alloy.

Harrysson et al. [42] used the EDM method to fabricate custom designed orthopedic components (Hip stem) from Ti6Al4V alloy such that they can tailor its mechanical properties and structural strength to minimize the stress shielding effect and bone remodeling. The mismatch between the stiffness of the prosthetic implant and the patient’s bone results in stress shielding which leads to bone resorption and loosening of the implant. The EBM method was shown to be a good candidate in manufacturing custom designed implants such as holed or grooved hip stems, hip stems with trabecular structure, or solid hip stems (See Figure 19).

The power from electron beam was also used to produce NiTi ingots. As mentioned earlier in this chapter, the conventional Vacuum Induction Melting (VIM) process lacks from high contamination of Carbon which comes from the graphite crucible and presence of Oxygen from the remnant air in the melting chamber. With Electron Beam Melting, a water-cooled copper crucible is used which eliminates the Carbon contamination and Oxygen contamination is minimized because of operation in high vacuum. It was shown that the carbon contamination is 4 to 10 times lower in EBM than VIM and the Oxygen content is dependent on the starting raw material [43][44].
Figure 19 Representative parts made via Electron Beam melting. (a) 60% porous cubes, (b) 95% porous cubes, (C) bending specimens, (d) hip stems with trabecular configuration, holed configuration, and solid [42].
1.2.4. Heat Treating and Shape Setting:

Nitinol and other shape memory alloy mill products - bars, wires, ribbons and sheets - are normally finished by cold working to achieve dimensional control and enhanced surface quality. Cold working suppresses the shape memory response of these alloys. It also raises the strength and decreases the ductility. However, cold working does not raise the stiffness of the material. Heat treating after cold working diminishes the effects of cold working and restores the shape memory response of SMAs. Therefore, in order to optimize the physical and mechanical properties of a Nitinol product and to achieve desired shape memory and/or superelasticity properties, the material is cold worked and heat treated.

The product suppliers normally provide the material in the cold worked condition. The maximum practical level of the cold work will be limited by the alloy and by the product section size. Binary superelastic NiTi alloy fine wires with As in the range of $-25$ to $+95^\circ C$ are typically supplied with cold drawing reduction (after the final annealing) in the range of 30 to 50%. Larger drawing reductions are sometimes used for very fine wires. These same alloys will be limited to about 30% maximum cold reduction in the larger diameter bars. Binary NiTi alloys with very low As in the range of $-50$ to $-60^\circ C$ will not sustain the higher levels of cold work without cracking.

Both superelastic and shape memory properties are optimized by cold working and heat treatment. This thermo-mechanical process is applied to all Nitinol alloys although different amounts of cold work and different heat treatments may be used for different alloys and property requirements [165].
Shape setting is accomplished by deforming the Nitinol part to the shape of the desired component, constraining the Nitinol by clamping, and then heat treating. This is normally done on the materials in the cold worked condition, for example cold drawn wires. However, annealed wires may be shape set with a subsequent lower temperature heat treatment.

In shape setting cold worked material, care must be taken to limit the deformation strain to prevent cracking of the material. Another approach is to partially anneal the wire prior to shape setting. Yet, another option is to shape set in incremental steps.

The electrical resistance of Nitinol makes it a good candidate for heating by electric current. Nitinol will be oxidized when heat treated in air. Therefore, surface requirements and atmosphere control are important considerations.

A wide range of temperature from 300 °C to 900°C can be chosen for the Shape-setting of Nitinol. However, in order to optimize the combination of physical and mechanical properties; heat treating temperatures for binary NiTi alloys are usually chosen in the narrower range of 325 to 525°C. Heat treating times are typically 5 to 30 minutes. Consideration must be given to the mass of the heat treating fixture as well as that of the product. Sufficient time must be allowed in the furnace to get the entire mass to the desired temperature [47].

In the case of shape setting SMA wires, a tooling fixture made of Stainless Steel can be used to hold the wire in a taut condition (See Figure 20). It is suggested to restrict the amount of the strain in the wire to 2% so that the fatigue properties (crack initiation) do not diminish. After heating, the wire will contract and get tightened; bolts and nuts with washers may be used to clamp the wire. Tying or coiling the wire is not suggested. It
is important to put the fixture in an oven while it has reached the desired temperature and take it out after the required amount of time and quench it [15].

Figure 20 The shape setting mold for preparing an NiTi helix.

The effect of time and temperature of shape setting on the shape recovery quality, Austenitie finish temperature, and nonlinear mechanical behavior of NiTi shape memory alloy was investigated in [45]. The shape setting process showed stable results where the Nitinol wire was constrained and treated on a mold at 500°C for aging times of longer than 10 min. Af temperature increased with the aging time and the peak values were obtained after aging at beyond 400°C. The upper and lower plateau stresses decreased with the aging time. The increase of Af with the aging time was consistent with the expected decrease in the Ni content of the Nitinol matrix (due to precipitation). At high temperatures, there is sufficient thermal energy to permit rapid diffusion of Ni and Ti
atoms in the matrix; but it becomes more difficult for the same atoms to form precipitate nuclei as the temperature increases. Higher nucleation rates will occur at lower temperature levels but diffusion rates will be slower [45].

As mentioned earlier, the phase transformation temperature of NiTi SMA depends on the chemical composition, the amount of cold working, and the heat treatment processing parameters. The heat treatment temperature and time as well as cooling rate can be significant parameters altering forward and reverse phase transformations between Austenite and Martensite. Yeung et al. [46] investigated the effect of these parameters for 3 stages of treatment processes; 1-solid solution, 2-solid solution followed by aging at high temperatures, and 3-solid solution followed by aging at low temperatures. Longer treatment times gave higher Ap (the peak temperature on the Differential scanning Calorimeter (DSC) reverse transformation plot, As<Ap<Af). The solid solution at different temperatures did not have significant effect on Ap but the cooling rate and the secondary aging could considerably change Ap. Secondary aging treatment between 400-480°C could increase Ap but the time duration had mild effect. Water quenching generally could give the highest transformation temperature change among other cooling methods.

Smith et al. [33] reviewed the types of furnaces and fixture hardware or mandrels that have been used for the heat treatment of Nitinol. Many types of furnaces were used including box furnaces, continuous belt hearth furnaces, tube furnaces, heated platen presses, vacuum furnaces, induction heaters, salt baths, and fluidized bed furnaces. Nitinol will be oxidized in a non-protected environment therefore care must be taken in selecting the type of the heat treatment furnace.
1.3. Objectives:

The main objective of this research is to design and numerically investigate the performance of an innovative next-generation pedicle screw to address the loosening and back-out problem in the osteoporotic bone. These are the major setbacks of the conventional pedicle screws in osteoporotic bone. To this end, an innovative pedicle screw design (SMArt™ pedicle screw) is proposed that utilizes the shape memory and superelasticity properties of Nitinol.

The design is comprised of NiTi tubes and wires that are wrapped around the shaft of a conventional pedicle screw. The expansion of this insert assembly by reaching to the body temperature will maintain the grip in the bone.

1.4. Approach:

In order to achieve the objectives set forth as for the current study, a framework for modeling the complex thermomechanical behavior of shape memory alloys was developed in COMSOL Multiphysics®. The model is capable of capturing the shape memory effect, superelasticity, and asymmetry in tension and compression and was validated against the published experimental data.

The Finite Element simulation of the wire and tube, the primary elements of the insert, was analyzed in COMSOL Multiphysics® utilizing the developed SMA model. The optimum geometry for the Nitinol assembly was selected based on the outcomes of this simulation and was proposed for the manufacturing phase of the first SMArtTM pedicle screw prototype.
1.5. Contributions:

The contribution of this work was two-fold. First of all, a novel pedicle screw design was proposed to overcome the shortcomings of these bone screws in anchoring osteoporotic bone which lead to a patent application. The functionality of the screw in enhancing the mechanical contact with osteoporotic bone was tested in simple mechanical tests. Second, a model that could simulate the behavior of shape memory alloys was presented in COMSOL Multiphysics® that did not existed before. The following papers were published based on the research performed in this work.

1.5.1. Publications:


1.5.2. Intellectual property:

Chapter Two

SMArt™ Pedicle Screw

2.1. Introduction:

Over the past 40 years shape memory alloys (SMAs) have been used for a variety of medical applications. These applications can be divided into two general categories: active and passive. In active applications, temperature of the material is controlled to induce phase transformation between Austenite and Martensite, which results in the desired thermo-mechanical behavior. By heating the SMA elements in an active endoscope, the device bends in the desired direction. Passive applications rely on the distinct thermo-mechanical characteristics, namely shape memory effect and super-elasticity. These effects allow alloys such as Nickel-Titanium (NiTi) to undergo large mechanically induced deformations and consequently to recover the original shape. An example of the passive use of SMAs: a coronary stent expands the blood vessel due to body heat. Most NiTi medical devices are made from 50.8 atomic percent Nickel and 49.2 atomic percent Titanium [48].

Shape memory effect can be employed to activate the medical devices in an operation through body heat or external sources of heat. Such designs could not be
realized with conventional alloys. Superelasticity-based applications, in general, take advantage of either the possibility of recovering large deformations (up to 10%) or the existence of a transformation stress plateau, which provides nearly constant stress over significant strain intervals.

The high-damping effect is the ability of the material to transform mechanical energy (e.g. provided by an applied force) into thermal energy (in the form of heat dissipation). This irreversible energy transformation allows the material to resist shocks and absorb vibrations; an indispensable feature for orthopedic implants (e.g. vertebral disk replacement devices).

An important requirement for any material to be used in human body is being biocompatible. Titanium is a biocompatible element; however excessive intake amount of Nickel may cause local and systemic toxicity, carcinogenic effects, and immune responses. Nickel in NiTi is chemically joined to the Titanium in a strong intermetallic bond, so the risk of reaction even in patients with Nickel-sensitivity, is extremely low. Surface treatments are also useful in enhancing the biocompatibility of shape memory alloys. A new surface treatment consists of a thermal oxidation, performed under low oxygen pressure to avoid Ni oxidation, which leads to the formation of a pure dioxide titanium (TiO$_2$) on NiTi surface. This TiO$_2$ oxide has been shown to efficiently protect NiTi surface from release of Ni ions into the exterior medium. Therefore this new surface treatment is expected to improve NiTi cytocompatibility by decreasing the risks of toxic reactions associated to Ni. Also, TiO$_2$ oxide on NiTi surfaces has similar electrochemical corrosion resistance properties to native pure titanium oxide. This could be of paramount importance when applying the Oxidization Treatment to NiTi devices.
for biomedical applications. It is worth mentioning that pure titanium is a highly biocompatible metallic material widely used in medicine because of the appropriate properties of its surface oxide [49] [50].

Moreover, using Nitrogen or Oxygen plasma immersion ion implantation (PIII) will lead to dramatically improved corrosion resistance and tribological properties such as surface hardness. The leaching of near-surface Ni concentration in NiTi alloys has been significantly suppressed by implanting atoms on the surface (either with N or O) using PIII. The effects can be attributed to the formation of a barrier layer consisting of TiN and TiO, respectively. Carbon plasma immersion ion implantation and deposition (PIII&D) is also proved to increase the corrosion resistance and other surface and biological properties of NiTi. The ion-mixed amorphous carbon coating produced via PIII&D or direct carbon PIII can improve the corrosion resistance and block the leakage of Ni and lead to enhanced surface mechanical and biomechanical properties [51] [52].

The good compatibility of NiTi to Magnetic Resonance Imaging (MRI) permits instruments made out of this material to be used directly in magnetic fields without distorting the outcome images. MRI Compatibility of Nickel–Titanium Alloy stents was shown to be better than 316L Stainless Steel Alloy ones; causing minor artifacting and allowing for improved visualization [53]. Despite the aforementioned facts, necessary regulatory approvals (FDA 510(k) and PMA) still must be received for each new application.

This chapter reviews the orthopedic applications of NiTi shape memory alloy and presents two designs for next-generation SMA pedicle screws. These screws mimic the bone growth and can compensate for bone loss due to osteoporosis.
2.2. Orthopedic Applications of NiTi Shape memory alloys:

Dai and his colleagues, based on a series of previous fundamental studies, first developed NiTi shape memory compression staples in 1981 and applied them for the treatment of transarticular fracture in human body in 1983 [54]. After that, NiTi opened its way in orthopedic implant applications:

- Compression staples/clamps for the treatment of bone fracture [54] [56] [59] [60] [62] [63] [64] [65] [67] [69] [70], and anterior fusion of the spine [71] [72] [73] [75],
- Intramedullary nails that are used to apply controlled forces to the bone [83],
- Fixator systems for suturing tissue in minimally invasive surgery [80],
- Fixation bone plates [57],
- Rods for the treatment of scoliosis [74] [76] [77] [78] [79].

In these cases, the Martensite start transformation temperature is usually set at 4-7 ºC. Martensitic NiTi is soft and malleable therefore the device can be easily deformed (upto 6-8%) while immersed in sterile ice-cold saline [55]. The recovery or Austenite start temperature, by which the original shape will be restored, is normally chosen around 37 ºC. This level of temperature can be attained either by just adapting the body temperature or by resistive heating the device via external electrical current. The recovery force will gradually increase by temperature. The extent of transformation strain is not to be exceeded more than 6-8% or the shape memory effect in the material would be damaged [55].
Several types of NiTi-based shape memory alloy staples are used to precipitate the healing process of the fractured bone through a continual compressive force. The device in its opened form is placed in the prepared site. By heating, the staple tends to close and exerts a compressive force on the fractured parts of the bone (See Figure 21 and Figure 22) [66].

Figure 21 The shape memory staple: (a) at body temperature the two prongs get closer and the loop tends to close. (b) At low temperatures the staple is deformed and implemented in the site [65].
Small size, simple procedure, minimally invasive surgery, and the advantage of compressive fixation make the compressive staples a suitable tool for extensive use in the following treatments: transarticular fracture, patella fracture [67], fracture of internal and external condyles of femur, distal fracture of the radius, and finally transversal and short oblique fracture of the short bones in the hand and foot [55] [65] [66].

While staples are not suitable for the fixation of long bone’s shaft fracture, shape memory saw-tooth arm internal fixators are used in this case. These devices have the advantages of effective resistance to bending, shearing, and torsion and at the same time keep certain axial compression stress on the fractured bone to accelerate healing and bone
remodeling [55] [69]. The embracing fixator developed by Dai, that can be either cylindrical or conical, consists of a body and a few pairs of saw tooth arms that implement shape memory effect to hold tight to the bone (See Figure 23) [61].

![Figure 23 Shape memory saw tooth arm embracing fixator [55].](image1)

A NiTi shape memory screw has been designed by Zhao which is used in the treatment of femur head fractures. Half of the front part of the screw is longitudinally split in two, which would open at body temperature and can prevent the fracture from displacement [68].

Bone plates are the surgical tools used to assist in the healing of broken and fractured bones. They are also made of shape memory alloys. Tension provided by the steel plates, due to the limited range of steel’s recoverable elastic strain, is diminished after only a few days of healing and the fracture site will no longer be under compression. This will lead to a slower healing process. However, SMAs can exert a longer-lasting constant homogeneous pressure that promote rapid and complete healing of the broken bone (See Figure 24) [55][66].
NiTi-based Shape memory devices are also used in spinal surgery. Zhao developed a Ω-shaped intervertebral artificial joint for cervical spine that reconstructs the height and biomechanical functions of it after decompression and replaces the traditional bone grafting and fusion. The device facilitates patients’ faster recovery, minimizes the degeneration in the adjacent discs and reduces the pain and complications associated with bone grafting [71]. Furthermore, shape memory staples are used in cervical anterior fusion. They have excellent functional capabilities for this task and improve fusion time, implant and graft stability and safety of surgical procedure. Moreover, compared to screw plate instrumentation, they have a lower profile and take a minimal amount of space, fit
easily and have no risk of damage to the spinal cord (See Figure 25). It is worth re-
mentioning that Nickel Titanium boasts mechanical behavior that is similar to the
behavior of ligament-cartilage structures replaced or reinforced by fixators and allows the
possibility of post-operative magnetic resonance imaging (MRI) [72] [73] [75].

Silberstein et al. [75] utilized an implant made of porous NiTi alloy for anterior
fusion of the spine instead of autologous bone graft. The implant had biomechanical
properties similar to those of the vertebral body. It successfully worked as a prosthesis in
the vertebral body for retention of the spine deformity correction (after removal of whole
or part of the injured vertebral body or disc) and provided stabilization in the operated
zone by in-growth of bone tissue into the pores of the implant.
Figure 25 (Top) Preparation of the device after cooling. (Bottom) Spinal Lumbar stenosis: (left) preoperative MRI (right) postoperative X-ray [73].
Scoliosis is the three dimensional deformity of the trunk in terms of lateral deviation and axial rotation of the spine. Since Harrington’s system for the correction of scoliosis, numerous such systems have been developed which are satisfactory but do not yield optimum results. It is due to the fact that the correction delivered is incomplete and a post-operative correction loss often occurs which is attributed to the viscoelastic behavior of the spine. Utilizing pseudo-elasticity and shape memory properties of an SMA rod and a number of anchors, it is possible to induce correction during and after operation through a continuous force (hence take advantage of the viscous behavior of the spine). In this way a three dimensional correction by lateral and anterior-posterior forces combined with an axial torque is applied to the deformed spine (See Figure 26) [74] [76] [77] [78] [79].

![Scoliotic spine before and after surgical operation. Implantable SMA scoliosis correction system with square cross section (Depuy holds the patent for this device) [76].](image)

In a case study, Wever et al. [77] performed an animal experiment to determine the in vivo functionality and biological safety of an SMA scoliosis correction device. In
the course of these experiments a scoliotic curve was induced instead of being corrected. The rod was capable of inducing significant scoliosis and there were no indications of corrosion or fretting around the rod. Histological examinations showed good tissue responses without evidence of foreign body response indicative of the biocompatibility of NiTi (See Figure 27).

Figure 27 (A) Transversal view of the device used for positioning of the rod on the rod-bridge interface. (B) An oblique view of the fixation of the rod on the bridge. (C) The implanted straightened rod with anchor system. (D) The recovered original curve of the rod [77].
The spinal vertebrae spacer is used in the treatment of scoliosis which can replace a damaged intervertebral disk (See Figure 28). The insertion of this spacer between two vertebrae assures the local reinforcement of the spinal vertebrae and prevents any traumatic motion during the healing process. The use of a NiTi shape memory spacer permits the application of a constant load regardless of the position of the patient, while preserving some degree of motion. The higher compliance and damping characteristics of NiTi alloy, compared to the high stiffness and low damping of other biomaterials such as Stainless Steel and Titanium, along with the possibility of deforming the device before implantation and then recovering the original shape through shape memory effect, make SMA one of the best choices for manufacturing effective spinal vertebrae spacers [66][81].

Figure 28 Shape memory intervertebral spacers in the Martensitic state (A) and in the original shape (B).
NiTi Shape memory double cup prosthesis of the hip, developed by Dai [82], is another exemplification of novel characteristics of NiTi shape memory alloys. Clinical practices showed some complications with the method of surface replacement of the hip joint including loosening or displacement of the prosthesis or late fracture of the femoral neck. The basis for the device operation is similar to the bone staples. The opening of the SMA cup had six anchor flukes that could be expanded before implantation and close after the operation. This way, the device would grip the femoral head and prevent cup loosening or displacement without the risk of fracture.

Yeung et al. [84] developed a spinal locking mechanism (Figure 29) that implemented the superelasticity and shape memory effect of Nitinol to overcome the fretting and corrosion loosening encountered in the conventional couplings. It has the ability to retighten once wear occurs and demonstrated experimentally better performance compared to the current nut and thread-bolt locking mechanisms in terms of axial and torsional resistance.

![Figure 29 SMA clamp gripping a superelastic spinal rod. The clamp will maintain a continual hold even in the case of wear and fretting [84].](image-url)
Porous NiTi SMAs, which represent a different material form, has been used as medical implants, especially artificial bone implants. As mentioned earlier, NiTi alloy combines the characteristics of shape memory effect and superelasticity with excellent corrosion resistance, wear resistance, mechanical properties, and good biocompatibility. Furthermore, NiTi alloy has two important mechanical characteristics similar to natural biomaterials such as bone. NiTi alloy has a recoverable strain of up to 8%, which is more comparable to that of bone (~2%) than the recoverable strain of stainless steel (0.2%). Also, NiTi alloy has a low elastic modulus (~48 Gpa), which is close to that of cortical bone (below 20 GPa); however, the elastic modulus of stainless steel can reach up to 193 GPa [128][129]. The mechanical properties of porous NiTi SMA, as compared with bulk NiTi alloy, can be adjusted to match those of the surrounding bone. This can be achieved by controlling the porosity and pore sizes through optimizing the synthesis and manufacturing conditions. In bone replacement applications, achieving the stiffness range of $E_{\text{bone}} = 12–17$ GPa while maintaining the lowest possible porosity in the NiTi implant is essential. It is worth mentioning that the closer the Young’s modulus and mechanical properties of the implant to those of replaced bony tissue, the lower the adverse effects of “stress shielding”.

Moreover, the porous structure of such implants allow the body tissues to grow inside and nutrients and body fluids to be transported through the interconnected pores; mechanisms critical to the precipitation of the healing process. The aforementioned characteristics make porous NiTi a promising biomaterial for use as artificial bone, tooth root implantation, etc [128] [129] [130] [131].

In addition to the preceding applications, there are a vast number of patented devices that pertain to the biomechanical implementation of NiTi shape memory alloys. The following are listed and described examples of the US patents attributed to the implants that exploit superelasticity and shape memory effect:

- Spinal implant and method of use [85]: This invention is a spinal disk implant that can be inserted via minimally invasive surgery methods. It tends to improve features of the both total disk replacement (TDR) devices and cage spacers. The implant consists of an outer housing composed of SMA material which has a memorized curved configuration and is radially compressible from one form to another in response to loading/unloading from the vertebral bodies (See Figure 30).

![Figure 30 Spinal implant and method of use [85].](image)

- Anchoring devices and implants for intervertebral disc augmentation [86]: This device, also, relates to spinal implants. It provides anchoring to adjacent vertebral
bodies in order to overcome some drawbacks in TDR devices i.e. implant migration and expulsion through an opening in the annulus fibrosis (See Figure 31).

Figure 31 Anchoring devices and implants for intervertebral disc augmentation [86].

- Apparatus for implantation into bone [87]: This device is intended for implantation into the spine or pelvis. It can be used for attaching and stabilizing adjacent vertebral bodies during the fusion process. It comprises of helical shape memory spikes with cutting tips that can penetrate into the bone or vertebral body by rotation (See Figure 32).
• Fusion implant [88]: Fusion cage intended for spinal stabilization. It can be inserted between the opposing vertebrae in a collapsed form. It allows for bone in-growth or addition of bone grafts (See Figure 33).

Figure 33 Fusion implant (original configuration) [88].
• Shape memory alloy staple [89]. (See Figure 34)

![Figure 34 Shape memory alloy staples [89].](image)

• Nitinol spinal instrumentation and method for surgically treating scoliosis [90]: The approach of this device is segmental fixation of an SMA rigid rod to the abnormally curved portion of the spine. The rod is shape set according to the desired configuration for the spine and is inductively heated after the operation for activation (See Figure 35).
Figure 35 Bone clamp for the scoliosis treatment device. (A) Deformed and (B) activated configurations [90].

- Multi-angle bone screw assembly using shape memory technology [91]: This device consists of a regular bone screw (e.g. pedicle screw) with a head that is capable of being connected to the spinal instrument rod at various angles and also maintaining the grip with the rod using shape memory compression elements (See Figure 36).

Figure 36 Multiaxial screw assembly and the receiver member [91].
- Bone anchor system and method of use [92]: An innovative device for fixation into the bone that does not utilize the conventional screwing method. The shaft of this bone anchor contains distributed shape memory thorns that expand upon activation by body temperature and engage the surrounding bone (See Figure 37).

![Figure 37 Shape memory bone anchor system after implantation](image)

- Methods and devices for stabilizing bone compatible for use with bone screws [93]: This device is a self-expanding stabilization device for repairing or implanting into the bone that has some attachment parts for receiving bone screws. It can be used in minimally invasive surgery or treat vertebral bodies affected by osteoporosis. The expanding part contains some struts that may expand either by applying force or use of shape memory effect. The struts undergo a continuous curvature through their length rather than bending at a hinge or a notch which helps the stability and
endurance of the device. By expanding, the struts cut through the cancellous bone and press against the cortical wall of the vertebrae (See Figure 38 below).

![Diagram of devices for stabilizing bone compatible for use with bone screws](image)

**Figure 38 Devices for stabilizing bone compatible for use with bone screws [93].**

In all of the aforementioned applications, Nitinol, due to its unique characteristics, provides a means of self-locking, self-expanding, and self-compressing for implants activated at body temperature (or heated via external sources).
2.3. Pedicle Screw in Osteoporotic Bones:

Metabolic bone diseases such as osteoporosis, osteomalacia, and Paget’s disease are usually linked, especially in elderly patients, with osteoporotic bone or a soft skeleton. Therefore, orthopedic procedures in elderly patients are costly and with the increasing age of the population, these costs will continue to grow. Due to its wide prevalence, osteoporosis has received a lot of attention over the past decades. Approximately 30% of postmenopausal Caucasian women in the United States have osteoporosis, and 16% have osteoporosis of the lumbar spine in particular; costing approximately $746 million in 1995 [95]. The adverse effects of osteoporotic fractures are likely to increase in the future with the growing number of the elderly people. For instance, the surgical treatment of deformities such as kyphosis and scoliosis can be very challenging, considering the poor bone quality and propensity for instrumentation placement in these people. On the other hand, people want to remain active and pain-free whenever possible. Therefore, there has been an increase in older patients willing to undergo the risks of surgery than before, making the situation even tenser.

Several advances in instrumentations, such as the use of laminar fixation (if available), multi-segment fixation, limited correction of the deformity, avoiding ending the instrumentation within the kyphotic segments, and augmentation of pedicle screw purchase through biologic and non-biologic fillers have been developed [95][96][109]. This section is devoted to the problems associated with osteoporotic bones and the existing solutions for mounting spinal implants to the affected bones.
2.3.1. Spinal Bone:

The spine consists of major types of cortical (compact; 5-30% porosity; ~1.8 g/cm³ density) and trabecular (cancellous; 30-90% porosity; 0.1-0.9 g/cm³ density) bone. (See Figure 39 and Figure 40)

The cortical bone demonstrated the properties listed in Table 2 in a review study.

Table 2 Mechanical Properties of cortical bone [117]

<table>
<thead>
<tr>
<th></th>
<th>Ultimate strength (MPa)</th>
<th>Elastic modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tension</td>
<td>92 - 188</td>
<td>7.1 – 28.2</td>
</tr>
<tr>
<td>Compression</td>
<td>133 - 295</td>
<td>14.7 – 34.3</td>
</tr>
<tr>
<td>Torsion</td>
<td>53 - 76</td>
<td>3.1-3.7</td>
</tr>
</tbody>
</table>

Trabecular (or cancellous) bone has a structure containing vertical pillars supported by horizontal struts and filled with bone marrow. Mechanical properties of the cancellous bone show high dependence on the loading direction. As an example, tensile strength of the cancellous bone was shown to be around 60-70% lower than its strength in compression [117]. In addition to being anisotropic, bone is also a viscoelastic material [132].

The structure of the bone is adjusted to its functional biomechanical loading. For instance the trabecular bone is stronger in the vertical direction in the vertebra and horizontal trabeculae acts as a support for the vertical pillars (See Figure 40).

The structure of the pedicular cancellous bone is somehow different from the vertebral body. The trabecular architecture within the pedicle isthmus is more isotropic
and plate-like. The thickness and number of trabeculae are greater than those of vertebral body trabeculae [116].

Figure 39 Cortical vs. trabecular bone.

Figure 40 Axial cross sectional view from human vertebral body. Thick rod and plate like trabeculae supported by horizontal trabeculae [117].
2.3.2. Osteoporosis effects on the bone:

*Bone mineral density* (BMD or Bone mass) is a measure of the amount of minerals (mainly calcium) contained in a certain volume of the bone. Bone mineral density (BMD) tests (also called bone mass measurement) are used to measure the bone density and determine the fracture risks in the case of osteoporosis. It may also be used to determine how effective an osteoporosis treatment is. There are different methods for the evaluation of osteoporosis. These include:

- *Jikei Osteoporosis Grading Scale*,
- *Dual-photon absorptiometry* (DPA),
- *Dual-energy x-ray absorptiometry* (DEXA) and
- *Metacarpal densitometry*.

According to Shigeru [106], all of the above methods offer good measures of the osteoporosis and pull-out force. Pull-out force, which is regarded as a standard way of assessing bone implants, correlates linearly with BMD. Among osteoporosis evaluation measures, Jikei scales can be determined from radiographic images. According to this scale, initial stages of osteoporosis entails a normal number of trabeculae with decreased bone density and thinner trabaculæ. For Grade I, transverse trabeculæ decrease in number while vertical trabeculæ and end plates remain prominent. In Grade II, transverse trabeculæ decrease more and vertical trabeculas also decrease. Finally by proceeding to the Grade III osteoporosis, transverse trabeculæ almost disappear and vertical trabeculæ become unclear like a ground glass image (See Figure 41 and Figure 42) [106][107].
2.4. **Pedicle screw:**

Bone screws have been used in the spinal fixation since the mid 1940’s. Boucher reportedly was the first to implant pedicle screws and Roy-Camille was the first to connect pedicle screws to a posterior plate. Later bone screw pioneers include Harrington, Cotrel, and Dubousset [124]. Pedicle screws are standard in posterior fixation.
procedures for the treatment of spinal instability caused by deformity, degenerative disc disease, fracture, spinal stenosis, spondylolisthesis, or tumors; however implanting pedicle screws in patients with osteoporosis presents surgeons with a challenge: the loss of the purchase (the grip between the bone and screw interface).

The pedicle is a small area of bone located on either side of the vertebral body and is the first to extend out from the back (posterior) of it. It is the connector between the vertebral body and the superior process that forms the facet joint (See Figure 43).

The pedicle screw, which is sometimes used as an adjunct to the spinal fusion surgery, provides a means of gripping a spinal segment. The screws themselves do not fixate the spinal segment but act as firm anchor points that can be connected with a rod. The screws are placed at two or three consecutive spine segments and then a short rod is used to connect the screws. This construct prevents motion at the segments that are being fused (see Figure 44) [120].
The invention and increased use of pedicle screws in spinal instrumentation improved the surgical management of the various types of spine lesions [107].

The pedicle screw fixation system is superior to the conventional posterior instrumentation methods due to capability of achieving 3D correction, maintaining anatomic or desired sagittal alignment, facilitating the instrumentation of short segments, strong fixation of the vertebrae, and reduction of the number of vertebrae to be engaged.
The pedicle has a relatively dense trabecular bone enclosed by cortical bone and its conical structure with ellipsoidal cross-section provides a significant means for screw placement. Since a pedicular fixation system consists of at least four screws connected to metallic rods, it can sustain high loads and provide an excellent stability for the fractured spine [106] [111] [117].

2.5. **Adverse effects of osteoporosis and enhancement methods:**

The very first concern regarding the use of spinal instrumentation in osteoporotic patients is the problem of hardware pull-out or loosening which may occur during surgery, while manipulating the instrumentation, or at a time after the surgery. The risk might be a change in the position of the hardware or even its collapse. If screw loosening occurs late after the surgery, depending on the case, two approaches may be taken: either revision of the instrumentation or supplementation with an anterior fusion which both incur complications and high costs. Therefore selection of appropriate instrumentation and a means to augment it would be crucial in osteoporotic patients [109] [117].

The results of a historic cohort study on patients treated for either degenerative spondylolisthesis or spinal fracture showed that 1.4% had loss of screw purchase during the surgery, while 3.5% had screw loosening or pull-out after the surgery. It is worth noting that the patients in the spondylolisthesis cohort (57.8 years old) who had pedicle screw fixation were significantly older than corresponding patients in the fracture cohort (35.7 years old), therefore they had significantly higher rates of intra-operative loosening (1.7% and 0.2% respectively) and pull-out (3.8% and 2.3% respectively) [114].

Screws that are inserted into osteoporotic vertebrae will compress the cancellous bone within the vertebrae whenever the spine is loaded. The cancellous bone will
continually compress until the screw contacts the endplates of the vertebrae or until enough bone is compressed and a stable column is formed against the screw which resists against the screws further displacement. Correspondingly, radiographs have shown that screw failure in the osteoporotic bone involves compaction of the enclosing cancellous bone during loading, unlike failure in the dense bone which entails screw bending without bone failure (See Figure 45) [117].

**Figure 45** Displacement of the pedicle screw within an osteoporotic human vertebra as a result of an in vitro long term cyclic test [116].

It is worth mentioning that most pedicle screws are evaluated biomechanically via axial pull-out tests (See Figure 46). In spite of that, studies demonstrated that transverse loosening is the primary mode of clinical failure for pedicle screws in the lumbar spine and applying cyclic loads in the cephalad-caudal direction (See Figure 47) to the screw is considered more realistic than simple pull-out loading [98] [101] [107] [117]. Also, as mentioned earlier, pedicle screw systems usually include a connecting rod between the screws in the different vertebrae levels so that the screws are locked with respect to
rotation. Hence, axial pull-out resistance tests appear to be a clinically more relevant failure indicator rather than torsional tests including torque measurements. Standard pull-out and cyclic tests are determined and defined by the American Society for Testing and Materials (ASTM F543-01 A3).

Figure 46 Typical of a pedicle screw pull-out test setup [104].
Figure 47 Schematic representation of vertebral body test specimen for axial pull-out test (A) and cyclic bending test in the cephalad-caudal direction (B) [97].

The other reason for extensive use of the axial pullout test might be the linear correlation between BMD and the maximum amount of axial force that screw instrumentation can tolerate. This relationship does not exist for cyclic load testing in the cephalad-caudal direction (See Figure 48).

Figure 48 Typical diagrams derived respectively from the tests in Figure 47 (CBC stands for bone cement augmented screws) [97]
A study by Inceoglu showed that the stress relaxation due to the viscoelastic properties of bone (that most likely occurs in vivo) significantly decreased the pull-out strength and stiffness of the screw compared to what the standard in vitro pullout tests could predict. It was suggested that the stress relaxation pull-out model was a better method to assess the screw’s performance [117] [132].

2.5.1. Pedicle screw augmentation methods:

Pedicle screw purchase and pullout resistance requires a solid interface between the screw and the surrounding bone it is implanted into. The amount of bone in contact with the implanted screw is reduced due to the progressive degradation of the cancellous bone and as a result the screw resistance to pullout diminishes. The screw strength in the bone depends on some main factors categorized and described as below.

- The geometry of the screw:

  Although the screw diameter is restricted by the pedicle isthmus width, increasing the major diameter of the screw to obtain more engagement within the endosteal cortex of the pedicle will lead to stronger purchase [101].

  Moreover, the more the thread depth and the more the engaged length of the screw, the better the screw pull-out resistance is [98]. The screws inserted through the opposite cortex of the vertebral body tolerated 430% more cyclic life than the ones inserted only up to 50% of the vertebral body (See Figure 49) [102].
Single and dual-lead pedicle screws did not show much difference in terms of the maximum attainable pull-out force; nonetheless dual-lead ones can be used to achieve a faster insertion time, without compromising the pullout force [104].

Results of a study by Abshire [116] indicated that conical screws offer improved initial fixation strength (17% increase in the pullout strength) compared to cylindrical screws of the same size and thread design (See Figure 50). The reason can be attributed to an increased minor diameter of Conical-shaped screws at the thread-shaft junction, which is the region of maximum strain in the case of bending load condition. Thus they are theoretically less likely to fracture or bend in this “at risk region” as compared with the equivalent cylindrical screws. Also, by matching the bell shape of the normal pedicle, conical screws are thought to provide more screw thread engagement of the pedicle cortical and cancellous bone at the cancellous–cortical interface. Their results suggest
that appropriately designed conical screws can be backed out 180 to 360 degrees for intraoperative adjustment without loss of pullout strength and stiffness [116].

Figure 50 Conical versus cylindrical pedicle screws [116].

- **The bone quality:**

As mentioned earlier, bone mineral density directly affects the pull-out resistance but not the cyclic behavior.

- **The quality of the fit:**

Pilot hole sizes of more than 72% of the screw outer diameter had adverse effects on the pull-out strength in the osteoporotic spine [103]. It might be due to the permanent damages caused in the pedicle cortical bone in the case of inserting screws that occupy more than 75% of the lumbar pedicle diameter [121]. Zdeblick findings suggest that the method of pedicle preparation i.e. either probing or drilling, does not affect the insertional torque of the screw or its ultimate pull-out strength. He also recommended the insertional
torque as a good predictor of the bone-metal interface failure. The reason was due to a linear correlation that existed between both the insertional torque, when tapping the hole or when inserting a screw, and the number of cycles to failure in an off-axis cyclic pull-out test [101].

Augmentation of the biomechanical implants, especially screws, using Polymethylmethacrylate has been accepted (FDA approved) for use in the body and the spine. Polymethylmethacrylate (PMMA) is a synthetic polymer of methyl methacrylate. This thermoplastic and transparent plastic has a good degree of compatibility with human tissue, and can be used as bone cement to affix implants and to remodel lost bone. It is supplied as a powder and with liquid methyl methacrylate (MMA). When mixed, these yield dough-like cement that gradually hardens. Although PMMA is biologically compatible, MMA is considered to be an irritant and a possible carcinogen. PMMA has also been linked to cardiopulmonary events in the operating room due to hypotension. Bone cement acts like a grout that fills the spaces between the prosthesis and the bone; and also inside the trabeculas of the cancellous bone thus prevents motion. A big disadvantage to this bone cement is that it heats up to quite a high temperature level while setting and because of this it kills the bone in the surrounding area [110].

Several investigators reported successful augmentation of the screw-bone interface purchase using PMMA (See Figure 48) [98] [102] [105] [106] [109] [111]. It was shown that filling of the trabecular portion of the vertebral body with pressurized bone cement (vertebroplasty) can increase the pull-out strength up to twice as much than that of a non-cemented pedicle screw. Vertebroplasty will also shift the mode of the hardware failure from stripping of the trabecular bone of the pedicle and vertebral body
by screw threads to the cortical bone fracture or full pedicle fracture in the osteoporotic spine. Nevertheless, this method has restricted acceptance due to the limitations described below [111].

Using PMMA imposes disadvantages as to the fact that undergoes an exothermic reaction while hardening hence is undesirable in close proximity to neural elements, especially if PMMA extrudes out of the cortical bone or pedicle. Therefore its use has been limited to the repair after screw stripping or the fracture of the pedicle during operation, with only small amounts of non-pressurized PMMA being applied. Other reasons contribute to its limited use such as infection, giant cell reaction causing bone resorption, and irremovable hardware [98] [99] [111] [113].

In an attempt to overcome some of the above-mentioned drawbacks, Cook et al. [105] tried to insert cement into the pedicle by means of the cannulated central portion of an expandable pedicle screw. Overall, there was a 250% increase in the mean pullout strength of the cemented expandable screw compared to that of a non-cemented expandable screw. Also, a cemented conventional screw achieved pullout strength similar to that of the non-cemented expandable screw. Therefore, they suggested the use of the expandable pedicle screw without cement in less severe osteoporosis as an excellent alternative to the cemented conventional screws in order to avoid potential PMMA complications [105].

The results of a study by Moore [113] indicated that calcium phosphate bone cements compare favorably with PMMA for augmentation of the pedicle screw purchase. Failure after augmentation by PMMA typically occurred by fracture at the base or through the pedicle, however screws augmented with calcium phosphate bone cement
failed through stripping of the bone cement. Therefore, pull-out resistance with Ca-P cement augmentation nearly is optimized to the strength of the pedicle. In addition to this, solidification of Ca-P cement involves hydration and is essentially not exothermic. It also has the benefit of being biocompatible and biodegradable [113].

Application of injectable carbonated apatite cancellous bone cement was shown to augment the pull-out strength by 68% and improve all the mechanical aspects of cyclic loading such as effective energy absorbed, initial and final peak loads, and post-test pull-out force by 30-63% [98]. This type of cancellous bone cement may provide an alternative to PMMA because it is biocompatible, remodelable, and almost non-exothermic at the time of hardening in situ [111].

The screw enhancement in osteoporotic spine via calcium apatite cement showed leakage in 5.5% of the dorsal screws at the pedicle corpus vertebra level [99].

In patients with spinal osteoporosis, the early achievement and maintenance of a biological bond between the pedicle screw and the bone is important to avoid the screw loosening complications. Applying a Hydroxyapatite (HA) coating on the transpedicular screws can accomplish this type of bonding. The use of Hydroxyapatite (HA) - coated implants may improve the stability of the bone–metal interface without the disadvantages of PMMA. Experimental and clinical studies have shown that both osteointegration and strength at the interface between bone and HA-coated pedicle screws are substantially better than those between bone and uncoated pedicle screws [97] [112] [115]. Hasegawa et al. [97] conducted a series of in vivo pedicle screw placement tests on dogs in which osteoporosis was induced by ovariectomy and a calcium-free diet. They showed that the resistance to pull-out force of the HA-coated pedicle screws is 1.6 times than that of
Titanium screws. The reason, as seen in histological sections, was attributed to the fact that the inter-spaces between the screw threads was filled with new bone of both woven and lamellar structures and good bonding was present between the bone and the apatite coating of the screw (See Figure 51). Also, in the HA-coated pedicle screws, the pull-out force increased as the BMD of each vertebra increased but they could not find any correlation between the BMD and the pullout force in the Titanium screws [97].

By modifying the thickness of the coating, an adequate enhancement of the screw purchase in the vertebra can be obtained, thus the extraction or revision of the instrumentation would be rendered feasible.

Using a combination of the pedicle screw and laminar hook on the same vertebrae increased the instrumentation stiffness by approximately 50%, suggesting that the combination method is valuable irrespective of the presence of spinal osteoporosis. Additional resistance gained by laminar hooks may be due to the fact that laminae is more cortical than cancellous and seems to be less affected by osteoporosis [107] [108] [109].
In order to overcome the problem of cement migration in bone augmentation via cement injection, balloon kyphoplasty has been used to create a pocket in the vertebral body for cement placement after pedicle preparation (but prior to screw placement). This has reduced the incidence of cement migration into the spinal canal, but paradoxically weakened the screw-bone interface initially by further destroying the remaining trabecular architecture [124].

The several methods that have been investigated for addressing screw loosening problem in osteoporotic and other patients can be summarized in the following categories:

- Extending the fusion to more levels to share the loads on the pedicle with other elements,
- Using pedicle hooks and laminar hooks to supplement the pedicle screw,
- Using large diameter screws for purchase in the cortical part of the pedicle,
- Using tapered screws for better bone compaction,
- Using longer pedicle screws to gain support from the anterior side of the vertebrae (bicortical purchase),
- Augmenting the bone and/or screw using bone cement (polymethylmethacrylate PMMA, calcium phosphate, or carbonated apatite) placed down the pedicle shaft prior to pedicle screw insertion,
- Using hydroxyapatite-coated pedicle screws, and
- Delivering the bone cement using fenestrated pedicle screws (screws designed with multiple holes on their shaft allowing for bone in-growth and/or influx of bone cement).
Finally, The aforementioned alternative surgical options are not ideal and entail drawbacks including increasing the time of surgery, increasing the risk of screw malpositioning, increasing the risk of injury to the spinal soft tissues, and sequestration of the bone cement in the spinal canal or unintended tissues (e.g. lung) leading to complications such as neurologic or vascular injury. Furthermore, some of these methods could cause damages to the bone and the spinal cord.

Regardless of the foregone techniques, fixation in the severely osteoporotic spine still represents a challenge.

2.5.2. Osteoporosis in other areas of Orthopedics:

All orthopedic devices are generally comprised of the following: bone-implant interface components (usually a screw), components to bridge across the fracture (e.g. bars or plates as well as connector clamps to the screw); and/or load sharing components (like spinal fixators) that must span across the vertebral discs and facets. Age related bone loss and the bone loss due to osteoporosis pose major problems for orthopedic fixation of the bone. The reason is not only due to the degraded bone in which fixation devices must find anchorage, but also because future bone formation at the site may fail to strengthen the construct or because future bone resorption may cause loosening and failure. Osteoporosis decreases the diameter of the trabeculae and yields a loss of interconnecting struts leading to a decrease in the ultimate compression and shear stresses at which the bone fails. In other words, a two-fold decrease in the density of the bone as a result of the osteoporosis will reduce the ultimate compressive stress by nearly a factor of four. Osteoporosis also affects bone cortex dimensions, especially in the femur and results in significant thinning of it. Cortical thinning reduces the length of the screw
engagement, the maximum screw torque that can be applied, and the frictional force between the plate and the bone. It also weakens the buttress support on the opposite cortex necessary for the plates or rods sustaining bending forces. Hence osteoporosis helps boosting the potential for fracture failure. Consequently, developing devices to supplement screws and gripping components is crucial for the success of internal fixation in the osteoporotic bone [122] [123].

2.6. Design of the SMArt™ Pedicle Screw:

In this section two SMArt™ pedicle screw (generally bone screw) designs are presented. These screws use NiTi’s superior thermo-mechanical properties to address the problem of pedicle screw loosening and back-out due to osteoporosis. It should be noted that these designs, although developed initially to enhance pedicle screw performance, are capable of being implemented in any situation where bone degradation enforces fixation difficulties. The research questions around each case and the steps to be taken towards the final design and ultimate commercialization will come in the next section.

2.6.1. Anchoring system with expandable thread inserts:

According to the aforementioned description on the adverse effects of osteoporosis on bone screw performance, an innovative screw instrumentation is proposed that is expected to augment the purchase of the bone-screw interface. The core idea is inspired from a screw thread system that is especially applicable to cases where the nut or internally threaded part is made from a soft material such as aluminum or magnesium. This system nowadays is vastly used in aviation industry. The stiffer screw in such cases is mated with an intermediate part known as thread lining or insert which
contains internal threads to hold the screw in place. If a conventional V-form screw is used without the insert, frequent loosening and tightening of the screw would cause rapid wear of the softer material from which the nut is made [118]; furthermore all the threads might not sustain the load evenly and only the first two threads would bear the whole load. By using a thread insert which is screwed in to the nut permanently, good wearing quality and load sharing between all the threads is obtained (See Figure 52).

![Figure 52 Screw Thread Inserts](image)

In the first design, this idea of the thread insert is combined with the unique characteristics of NiTi shape memory alloys to realize a segmented insert. This insert is mated with a pedicle screw to extend itself while placed in situ and is expected to
augment the screw purchase as the bone goes through osteoporosis (See Figure 53, Figure 54, and Figure 55).

Figure 53 NiTi insert. (A) Initial low-temperature form; (B) final form when reached to the body temperature. A portion of the insert from both ends expands and the remaining contracts to grip the screw.
Figure 54 The screw assembly before placement.

Figure 55 The screw assembly after placement.
This design uses both the shape memory and superelasticity properties of NiTi SMA. The expandable insert in the original (Figure 53-B) and deformed (Figure 53-A) configurations is shown in Figure 53. The insert in its initial high temperature form consists of two parts: one retractor and the other protractor. The protractor activates at the body temperature and tends to expand the insert. This expansion is such that only a portion of each insert from both ends straightens while the remaining contracts and tends to firmly grip the screw body (Figure 53 bottom). On the other hand, the retractor which has its Austenite transformation temperature (Af) higher than body temperature; can be activated by heating the assembly. The original form of the retractor is shown in Figure 53 (top). Upon heating above body temperature, the assembly folds to a form that can be easily removed by just unscrewing. Therefore, the whole system comprising a screw and a number of helical inserts (7 in the current design); kept at low temperature via iced saline solution, is inserted in the bone (See Figure 54). In terms of a healthy cancellous bone, the system acts as a regular screw with an insert that distributes the load on all of the threads. In case the bone goes through degradation and loss of purchase with the assembly, inserts that now have reached to steady state body temperature, unfold (See Figure 55) to compensate for the bone loss thus avoiding the screw-bone interface loosening and the whole implant failure. Should the screw need to be removed due to any reason, applying heat to the assembly will make the protrusions to fold back. The temperature by which the device activates can be adjusted by applying modifications to the alloying elements and heat treatment of the implant. So it can be set to a level that does not harm the surrounding bone and tissue. The temperature range reported dangerous for bone tissue is 47-50°C. The maximum endurable temperature above which
bone necrosis will happen is described as 53°C [127]. The heat can be provided utilizing a resistive component placed inside the screw body through connecting it to electric current. The heat is then spread throughout the whole structure via conduction. An alternative approach is induction heating. In this way, the assembly is engulfed by an alternating magnetic field, provided from an external device, which heats the implant’s surface up; exactly where the insert is located.

The thread insert design is such that the protractor and retractor parts can be manufactured via processes such as extrusion or rolling. In addition, the retractor and protractor inserts must be shape-set to their desired high temperature configurations. Shape setting is a heat treatment process intended to instill a desired memorized shape in a shape memory alloy component. Finally, the retractor can be slid in to the protractor (or vice-versa) and the assembly wrapped around a conventional screw.

Such an anchoring system can be used not only in the spinal instrumentation and as a transpedicular screw but also in every situation wherein a device is sought to be attached to bone, specifically osteoporotic bone. The general specifications and advantages of this innovative structure include:

a) Tackling the unsettled problem of loosening and back-out in the bone screws that occur due to osteoporosis and to some extent eliminating the need for bone cements.

b) This anchoring implant is also removable without stripping the tissue around and damaging the bone structure.

c) Dismissing the need for designing and producing a new screw since the insert can be modified readily to mate with any type of bone screw.

d) Straightforward production and manufacturing method for the insert.
e) Applicability to other orthopedic implants that have such loosening problem. For instance the screw-plates used for fixation of the long bone fractures, devices employed for fixation of the proximal and distal femoral fractures, stabilizing nail fixation of tibial or proximal humerus fractures, etc.

f) Relevance to industrial purposes where a structure should be attached to a softer or degradable base such as fastening metal to plastics or thermoplastics.

The primary concept design of the implant was described above, which in order to reach the concluding commercial form, must certainly go through a series of modifications and alterations.

Below are listed some research questions related to the improvement of this primary design up to an ultimate final outline:

- What are the optimum transformation temperature ranges for the helical insert (both retractor and protractor parts)?
- What is the best possible section profile of the insert so that the protractor and retractor can antagonistically act against each other and perform the desired folding and unfolding displacements, considering the effect of the surrounding trabecular bone?
- Does the partial expansion of the insert enhance the bone-instrument interface purchase?
- Does the partial gripping effect of the squeezing section of the insert provide required friction and strength with the screw in order to withstand various biomechanical loadings?
Does the induction or resistive heating of the system raise its temperature to the desired level consistently and evenly through whole structure? Is that level of temperature a menace to the adjacent live tissue?

What is the best and safest approach to heating the device?

In order to address these questions a finite element model is developed to evaluate the effect of different geometrical and material characteristics on the performance of the screw.

2.6.2. Bone screw with expandable legs:

The second novel screw design comprises two parts: a shape memory interior and a super-elastic exterior shown respectively in Figure 56, Figure 57 and Figure 58.

Half of both the interior and exterior shanks are split longitudinally into four legs.

![Figure 56 Close view of the expandable interior part. (1) Expandable leg. (2) cross-like ledge for engagement into the same-shaped slots of the exterior (3) longitudinal split.](image)
Figure 57 Close view of the exterior part. (1) Super-elastic leg with cross-like slot (2) longitudinal split (3) cancellous thread.

Figure 58 Superelastic Exterior part of the expandable leg implant at initial form.

The inner part legs have each a cross-like ledge that can be guided through same shaped slots in the exterior part (See Figure 56 and Figure 57) which prevent any relative rotation of the two components. The interior part also has a regular metric thread created
at its head which can be used for pushing or pulling it in and out the slots of the exterior part of the screw. The exterior includes regular cancellous thread on the surface and a knob on the top for attaching connection components to the screw.

The interior has shape memory characteristic meaning that upon heating to body temperature will tend to recover its high temperature original form. As shown in Figure 59, at its memorized shape all the legs are expanded.

![Figure 59 high-temperature Austenite form of the interior part.](image)

The exterior is superelastic with austenite high temperature form as shown in Figure 58 wherein all legs are closed. The transformation temperature of the interior part is adjusted near 37 ºC and that of the exterior well below 37ºC.

The assembly of interior and exterior parts is illustrated in Figure 60, Figure 61, and Figure 62. This assembly is placed similar to regular pedicle or bone screws in the bone despite the fact that it should be kept at a low temperature. After placement, the
structure will gradually reach to the body temperature upon which the inner piece activates and forces to open the screw exterior legs with it. In case the bone encompassing the screw degrades and loses strength, this feature causes the assembly to retain the purchase via extending outwards (Figure 63).

Figure 60 Assembly of the exterior and interior parts of the implant at low-temperature.
Figure 61 Close view (axial section) of the implant assembly.

Figure 62 Back section view of the implant assembly.
Figure 63 Implant assembly at the high-temperature (body temperature) illustrating the extended configuration.

The proposed screw is removable so that if the screw assembly needs to be revised or removed, a specially designed driver can be attached to the thread built at the top of the inner part and pull the interior out of the screw exterior while safely holding the exterior part. As mentioned earlier, the exterior is superelastic with closed original shape therefore (after pulling the interior out) will retract its legs and can be easily unscrewed out of the bone by turning.

The typical ranges of the transformation temperature in order for the two parts of the assembly to achieve the described functionality are shown in Figure 64. As and Af refer to Austenite start and finish temperatures for the interior part respectively and Ās and Āf are those of the exterior.
As it is implied from the figure, the exterior part is always in the Austenite phase throughout the operating stress-temperature range and the interior part transforms around body temperature. A typical path the interior part may follow during operation is also graphed in Figure 64.

Figure 64 Typical stress-temperature operation cycle for the implant. (1) Transformation region of the exterior part implying its superelasticity at the operation temperature range. (2) Transformation region of the interior part.

One important aspect in designing shape memory devices is the maximum strain imposed. The maximum strain that can be recovered through shape memory effect in NiTi is approximately 6-8%. Moreover, the fatigue properties of NiTi will diminish drastically if the maximum sustained strain in the component passes 3% under cyclic loading. A rough analysis via FEA, demonstrated in Figure 65, suggested that under a gap of 60 degrees between the assembly legs, the maximum strain to which the screw undergoes is in the order of 6.6% which is acceptable.
Figure 65 The strain distribution in the implant for the opening angle of 60º. The maximum strain is approximately 6.6%.

In terms of manufacturing, the processes utilized for manufacturing regular pedicle screws and other biomedical implants are applicable in this case and no implications seems to exist.

In conclusion based on the above descriptions, the prominent advantages of this anchoring system can be listed as below:

a) The implant is intended to address the issues related to osteoporotic bone degradation and screw loosening.

b) Moreover, such is the configuration of the implant that enables uncomplicated removing and revision without the need for externally heating or cooling the device.
c) Similar to the previous design, it can be used in other biomedical areas as well as industrial implementations.

The research questions listed in the previous section, namely the functionality analysis, failure analysis, design parametric analysis, manufacturability modifications, etc. are also the case for this design.
Chapter Three

Finite element modeling of shape memory alloys’ behavior

This chapter presents an extensive Finite Element model that simulates the complex thermo-mechanical behavior of shape memory alloys. Initially, the one dimensional model developed under the framework of COMSOL Multiphysics® is described. The generalization of this model to three dimensional problems is also discussed in this chapter. The finite element model is used to estimate the performance of the SMArt™ pedicle screw.

3.1. Introduction:

In order to predict and utilize the mechanical behavior of NiTi and other shape memory alloys in any field of engineering, the thermomechanical transformation underlying SM and SE must be thoroughly understood and sufficiently modeled.

For NiTi, a reversible solid sate displacive crystalline phase transformation dominated by shear between a high symmetry parent phase (Austenite in the form of ordered body-centered cubic (bcc) superlattice β phase in the case of Ni₅₀.₀Ti₄₀.₀) and a low symmetry product phase (Martensite in the form of monoclinic distortion of a B19
lattice) underpins both SE and SM effects which occurs due to the application of both stress and temperature [1] [4]. Fundamental and complex nature of the SE and SM due to the crystallographic phase of the material and the thermomechanics of transformation lead to various modeling approaches for SMAs [4] [7]. These modeling approaches are briefly explained in this section.

**Micromechanical models** consider the elastic, thermal and chemical free energies of thermodynamics from a microscopic standpoint. This approach homogenizes the local relations to obtain the stress-strain and transformation behavior [5] [6].

**Mesoscopic or lattice models** develop energy relations for a representative lattice and homogenize that control volume to reach to macroscopic constitutive behavior [8].

Models describing the macro-scale behavior of SMAs, also known as the **phenomenological models**, are developed based on the assumption that the state of each point of the material can be represented as a mixture of phases rather than segregated and distinct areas for each phase. The macro-scale models cover a range of theory from irreversible thermodynamics principles [135] to Preisach models [136]. The differences among these models come from the internal variables selected, type of the kinetic transformation equations, energy relations, and the level of thermodynamic consistency through using the energy conservation principle and the Clausius Duham inequality. The main parameters as well as the state variables in the phenomenological models are of engineering nature and easy to measure. Therefore, along with their simplicity, these models are easier for implementation into numerical computations.

One of the first models in the group of phenomenological models was presented by Tanaka and Nagaki [137]. In this model, strain $\varepsilon$ and temperature $T$ were considered
as state variables and phase fraction of Martensite $\zeta$, $0 \leq \zeta \leq 1$, was employed as the internal variable. The state variables were meant to be time/space averaged on a sub-Macroscale level with a length scale at least an order of magnitude larger than the average grain diameter. This model was later extended by Liang and Rogers [138] and Brinson [139] [140] [141] who incorporated phase fractions of twinned and detwinned Martensite as internal variables to capture SE and SM effects based on the loading path of an experimentally defined stress-temperature phase diagram. It was also shown that various 1D phenomenological SMA constitutive laws are similar by essence and differ in the formulation of the transformation kinetics [140].

Gao et al. [141] provided an extension to the previous work by Brinson and Lammering [150] where the authors described a nonlinear 1D finite element procedure for truss elements to analyze the behavior of shape memory alloys. In the extended model, the kinetics law developed by Bekker and Brinson [142] was utilized and modified to cover the entire phase diagram. The SMA constitutive and the phase-diagram-based kinetics laws were implemented into the ABAQUS finite element software package. Finally, the developed code was verified against super-elastic and shape memory loading experiments.

Jaber et al. [151] proposed a finite element model using an adapted 3D constitutive law for the SMA behavior which was based on the strain and temperature as control variables. A structural model was developed to analyze 3D SMA structures made out of thick beam elements with features such as taper and curvature. The combination of the above models was numerically evaluated using the return mapping algorithms. The
results of the numerical solution showed good agreement with the experimental data attained from the literature.

Gillet et al. modeled [152] SMA behavior considering the nonsymmetrical behavior of these alloys in tension and compression. This model was included in the framework of the beam theory. The material properties of the model were derived from tension and compression tests conducted. The results of the simulation were then successfully compared with the experimental outcomes performed on superelastic beams and springs made of copper-based SMA.

Thiebaud et al. [148] employed a phenomenological model based on the previously developed Raniecki [149] model in COMSOL Multiphysics® software to simulate the pseudoelastic behavior and also the dynamic response of SMAs. The structural mechanics module of the software was coupled with its Partial Differential Equation (PDE) module to solve the weak form of the phase transformation problem. Also, the stiffness and damping properties of the material under offset harmonic strain loading were evaluated using an Equivalent Complex Young’s Modulus approach.

The Tanaka model was utilized in this study to simulate the behavior of SMA; namely shape memory effect and superelasticity. COMSOL Multiphysics® software package was employed to prepare a 3D framework for evaluating the functionality of components made of SMAs. To this end, three application modules namely the Structural Mechanics, Partial Differential Equation (PDE), and Heat Transfer module were tied together to solve the problem. The structural mechanics module solves the equations of elasticity with dependant variables of displacement components in Cartesian coordinates. The kinetics of Martensite transformation was modeled through the PDE module with
detwinned Martensite fraction and twinned Martensite fraction in positive and negative axial directions as dependant variables. From this module, the transformation strains were obtained and integrated into the solid mechanics equations. For the purpose of this research, only the stress in the axial direction was considered as driving the transformation which is an acceptable approximation since the stresses in the transverse directions, for the case of a beam, are negligible and do not significantly contribute to the critical level of inducing Martensite transformation in the specimen. Also, the heat transfer module was responsible for solving the heat equation and providing the solution as temperature to the SMA PDE module.

The developed model can be used to estimate the performance of a smart pedicle screw; an illustration of the applicability of novel SE and SM properties in orthopedics.

3.2. Modeling of the SMA behavior:

In order to characterize the behavior of shape memory alloys, the Tanaka model introduced in the previous section was modified. The model considers strain and temperature as field variables and volume fraction of Martensite in the material as internal variable. Martensite transformation can be triggered with either change of temperature or application of stress; therefore the fraction of Martensite was divided into stress-induced and temperature-induced Martensite. The temperature induced or twinned Martensite, $\zeta_d$, consists of a self accommodated combination of Martensitic variants. On the other hand, the stress induced Martensite, $\zeta_s$, represents the extent of material transformation into a single Martensitic variant corresponding with the direction of the loading. As the result of the applied stress, each of the 6 face-diagonal planes of the austenitic NiTi lattice can shear in 2 directions and shift in 2 directions which constitute
24 possible Martensite variants in 3D. Because in bending of beams (the approximation for this application) the upper and lower layers undergo stresses in two opposite directions, the stress induced Martensite is correspondingly divided into two variables to capture the variants of Martensite which correspond to positive and negative stress directions. Also, an empirically developed stress-temperature phase transformation diagram was considered to distinguish between the transformation and non-transformation regions and paths. Cosine transformation kinetics laws in the rate form were used to define the evolution of the negative and positive stress-induced as well as the temperature-induced Martensite fractions. With this distinction, the model can predict the pseudoelastic, shape memory effect, and cyclic behaviour in SMAs and take into account the tension-compression dissymmetry.

3.2.1. Constitutive law:

The 1D constitutive equation relating the second Piola-Kirchoff stress $S$ to the thermomechanical variables Green-Lagrange strain $E$, volume fraction of stress induced Martensite $\zeta_s$, and temperature $T$ is:

$$S - S_0 = D (E - E_0) + \Omega (\zeta_s - \zeta_{s_0}) + \Theta (T - T_0)$$ (1)

The $0$ subscript here denotes the initial condition of that variable. $\Theta$ is the coefficient of thermal expansion for the SMA material. $D$ is representative of the modulus of SMA material and is taken different for Martensite and Austenite structures. It is reasonably assumed that the overall modulus of the SMA structure, according to the rule of mixture, depends on the volumetric fraction of Martensite, $\zeta$, as below [139]:

$$D = D_a + \zeta (D_m - D_a)$$ (2)
Where $D_a$ and $D_m$ are respectively the modulus value of the fully Austenitic and fully Martensitic SMA material.

$\Omega$ is the transformation coefficient and can be shown to be:

$$\Omega = -\varepsilon_L D$$  \hspace{1cm} (3)

$\varepsilon_L$ is the maximum residual strain of an SMA and is found to be a constant at temperatures below Austenite finish temperature, Af. The volume fraction of Martensite is:

$$\zeta = \zeta_d + \zeta_s$$  \hspace{1cm} (4)

The stress induced Martensite, $\zeta_s$, is in turn decomposed into positive, $\zeta_{sp}$, and negative, $\zeta_{sn}$, constituents which respectively correspond to the positive and negative directions of the applied stress:

$$\zeta_s = \zeta_{sp} + \zeta_{sn}$$  \hspace{1cm} (5)

The Tanaka-based models were initially derived from the thermodynamics principles; however, they can be represented via the micromechanics Voigt model as well [140]. This requires assuming uniform distribution of the strain over the averaged volume element containing transformed and non-transformed material. (Quantities in bold face represent tensorial/vector objects) The Green-Lagrange strain tensor $\mathbf{E}$ can be decomposed into elastic $\mathbf{E}_{el}$, thermal $\mathbf{E}_{th}$, and transformation strain $\mathbf{E}_{tr}$ components (See Figure 66):

$$\mathbf{E} = \mathbf{E}_{el} + \mathbf{E}_{th} + \mathbf{E}_{tr}$$  \hspace{1cm} (6)
The large deformation framework is adopted here, although it is possible to switch back to small deformation wherever the approximation is reasonable. X, Y, and Z are the referential coordinates in the undeformed state of the material. The displacement components in such a coordinate system are taken to be u, v, and w. The deformation gradient tensor $F$ is defined as:

$$
F = \begin{bmatrix}
1 + \frac{\partial u}{\partial X} & \frac{\partial u}{\partial Y} & \frac{\partial u}{\partial Z} \\
\frac{\partial v}{\partial X} & 1 + \frac{\partial v}{\partial Y} & \frac{\partial v}{\partial Z} \\
\frac{\partial w}{\partial X} & \frac{\partial w}{\partial Y} & 1 + \frac{\partial w}{\partial Z}
\end{bmatrix}
$$

(7)

The Green-Lagrange strain, which is a measure of deformation in the material based on the square of change of length without including rigid body displacement or rotation, can be proved to be:

$$
E = \frac{1}{2} (F^T \cdot F - I)
$$

(8)
\( \mathbf{I} \) is the second order identity tensor. On the other hand, the infinitesimal strain tensor \( \mathbf{\varepsilon} \) is derived by neglecting the nonlinear elements of \( \mathbf{E} \):

\[
\mathbf{\varepsilon} = \frac{1}{2} (\mathbf{F}^T + \mathbf{F}) - \mathbf{I} = \begin{bmatrix}
\frac{\partial u}{\partial X} & \frac{1}{2} \left( \frac{\partial u}{\partial Y} + \frac{\partial v}{\partial X} \right) & \frac{1}{2} \left( \frac{\partial u}{\partial Z} + \frac{\partial w}{\partial X} \right) \\
\frac{1}{2} \left( \frac{\partial u}{\partial Y} + \frac{\partial v}{\partial X} \right) & \frac{\partial v}{\partial Y} & \frac{1}{2} \left( \frac{\partial v}{\partial Z} + \frac{\partial w}{\partial Y} \right) \\
\frac{1}{2} \left( \frac{\partial u}{\partial Z} + \frac{\partial w}{\partial X} \right) & \frac{1}{2} \left( \frac{\partial v}{\partial Z} + \frac{\partial w}{\partial Y} \right) & \frac{\partial w}{\partial Z}
\end{bmatrix}
\]

(9)

The Cauchy stress tensor \( \sigma \) is basically defined as the force per unit of the deformed area. The strain measure that is appropriate to use with the Cauchy stress tensor \( \sigma \) is the small deformation strain tensor \( \mathbf{\varepsilon} \). The problem with using the Cauchy stress tensor for analyzing materials undergoing large deformation is that the area in the deformed configuration is generally not known. Therefore, there is a need for a stress measure that can be used in the reference or undeformed configuration. The 2nd Piola-Kirchhoff stress tensor \( \mathbf{S} \) is defined as the force mapped to the undeformed configuration per unit of the undeformed area. \( \mathbf{S} \) is symmetric and energetically consistent with the Green-Lagrange strain \( \mathbf{E} \). In other words, the elastic strain energy density calculated using the 2nd Piola-Kirchhoff stress tensor with the Green-Lagrange strain will be the same as that calculated with the Cauchy stress tensor and the small deformation strain tensor:

\[
\mathbf{\sigma}: \mathbf{\varepsilon} = \mathbf{S}: \mathbf{E}
\]

(10)

The elastic stress-strain relationship implies that:

\[
\mathbf{S} = \mathbf{C} : (\mathbf{E} - \mathbf{E}_{\text{th}} - \mathbf{E}_{\text{tr}})
\]

(11)

\( \mathbf{C} \), the elastic stiffness tensor, can be defined as before by the rule of mixture:

\[
\mathbf{C} = \mathbf{C}_A + \zeta (\mathbf{C}_M - \mathbf{C}_A)
\]

(12)
Due to its insignificance compared to the transformation strain, the thermal strain will not be considered in this study.

The 2nd Piola-Kirchoff (PK) stress has the following relationship with the Cauchy stress:

\[ S = JF^{-1} \cdot \sigma \cdot F^{-T}, \quad \sigma = J^{-1} F \cdot S \cdot F^T, \quad J = \det(F) \]  \hspace{1cm} (13)

Principle of virtual work in the quasi-static form (neglecting the inertial terms) is implemented to solve for the stress/strain state of the material. The relationship between the 2nd PK stress \( S \) in the undeformed (reference) body \( V_0 \), variation of the strain \( \delta E \), density of the external body forces per unit mass \( f \), the variation of the displacement field \( \delta u \), and the field of tractions \( T \) (stress vectors) acting upon the deformed surface \( S \) (stress boundary condition) can be written as [153]:

\[ \int_{V_0} S : \delta E \ \mathrm{dv}_0 = \int_{V_0} \rho_0 f \cdot \delta u \ \mathrm{dv}_0 + \int_S T \cdot \delta u \ \mathrm{ds} \]  \hspace{1cm} (14)

Where \( \rho_0 \) is the material density in the undeformed state. For small deformation condition equation 14 can be written in the following form:

\[ \int_V \sigma : \delta \varepsilon \ \mathrm{dv} = \int_V \rho f \cdot \delta u \mathrm{dv} + \int_S T \cdot \delta u \mathrm{ds} \]  \hspace{1cm} (15)

Here \( V \) and \( \rho \) correspond to the deformed body.

**3.2.2. Transformation kinetics law**

The transformation equations and transformation stresses have been developed based on an empirically-derived cosine model for defining the relationship between the Martensite fraction, stress, and temperature during the transformation. They should be slightly modified to incorporate the decomposition of stress induced Martensite into positive and negative portions. The description of the SMA kinetics law is based on the
loading path on a Cauchy stress-temperature phase diagram illustrated in Figure 67. The fraction of Martensite depends on both the current position on the meta-equilibrium (σ-T) phase diagram and the history of the thermomechanical loading. The compression part of the diagram can approximately be a replicate of the tensile part in the opposite direction [142]; however, it is possible to alter the critical values of the stress for start of the transformation or the slopes of the transformation bands according to findings from the thermomechanical experiments on the material. Also, some researchers have proposed modifications (not included here) to this diagram such as linear increase in the critical values of the stress required for detwinning in the temperatures below Ms or distinction between transformation from twinned Martensite to Austenite than from detwinned Martensite to Austenite [135].
Figure 67 Empirical stress-temperature phase diagram showing different paths of transformation; detwinned Martensite Md, twinned Martensite in the positive Mtp and negative Mtn directions, and Austenite A.
As shown in Figure 67, the diagram here is divided into transformation regions over which the transformation to the corresponding phase occurs. In this figure, \( M_s \), \( M_f \), \( A_s \), and \( A_f \), are respectively Martensite start and finish transformation temperatures and Austenite start and finish transformation temperatures. Furthermore, \( \sigma_{sp}^{cr} \) and \( \sigma_{fp}^{cr} \) denote the critical stresses for the start and finish of the transformation into stress-induced Martensite in temperature ranges below \( M_s \).

The trend in the critical stress value at the start and end of the transformation is adequately expressed as a linear function of the temperature (according to Clausius-Clapeyron relation assuming equal stiffness and thermal expansion coefficient for Martensite and Austenite) with a slope of \( C_M \) for Martensite and \( C_A \) for Austenite transformation [139]. The stress influence factors can be different for the positive, \( C_{MP} \) & \( C_{AP} \), and negative, \( C_{MN} \) & \( C_{AN} \), directions.

The stress-temperature paths represent the following transformations:

**Paths 1 and 3 in Figure 67** Forward transformation to twinned Martensite in the positive direction \( M_{tp} \):

\[
\{1\}: \quad \text{if } T < M_s , \text{ and } \sigma_{sp}^{cr} < \sigma < \sigma_{fp}^{cr} , \text{ and } \dot{\sigma} > 0
\]

\[
\zeta_{sp} = \frac{1 - \zeta_{sp0}}{2} \cos \left( \frac{\pi}{\sigma_{sp}^{cr} - \sigma_{fp}^{cr}} \left[ \sigma - \sigma_{fp}^{cr} \right] \right) + \frac{1 + \zeta_{sp0}}{2}
\]

\[
\zeta_d = \zeta_{d0} \left( \frac{1 - \zeta_{sp}}{1 - \zeta_{sp0}} \right), \quad \zeta_{sn} = \zeta_{sn0} \left( \frac{1 - \zeta_{sp}}{1 - \zeta_{sp0}} \right), \quad \zeta_s = \zeta_{sp} + \zeta_{sn}
\]

\[
\{3\}: \quad \text{if } T > M_s , \text{ and}
\]

\[
\sigma_{sp}^{cr} + C_{MP} (T - M_s) < \sigma < \sigma_{fp}^{cr} + C_{MP} (T - M_s) , \text{ and } \dot{\sigma} > T C_{MP}
\]
\[
\zeta_{sp} = \frac{1 - \zeta_{sp_0}}{2} \cos \left\{ \frac{\pi}{\sigma_{sp}^{cr} - \sigma_{fp}^{cr}} \left[ \sigma - \sigma_{fp}^{cr} - C_{MP} (T - M_s) \right] \right\} + \frac{1 + \zeta_{sp_0}}{2}
\]

\[
\zeta_d = \zeta_{d_0} \left( \frac{1 - \zeta_{sp}}{1 - \zeta_{sp_0}} \right), \quad \zeta_{sn} = \zeta_{sn_0} \left( \frac{1 - \zeta_{sp}}{1 - \zeta_{sp_0}} \right), \quad \zeta_s = \zeta_{sp} + \zeta_{sn}
\]

The reason behind the third condition for the above equations can be clarified by referring to Figure 68. The trajectory of the state of stress and temperature on the stress-temperature phase diagram should be appropriate for the transformation to take place. The transformation to twinned Martensite occurs only if the rate of change for the stress and temperature follows the circle-dotted line which means if \( \dot{\sigma} > \dot{T}_{C_{MP}} \). By the same token, the reverse transformation to Austenite happens on the square-dotted line i.e. only if \( \dot{\sigma} < \dot{T}_{C_{MP}} \).

Figure 68 The path conditions for transformation to Martensite or Austenite.
(Paths 2 and 4 in Figure 67) Forward transformation to twinned Martensite

in the negative direction Mtn:

{2}: if $T < M_s$, and $\sigma_{fn}^{cr} < \sigma < \sigma_{sn}^{cr}$, and $\dot{\sigma} < 0$ \hspace{1cm} (18)

\[
\zeta_{sn} = \frac{1 - \zeta_{sn_0}}{2} \cos \left( \frac{\pi}{\sigma_{sn}^{cr} - \sigma_{fn}^{cr}} [\sigma - \sigma_{sn}^{cr}] \right) + \frac{1 + \zeta_{sn_0}}{2}
\]

\[
\zeta_d = \zeta_{d_0} \left( \frac{1 - \zeta_{sn}}{1 - \zeta_{sn_0}} \right), \quad \zeta_{sp} = \zeta_{sp_0} \left( \frac{1 - \zeta_{sn}}{1 - \zeta_{sn_0}} \right), \quad \zeta_s = \zeta_{sp} + \zeta_{sn}
\]

\[
\zeta_{sp} = \zeta_{sp_0} \left( \frac{1 - \zeta_{sn}}{1 - \zeta_{sn_0}} \right), \quad \zeta_s = \zeta_{sp} + \zeta_{sn}
\]

{4}: if $T > M_s$, and

\[
\sigma_{fn}^{cr} + C_{Mn} (T - M_s) < \sigma < \sigma_{sn}^{cr} + C_{Mn} (T - M_s), \text{ and } \dot{\sigma} < \dot{T} C_{Mn}
\]

\[
\zeta_{sn} = \frac{1 - \zeta_{sn_0}}{2} \cos \left( \frac{\pi}{\sigma_{sn}^{cr} - \sigma_{fn}^{cr}} [\sigma - \sigma_{sn}^{cr} - C_{Mn} (T - M_s)] \right) + \frac{1 + \zeta_{sn_0}}{2}
\]

\[
\zeta_d = \zeta_{d_0} \left( \frac{1 - \zeta_{sn}}{1 - \zeta_{sn_0}} \right), \quad \zeta_{sp} = \zeta_{sp_0} \left( \frac{1 - \zeta_{sn}}{1 - \zeta_{sn_0}} \right), \quad \zeta_s = \zeta_{sp} + \zeta_{sn}
\]

(Paths 5 and 6 in Figure 67) Reverse transformation to Austenite:

{5}: if $T > A_s$, and

\[
C_{An} (T - A_s) < \sigma < \min \left[ 0, C_{An} (T - A_f) \right], \text{ and } \dot{\sigma} > \dot{T} C_{An}
\]

\[
\zeta_{sp} = \frac{\zeta_{sp_0}}{2} \left\{ \cos \left[ a_A \left( T - A_s - \frac{\sigma}{C_{An}} \right) \right] + 1 \right\}
\]

\[
\zeta_{sn} = \frac{\zeta_{sn_0}}{2} \left\{ \cos \left[ a_A \left( T - A_s - \frac{\sigma}{C_{An}} \right) \right] + 1 \right\}
\]
\[
\zeta_d = \frac{\zeta_{d0}}{2} \left\{ \cos \left[ a_A \left( T - A_s - \frac{\sigma}{C_{an}} \right) \right] + 1 \right\}
\]

\[
\zeta = \zeta_d + \zeta_{sp} + \zeta_{sn}
\]

\{6\}: \text{if } T > A_s, \text{ and}

\[
\max(0, C_{Ap} (T - A_f)) < \sigma < C_{Ap} (T - A_s), \text{ and } \dot{\sigma} < \dot{T} C_{Ap}
\]

\[
\zeta_{sp} = \frac{\zeta_{sp0}}{2} \left\{ \cos \left[ a_A \left( T - A_s - \frac{\sigma}{C_{Ap}} \right) \right] + 1 \right\}
\]

\[
\zeta_{sn} = \frac{\zeta_{sn0}}{2} \left\{ \cos \left[ a_A \left( T - A_s - \frac{\sigma}{C_{Ap}} \right) \right] + 1 \right\}
\]

\[
\zeta_d = \frac{\zeta_{d0}}{2} \left\{ \cos \left[ a_A \left( T - A_s - \frac{\sigma}{C_{Ap}} \right) \right] + 1 \right\}
\]

\[
\zeta = \zeta_d + \zeta_{sp} + \zeta_{sn}
\]

(Path 7 in Figure 67) Forward Transformation to twinned Martensite Md:

\{7\}: \text{if } M_f < T < M_s, \text{ and } \sigma_{fr}^{cr} < \sigma < \sigma_{fr}^{cr}, \text{ and } \dot{T} < 0

\[
\zeta_d = \frac{1 - \zeta_{sp} - \zeta_{sn} - \zeta_{d0}}{2} \{ \cos[a_M (T - M_f)] \} + \frac{1 - \zeta_{sp} - \zeta_{sn} + \zeta_{d0}}{2}
\]

\[
\zeta = \zeta_d + \zeta_{sp} + \zeta_{sn}
\]

In the above equations, \(\dot{\sigma}\) and \(\dot{T}\) are the rate of change of stress and temperature respectively; also \(a_M = \frac{\pi}{M_s - M_f}\), and \(a_A = \frac{\pi}{A_f - A_s}\).
The same argument, as depicted in Figure 68, can be set forth regarding the path conditions for the rest of the transformation equations. The direction of the thermomechanical loading path is important for the transformation to occur and should be such that its normal distance to the destination phase boundary does continuously reduce. Furthermore, it should be noted that the zero value for different variables (e.g. \( \zeta_{sp} \)) are the amount of that variable at the start (or re-start) of the transformation process.

The initial or 0 values are described according to the following equations:

\[
\begin{align*}
\{1\} & \quad \zeta_{sp_0} = \frac{2\zeta_{sp} - 1 - \cos \left\{ \frac{\pi}{\sigma_{sp}^{cr} - \sigma_{fp}^{cr}} [\sigma - \sigma_{fp}^{cr}] \right\}}{1 - \cos \left\{ \frac{\pi}{\sigma_{sp}^{cr} - \sigma_{fp}^{cr}} [\sigma - \sigma_{fp}^{cr}] \right\}}, \\
\zeta_{sn_0} &= \zeta_{sn} \frac{1 - \zeta_{sp_0}}{1 - \zeta_{sp}}, \quad \zeta_{d_0} = \zeta_{d} \frac{1 - \zeta_{sp_0}}{1 - \zeta_{sp}}.
\end{align*}
\]

\[
\begin{align*}
\{2\} & \quad \zeta_{sn_0} = \frac{2\zeta_{sn} - 1 - \cos \left\{ \frac{\pi}{\sigma_{sn}^{cr} - \sigma_{fn}^{cr}} [\sigma - \sigma_{fn}^{cr}] \right\}}{1 - \cos \left\{ \frac{\pi}{\sigma_{sn}^{cr} - \sigma_{fn}^{cr}} [\sigma - \sigma_{fn}^{cr}] \right\}}, \\
\zeta_{sp_0} &= \zeta_{sp} \frac{1 - \zeta_{sn_0}}{1 - \zeta_{sn}}, \quad \zeta_{d_0} = \zeta_{d} \frac{1 - \zeta_{sn_0}}{1 - \zeta_{sn}}.
\end{align*}
\]

\[
\begin{align*}
\{3\} & \quad \zeta_{sp_0} = \frac{2\zeta_{sp} - 1 - \cos \left\{ \frac{\pi}{\sigma_{sp}^{cr} - \sigma_{fp}^{cr}} [\sigma - \sigma_{fp}^{cr} - C_{Mp} (T - M_s)] \right\}}{1 - \cos \left\{ \frac{\pi}{\sigma_{sp}^{cr} - \sigma_{fp}^{cr}} [\sigma - \sigma_{fp}^{cr} - C_{Mp} (T - M_s)] \right\}}, \\
\zeta_{sn_0} &= \zeta_{sn} \frac{1 - \zeta_{sp_0}}{1 - \zeta_{sp}}, \quad \zeta_{d_0} = \zeta_{d} \frac{1 - \zeta_{sp_0}}{1 - \zeta_{sp}}.
\end{align*}
\]
\{4\} \quad \zeta_{sn_0} = \frac{2\zeta_{sn} - 1 - \cos\left\{\frac{\pi}{\sigma_{sn}^c - \sigma_{fn}^c}\left[\sigma - \sigma_{fn}^c - C_{Mn} (T - M_s)\right]\right\}}{1 - \cos\left\{\frac{\pi}{\sigma_{sn}^c - \sigma_{fn}^c}\left[\sigma - \sigma_{fn}^c - C_{Mn} (T - M_s)\right]\right\}},

\zeta_{sp_0} = \zeta_{sp} \frac{1 - \zeta_{sn_0}}{1 - \zeta_{sn}}, \quad \zeta_{d_0} = \zeta_{d} \frac{1 - \zeta_{sn_0}}{1 - \zeta_{sn}}.

\{5\} \quad \zeta_{sp_0} = \frac{2\zeta_{sp}}{\left\{\cos\left[a_A \left(T - A_s - \frac{\sigma}{C_{An}}\right)\right] + 1\right\}},

\zeta_{sn_0} = \frac{2\zeta_{sn}}{\left\{\cos\left[a_A \left(T - A_s - \frac{\sigma}{C_{An}}\right)\right] + 1\right\}},

\zeta_{d_0} = \frac{2\zeta_{d}}{\left\{\cos\left[a_A \left(T - A_s - \frac{\sigma}{C_{An}}\right)\right] + 1\right\}},

\{6\} \quad \zeta_{sp_0} = \frac{2\zeta_{sp}}{\left\{\cos\left[a_A \left(T - A_s - \frac{\sigma}{C_{Ap}}\right)\right] + 1\right\}},

\zeta_{sn_0} = \frac{2\zeta_{sn}}{\left\{\cos\left[a_A \left(T - A_s - \frac{\sigma}{C_{Ap}}\right)\right] + 1\right\}},

\zeta_{d_0} = \frac{2\zeta_{d}}{\left\{\cos\left[a_A \left(T - A_s - \frac{\sigma}{C_{Ap}}\right)\right] + 1\right\}},

\{7\} \quad \zeta_{d_0} = \frac{2\zeta_{d} - (1 - \zeta_{sp} - \zeta_{sn})\{1 + \cos[a_M (T - M_f)]\}}{\{1 - \cos[a_M (T - M_f)]\}}.

There is a problem of division by zero in the initial condition equations. It was circumvented by substituting the Taylor series expansion (about zero) of the trigonometric functions in such cases.
Following is the transformation kinetics relations for the aforementioned thermomechanical paths in the rate form:

\[
\dot{\zeta} = \begin{bmatrix} \dot{\zeta}_{sp} \\ \dot{\zeta}_{sn} \\ \dot{\zeta}_{d} \end{bmatrix}^T = A \cdot C^d \quad \text{or} \quad \dot{\zeta}_i = A_{ij} C^d_j
\]  

(23)

Matrix \( A \) contains the rate of change of different Martensite phases with respect to the pseudo-time and is defined as below:

\[
A_{11} = \frac{1 - \zeta_{sp}}{2} \left( -\frac{\pi \sigma}{\sigma_{sp}^c - \sigma_{fp}^c} \right) \sin \left\{ \frac{\pi}{\sigma_{sp}^c - \sigma_{fp}^c} \left( \sigma - \sigma_{fp}^c \right) \right\},
\]

(24)

\[
A_{21} = \zeta_{sn} \frac{-A_{11}}{1 - \zeta_{sp}}, \quad A_{31} = \zeta_d \frac{-A_{11}}{1 - \zeta_{sp}};
\]

\[
A_{12} = \zeta_{sp} \frac{-A_{22}}{1 - \zeta_{sn}},
\]

\[
A_{22} = \frac{1 - \zeta_{sn}}{2} \left( -\frac{\pi \sigma}{\sigma_{sn}^c - \sigma_{fn}^c} \right) \sin \left\{ \frac{\pi}{\sigma_{sn}^c - \sigma_{fn}^c} \left( \sigma - \sigma_{fn}^c \right) \right\},
\]

\[
A_{32} = \zeta_d \frac{-A_{22}}{1 - \zeta_{sn}};
\]

\[
A_{13} = \frac{1 - \zeta_{sp}}{2} \left( -\frac{\pi (\sigma - C_{M_p} \dot{T})}{\sigma_{sp}^c - \sigma_{fp}^c} \right) \sin \left\{ \frac{\pi}{\sigma_{sp}^c - \sigma_{fp}^c} \left[ \sigma - \sigma_{fp}^c - C_{M_p} (T - M_s) \right] \right\},
\]

\[
A_{23} = \zeta_{sn} \frac{-A_{13}}{1 - \zeta_{sp}}, \quad A_{33} = \zeta_d \frac{-A_{13}}{1 - \zeta_{sp}}; \quad A_{14} = \zeta_{sp} \frac{-A_{24}}{1 - \zeta_{sn}},
\]

\[
A_{24} = \frac{1 - \zeta_{sn}}{2} \left( -\frac{\pi (\sigma - C_{M_n} \dot{T})}{\sigma_{sn}^c - \sigma_{fn}^c} \right) \sin \left\{ \frac{\pi}{\sigma_{sn}^c - \sigma_{fn}^c} \left[ \sigma - \sigma_{fn}^c - C_{M_n} (T - M_s) \right] \right\},
\]

(23)
\[
A_{34} = \frac{-A_{24}}{1 - \zeta_{sn_0}};
\]

\[
A_{15} = -\frac{a_A}{2} \zeta_{sp_0} (\dot{T} - \frac{\dot{\sigma}}{C_{An}}) \sin \{a_A (T - A_s - \frac{\sigma}{C_{An}})\},
\]

\[
A_{25} = -\frac{a_A}{2} \zeta_{sn_0} (\dot{T} - \frac{\dot{\sigma}}{C_{An}}) \sin \{a_A (T - A_s - \frac{\sigma}{C_{An}})\},
\]

\[
A_{35} = -\frac{a_A}{2} \zeta_{d_0} (\dot{T} - \frac{\dot{\sigma}}{C_{An}}) \sin \{a_A (T - A_s - \frac{\sigma}{C_{An}})\};
\]

\[
A_{16} = -\frac{a_A}{2} \zeta_{sp_0} (\dot{T} - \frac{\dot{\sigma}}{C_{Ap}}) \sin \{a_A (T - A_s - \frac{\sigma}{C_{Ap}})\},
\]

\[
A_{26} = -\frac{a_A}{2} \zeta_{sn_0} (\dot{T} - \frac{\dot{\sigma}}{C_{Ap}}) \sin \{a_A (T - A_s - \frac{\sigma}{C_{Ap}})\},
\]

\[
A_{36} = -\frac{a_A}{2} \zeta_{d_0} (\dot{T} - \frac{\dot{\sigma}}{C_{Ap}}) \sin \{a_A (T - A_s - \frac{\sigma}{C_{Ap}})\};
\]

\[
A_{17} = A_{27} = 0,
\]

\[
A_{37} = -a_M \frac{(1 - \zeta_{sp} - \zeta_{sn}) - \zeta_{d_0}}{2} \dot{T} \sin \{a_M (T - M_f)\} - \frac{\zeta_{sp} + \zeta_{sn}}{2} (1 + \cos \{a_M (T - M_f)\})
\]

The vector $C^d$ holds the conditions of transformation for each path. It ensures that no transformation occurs while loading along the so-called dead directions or acting in the dead zones. It can be described as below:

\[
C^d_{1} = \langle T < M_s \rangle \ast \langle \sigma < \sigma_{fp}^{cr} \rangle \ast \langle \sigma_{sp}^{cr} < \sigma \rangle \ast \langle 0 < \dot{\sigma} \rangle,
\]

\[
C^d_{2} = \langle T < M_s \rangle \ast \langle \sigma < \sigma_{sn}^{cr} \rangle \ast \langle \sigma_{fn}^{cr} < \sigma \rangle \ast \langle \dot{\sigma} < 0 \rangle,
\]
\[
C^d_3 = (M_s \leq T) \ast (\sigma < \sigma^c_{fp} + C_{Mp}(T - M_s)) \ast (\sigma^c_{sp} + C_{Mp}(T - M_s) < \sigma) \\
\ast (C_{Mp} \dot{T} < \dot{\sigma}),
\]

\[
C^d_4 = (M_s \leq T) \ast (\sigma < \sigma^c_{sn} + C_{Mn}(T - M_s)) \ast (\sigma^c_{fn} + C_{Mn}(T - M_s) < \sigma) \\
\ast (\dot{\sigma} < C_{Mn} \dot{T}),
\]

\[
C^d_5 = (A_s \leq T) \ast (\sigma < \min[t = 0, C_{An}(T - A_f)]) \ast (C_{An}(T - A_s) < \sigma) \\
\ast (C_{An} \dot{T} < \dot{\sigma}),
\]

\[
C^d_6 = (A_s \leq T) \ast (\sigma < C_{Ap}(T - A_s)) \ast (\max[0, C_{Ap}(T - A_f)] < \sigma) \\
\ast (\dot{\sigma} < C_{Ap} \dot{T}),
\]

\[
C^d_7 = (T < M_s) \ast (M_f < T) \ast (\sigma < \sigma^c_{fp}) \ast (\sigma^c_{fn} < \sigma) \ast (\dot{T} < 0)
\]

The quantity \(\ast\) equals one if the logical expression inside it is true; otherwise it is zero.

Since in this study only 1D and cantilever bending situations are investigated, the components of the transformation strain other than axial (z direction) are neglected. Therefore there will be:

\[
E_{zz}^{tr} = \varepsilon_{Lp} \zeta_{sp} + \varepsilon_{Ln} \zeta_{sn}
\]  \(26\)

\(\varepsilon_{Lp}\) and \(\varepsilon_{Ln}\) are the maximum transformation strains in tension and compression respectively. The coefficient of asymmetry \(\tau\) is defined as the following proportionalities:

\[
\tau = -\frac{C_{An}}{C_{Ap}} = -\frac{C_{Mn}}{C_{Mp}} = -\frac{\sigma^c_{sn}}{\sigma^c_{sp}} = -\frac{\sigma^c_{fn}}{\sigma^c_{fp}} = -\frac{\varepsilon_{Lp}}{\varepsilon_{Ln}}
\]  \(27\)

Although NiTi was shown to have asymmetric properties in tension and compression [143] [144] [156], the transformation properties in compression are
considered to be the mirror opposite (unless otherwise stated) of their tensional counterparts; i.e. $\tau = 1$.

3.3. One-dimensional modeling via COMSOL Multiphysics®:

The nonlinear equations mentioned so far (stress-strain relations and phase transformation kinetics) form a system of algebraic-differential equations (ADE). For the case of the 1D situation in a shape memory rod (See Figure 69), the principle of virtual work in the small displacements framework reduces to the equilibrium equation as:

$$\sigma_{ij, j} = 0 \implies \frac{\partial \sigma}{\partial x} = 0$$ (28)

Where $\sigma$ is the axial stress in the rod. The cross section area of the rod is considered to be constant.

![Figure 69 SMA rod under axial force.](image)

The heat transfer equation considering conduction along the SMA rod can be written as:

$$\nabla \cdot (k\nabla T) + \dot{q} = \rho c_p \frac{\partial T}{\partial t} \implies k \left( \frac{\partial^2 T}{\partial x^2} \right) = \rho c_p \frac{\partial T}{\partial t}$$ (29)

In which $k$ is the thermal conductivity, $\rho$ is the material density assumed here to be independent of the phase fraction, $C_p$ is the specific heat, and $\dot{q}$ is the heat generation
per unit volume. \( \dot{q} \) can account for the exothermic or endothermic reverse and forward transformations.

\[
\dot{q} = h_{sp} \dot{\zeta}_{sp} + h_{sn} \dot{\zeta}_{sn} + h_{d} \dot{\zeta}_{d} \tag{30}
\]

For the purpose of this model, latent heats \((h_{sp}, h_{sn}, h_{d})\) are neglected which is consistent with what the operational circumstances of the \textit{SMArt} TM pedicle screw in the human vertebrae impose.

The system of ADE is solved via COMSOL Multiphysics® PDE module. The system below is generally solved with the Galerkin method after discretization of the domain.

\[
\begin{align*}
\sum_{i} d_{ii} \frac{\partial \chi_i}{\partial t} + \frac{\partial \Gamma_{ij}}{\partial x_j} &= F_{i} & \text{in } V \\
-n_j \Gamma_{ij} &= G_{i} + \frac{\partial R_m}{\partial u_l} \mu_m & \text{on } S \\
0 &= R_m & \text{on } S
\end{align*}
\tag{31}
\]

Where \( V \) is the computational domain over which the PDE system (the first equation in 31) is defined. The second and the third equations are respectively the generalized Neumann and Dirichlet boundary conditions defined on \( S \), the domain boundary.

\( \chi \) is the vector of dependent variables, to find whom the equation is solved, and \( d \) is the matrix of mass coefficient. The vectors \( \Gamma, F, G, \) and \( R \) are coefficient vectors and can be functions of the spatial coordinates, the solution \( \chi \), and the space derivatives of \( \chi \).

\( \mu \) is a dependant variable, called the Lagrange multiplier, and represents the reaction forces in the structural mechanics problems.

Finally, \( n \) is the outward unit vector normal to \( S \).
For the current study:

$$\chi = [u \ \zeta_{sp} \ \zeta_{sn} \ \zeta_{d} \ T]^T$$  \hspace{1cm} (32)

$$\Gamma = [\sigma \ 0 \ 0 \ 0 \ (-k \frac{\partial T}{\partial x})]^T$$

$$F = [0 \ A_1 j C_j^d \ A_2 j C_j^d \ A_3 j C_j^d \ 0]^T$$

As illustrated in Figure 69, one side of the SMA rod modeled here is fixed in the space and under a temperature boundary condition (B.C.). This means the Dirichlet boundary condition (the third equation in 31) for the fixed end should be defined as:

$$R = [u \ 0 \ 0 \ 0 \ (T - \text{tempinc})]^T$$  \hspace{1cm} (33)

The other end of the rod is under application of an external force. Thus the Neumann boundary condition (the second equation in 31) for the loaded end is:

$$G = [(-\text{forceinc}) \ 0 \ 0 \ 0 \ 0]^T$$  \hspace{1cm} (34)

In which \text{forceinc} and \text{tempinc} are the functions of pseudo-time that define the applied external force and temperature respectively.

The problem, reworded in matrix notation, is as following:

$$
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & -h_{sp} & -h_{sn} & -h_{d} & \rho c_p \\
\end{bmatrix}
\begin{bmatrix}
\dot{u} \\
\dot{\zeta}_{sp} \\
\dot{\zeta}_{sn} \\
\dot{\zeta}_{d} \\
\end{bmatrix}
+ \frac{\partial}{\partial x}
\begin{bmatrix}
\sigma \\
0 \\
0 \\
\end{bmatrix}
= \begin{bmatrix}
0 \\
A_1 j C_j^d \\
A_2 j C_j^d \\
A_3 j C_j^d \\
\end{bmatrix}
$$

$$(\text{fixed end}) \rightarrow R = \begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
\end{bmatrix} = \emptyset$$
The foregone axial problem is solved under various loading and boundary conditions to represent the capabilities of the model. The developed model herein can adequately capture shape memory effect, superelasticity, partial loading/unloading, and asymmetric thermomechanical properties of shape memory alloys in tension and compression.

### 3.4. Two-dimensional/Three-dimensional generalization of the model:

The system of equations described in a 1D platform, as the material of the last section 3.3., is now generalized to 2D/3D considering the evolution of phases to occur only in the axial direction bearing the dominant stress values. It is worth mentioning that although the dissymmetry effect has been proved for some shape memory alloys, Rejzner et al. [145] showed that neglecting this dissymmetry effect doesn’t have a significant influence on the predictions of the SMA NiTi beam behavior.

Three application modules namely the Structural Mechanics, Partial Differential Equation (PDE) solver, and Heat Transfer module were used to solve the problem. The structural mechanics module was responsible for solving the equations of virtual work (See equations 14 and 15) with dependant variables of displacement components in the Cartesian coordinates; u, v, and w. The kinetics of the Martensite transformation was
modeled through the PDE module using the same approach and equation system as in the 1D situation. From this module, the transformation strains were obtained and integrated into the solid mechanics equations. Also, the heat transfer module was supposed to solve the heat equation for heat conduction in the component and possible convection interactions with the environment. Figure 70 illustrates the interaction between different modules to solve this problem.

![Diagram showing the interaction between different modules of COMSOL Multiphysics to model 2D/3D SMA applications.](image)

The resulted system of nonlinear PDEs is solved by a damped Newton Iteration method. The nonlinear problem is discretized into linearized integration steps by forming a Jacobian (stiffness) matrix.

The equation of virtual work for a 3D model reduces to the following equilibrium equation in the matrix form:
Where \( \nu \) is the Poisson ratio and follows the mixture rule, like the modulus \( D \). In addition:

\[
\begin{align*}
\frac{E_{zz}^{el}}{E_{zz}^{tr}} = & E_{zz} - \left( \varepsilon_{Lp} \zeta_{sp} + \varepsilon_{Ln} \zeta_{sn} \right) \\
D &= D_a + \zeta (D_m - D_a) \\
\nu &= \nu_a + \zeta (\nu_m - \nu_a) \\
\zeta &= \zeta_{sp} + \zeta_{sn} + \zeta_d
\end{align*}
\]

For the special case of a 2D plane stress problem, the above equations are modified accordingly to exclude the neglected dimension and its corresponding stresses.

**3.5. Finite Element Simulation of the SMArt™ pedicle screw**

Pedicle screws, which are used as an anchoring point for implanting spinal instrumentations in the spinal fracture and deformity treatments, entail a major drawback i.e. loosening and back-out in the osteoporotic bone. The strength of the screw contact with the surrounding bone diminishes as the bone degrades e.g. due to osteoporosis.
A *SMArt*™ pedicle screw design was previously developed to address this issue which uses NiTi superelastic-shape memory coils wrapped around it. The smart assembly consists of an external superelastic tube which is responsible for expanding the design protrusions when reached to body temperature; also an internal shape memory wire, inserted into the tube, is sought to retract the assembly while locally heated to above the body temperature (Refer to section 2.6. for more details).

The whole assembly can be evaluated and optimized as for the interaction of the superelastic tube and shape memory wire using the model developed in COMSOL Multiphysics.

**3.5.1. Definition of the problem:**

Bone screws have been used in spinal instrumentation since the 1940s. A pedicle screw is a particular type of bone screw designed for implantation into a vertebral pedicle. The pedicle screw provides a means of gripping a spinal segment. The screws themselves do not fixate the spinal segment, yet act as firm anchor points that can be connected with other spinal instrumentations. One major drawback in spinal surgery using pedicle screws is due to the adverse effects of osteoporosis. Osteoporotic bone, because of the degradation of the supporting bone structures, cannot provide enough anchoring foundation for the screw to be implanted into; therefore pedicle screw placement in the osteoporotic bone involves the risk of intra-operation or post-operation screw pull-out/loosening.

One proposed solution to enhance the performance of the pedicle screws in the osteoporotic bone utilizes shape memory-superelastic NiTi antagonistic beam assembly. The β version of the *SMArt*™ screw consists of a base screw and a few assemblies of
SMA wire and tube. The base screw is similar to the conventional pedicle screws except for an additional circular thread cut on the minor surface as well as transverse.

The SMA wire-tube assembly will be inserted and fixated into these holes. The wire should activate at above body temperature and it should be in Martensite phase when in body temperature. The tube, made of another composition of NiTi, has an activation temperature around body temperature.

The wire should be inserted into the tube. Then the assembly of wire and tube is wrapped around the base screw and fitted in the circular cut on the surface of the screw. The stem of the wire-tube assembly is welded to the screw for achieving better fixation. The assembly of the wire and tube is depicted in Figure 71.

Figure 71 The SMA helical insert is welded to the transverse holes on the body of the screw. (Shown as assembled for more clarity)
3.5.2. Antagonistic shape memory-superelastic beam assembly:

The assembly consists of a superelastic NiTi (with lower Af temperature) tubular beam and a shape memory NiTi (with higher Af temperature) circular beam; as illustrated in Figure 72. Moreover according to Figure 73, the initial memorized shapes of both the tube and the wire are bent off the centerline in opposite directions. The basis of operation is the difference in the transformation temperatures between the wire and the tube. At a so-called low temperature (body temperature 37°C for the present biomedical purpose), the tube is superelastic and the wire is shape memory. On the other hand, at a higher temperature level (suppose 70°C) the wire also becomes superelastic. Beyond this level of temperature, both the wire and the tube exist in Austenite state, at which their memorized shape is stable. This process is depicted in Figure 74. Suppose the operation process begins from a very low temperature at which the assembly resides in a straight state; deformed compared to the memorized shapes. By reaching the lower temperature level as the second stage, the tube will transform to the stiffer Austenite form while the wire will remain in the flexible Martensite form; hence the tube tends to raise the assembly upwards towards its memorized situation. The third stage is to heat the assembly to the high temperature level. By that point, the wire also will have become Austenite and have acted against the current situation, pushing the assembly down.
Figure 72 The antagonistic beam assembly.

Figure 73 Initial memorized shapes of the assembly components.

Figure 74 Assembly at (a) low temperature (second stage), (b) high temperature (third stage).
Figure 75 (a) The assembly in the straight condition, (b) desired low temperature form (37°C) after activation of the tube: the assembly is bent upwards, (c) desired high temperature form (70°C) after activation of the wire: the assembly is re-bent downwards.

Functioning of the smart pedicle screw requires that the amount by which the assembly moves upwards at body temperature (Figure 75-b) to be large. In addition, the amount of bending downwards at high temperature (Figure 75-c) should be such that the assembly gets back as much as possible to the zero straight condition (Figure 75-a).

These requirements necessitate a parametric analysis to be performed so that the optimum configuration in terms of the several variables forming the assembly could be found. These variables include:

- The diameters of the wire and the tube,
- The transformation temperatures of the wire and the tube,
- The Austenite-Martensite moduli,
- The initial memorized deflection of the wire and the tube, etc.
The physical and shape memory properties of SMAs are virtually imposed by the supplier of the material and therefore are not considered as variable in this study. In the next section of this study, two NiTi alloys will be considered with different transformation and thermomechanical properties. The analysis will then be focused on the geometrical aspects’ of the assembly; namely the diameters and initial deflections.

3.5.3. Proposed solution approach:

Thus far, the problem of the SM-SE antagonistic beam assembly is defined. Various nonlinearities have been introduced by considering the shape memory effect, large deformation framework, and the wire-tube contact so that the problem is not efficiently solvable. Therefore, there is a need for a simplified approximation that moderates the cost of the original severely nonlinear problem.

To this end, a shortcut objective process is proposed that is schematically drawn in Figure 76. $\delta_{B_1}$ and $\delta_{A_1}$ are the initial tip deflections of the tube B and the wire A in their memorized shapes respectively. For the purpose of simplicity, the two mating beams are modeled as two serially connected springs with nonlinear stiffness properties. Some approximations are included herein: firstly, the shear force between the wire and the tube is neglected therefore the problem reduces to two entangled beams having the same curvature at every cross section. Secondly, the hysteresis effect during the unloading of the superelastic beam and the linear elastic unloading of the shape memory beam are also disregarded. Thus, the behavior of the beams is modeled as nonlinear elastic materials with stiffness properties shown later on. In fact, it could be proved that the hysteresis or linear loading of the material tends to help further achieve the objective functionality of the assembly and neglecting them is a conservative assumption.
According to Figure 76, the overall deflection of the system at low temperature, \( \Delta_L \), can be solved via this system of nonlinear equations:

\[
\begin{align*}
\{ & F_{A2} - F_{B2} = 0 \\
& \delta_{A2} + \delta_{B2} - \delta_{B1} - \delta_{A1} = 0
\}
\tag{37}
\end{align*}
\]

\[ \Delta_L = \delta_{B1} - \delta_{B2} = \delta_{A2} - \delta_{A1} \]

By the same token, the overall deflection of the assembly at high temperature, \( \Delta_H \), can be found by:

\[
\begin{align*}
\{ & F_{A3} - F_{B3} = 0 \\
& \delta_{A3} + \delta_{B3} - \delta_{B1} - \delta_{A1} = 0
\}
\tag{38}
\end{align*}
\]

\[ \Delta_H = \delta_{B1} - \delta_{B3} = \delta_{A3} - \delta_{A1} \]
Figure 76 Schematic procedure representing the approximate functionality of the antagonistic beam assembly.
Chapter Four

Results and discussions

4.1. 1D preliminary simulations:

The results of the simulation of a 1D SMA rod are presented in this section. The NiTi SMA has the mechanical/transformation properties as tabulated in Table 3.

Table 3 Material properties for NiTi [139][146][147]

<table>
<thead>
<tr>
<th>Moduli</th>
<th>Transformation temperatures (°C)</th>
<th>Transformation constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_a = 67 \times 10^3$ MPa</td>
<td>$M_f = 9$</td>
<td>$C_M = 8$ MPa/°C</td>
</tr>
<tr>
<td>$D_m = 26.3 \times 10^3$ MPa</td>
<td>$M_s = 18.4$</td>
<td>$C_A = 13.8$ MPa/°C</td>
</tr>
<tr>
<td>$\Theta = 0.55$ MPa/°C</td>
<td>$A_s = 34.5$</td>
<td>$\sigma_s^{cr} = 100$ MPa</td>
</tr>
<tr>
<td>$\nu = 0.33$</td>
<td>$A_f = 49$</td>
<td>$\sigma_f^{cr} = 170$ MPa</td>
</tr>
<tr>
<td>Maximum residual</td>
<td>Density (Kg/mm3)</td>
<td>Specific heat (J/Kg °C)</td>
</tr>
<tr>
<td>strain (%)</td>
<td>$\varepsilon_L = 6.7$</td>
<td>$\rho = 6.45 \times 10^{-6}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$k = 10$</td>
</tr>
</tbody>
</table>
A rod of NiTi SMA is supposed to be held fixed at one side and undergo an axial force from the other side (See Figure 69). Various instances of preliminary thermomechanical loadings are applied in this simulation with the purpose of examining the functionality and accuracy of the proposed model.

**Preliminary test 1:**

In the first example, force and temperature were altered separately in the rod according to Figure 77 and Figure 78.

![Figure 77 Force profile for the preliminary test #1.](image)
The rod was initially unstressed and fully in detwinned Martensite. As it was mentioned before, time in this study is the pseudo-time and defines the evolution of the dependant variables. The stress was cycled to an amount more than the critical value to finish the detwinning process in both tension and compression at a temperature below Mf and then was kept zero while the temperature was elevated to above Af. Figure 79 illustrates the evolution of different phases due to this loading procedure.
The detwinned Martensite was vanished as a result of two stages of completed reorientation and detwinning to stress-induced Martensite in tension and compression. The Martensite phases were totally transformed by the time temperature had passed Austenite finish 49°C and the developed Austenite finally transformed into twinned (or self-accommodated) Martensite while the temperature fell below Mf.

This process is further clarified in Figure 80 where the change of Martensite fraction ($\zeta = \zeta_{sp} + \zeta_{sn} + \zeta_{d}$) with respect to the temperature is depicted. The smooth transformation curves are developed as a result of using cosine form of the kinetics law. Also, the start and finish of the transformation are accurately specified at the corresponding temperatures.
Figure 80 Evolution of the Martensite fraction with respect to the change of temperature in preliminary test #1.

Moreover, this simulation exemplifies the shape memory effect as observed in Figure 81 which depicts the stress-strain graph for the rod. The nonlinearity and formation of transformation strains in both negative and positive directions can be clearly seen from this figure. The residual strain after unloading from the rod is recovered by raising the temperature up to Af whereas the formation of detwinned Martensite does not incur any shape change as predicted.
Preliminary test 2:

The temperature for the second example was maintained constant at 10 °C (below As); however the force was cycled such that the stress followed the profile shown in Figure 82. The rod was fully detwinned Martensite before the start of the loading. This test manifests the partial loading/unloading behavior in shape memory alloys. The stress increased up to a level not enough for the finish of detwinning transformation but rose again after a relatively small decline. No transformation occurred during the partial unloading according to Figure 83, which depicts the evolution of various Martensite fractions.
Figure 82 Stress profile for the preliminary test #2; the temperature was kept constant at 10°C.

Figure 83 Evolution of various Martensite fractions in response to the loading in Figure 82.

Stress-strain behavior for this test is depicted in Figure 84.
Preliminary test 3:

The SMA rod in this test is kept at 60 °C, a temperature well above Af. The loading, shown in Figure 85, was applied to the rod while it is in full Austenite state. This test demonstrates the superelastic behavior of shape memory alloys in terms of loading in tension and compression. The response to partial loading followed by unloading and partial unloading followed by loading in both tension and compression is obvious in the Martensite fraction-stress plots in Figure 86 and Figure 87 as well as stress-strain plot in Figure 88.
Figure 85 Loading profile for the superelastic SMA rod in the bottom line test #3.

\[ \zeta = \zeta_{sp} + \zeta_{sn} + \zeta_d \]

Figure 86 The evolution of Martensite fractions in response to the loading in Figure 85.
Figure 87 Change of Martensite fractions with respect to stress in the preliminary test #3.

Figure 88 Stress-strain plot showing superelasticity effect (preliminary test #3).
Preliminary test 4:

The fourth example is also a case pertaining to superelasticity and partial transformation. The rod is loaded, according to Figure 89, from 100% Austenite while kept at a temperature above Af (60°C).

![Stress Profile](image.png)

**Figure 89 Loading profile in the isothermal test #4, T=60°C**

The stress oscillates in the transformation band such that the fraction of stress-induced Martensite follows a graph shown in Figure 90. Also, the relationship between Martensite fraction and stress is shown in Figure 91.

The stress-strain curve is illustrated in Figure 92. As it can be seen from this figure, the internal loops correspond to partial transformation and agree well with the applied loading path; the envelope curve shows the recovery of transformation strain upon unloading which is the superelasticity effect.
Figure 90 Evolution of Martensite fractions as a result of cyclic loading in Figure 89.

Figure 91 Internal loops in the transformation-stress graph (preliminary test#4).
Rena et al. [154] performed a cyclic loading test on a superelastic NiTi wire of 1 mm diameter. The cyclic loading path with partial loading/unloading and the stress-strain response of the wire is shown in Figure 93. The cyclic loading results in stress plateaus in the wire that shift up or down during the loading and unloading that follow an incomplete transformation. This effect, as foregone in Figure 92, is qualitatively captured through the current model. Tanaka et al. [155] attributed this feature to the microscopic residual stresses that form in the vicinity of the defects caused by accumulation of the local dislocations during the cycling loading. The ensuing buildup of the Martensite phase does not contribute to the subsequent transformations. It is worth mentioning that this shift of the plateaus in the stress-strain cyclic loops eventually converges to an envelope loop if the wire has been trained by enough number of cycling before the experiment [154][155].
Figure 93 Cyclic loading/unloading applied to an NiTi superelastic wire and the resulting stress-strain response [154].

**Preliminary test 5:**

A constant stress test is performed in this example. The initially 100% detwinned martensite rod is compressed, while kept at a temperature below Ms (0°C), to a stress level enough for the completion of the transformation in the negative direction (See
Afterwards the temperature is cycled according to Figure 95 while the load is maintained unvarying.

The effect of this cyclic temperature loading on the fraction of stress-induced Martensite in the negative direction is illustrated in Figure 96.
The evolution of Martensite fraction in response to the cyclic thermal loading in Figure 95.

The hysteresis loop in a partial cycle of Martensitic transformation, taken from [157], is shown in Figure 97. This graph is quantitatively comparable to Figure 96, reasserting the potentialities of the current model in capturing the cyclic response of the SMAs.

Martensitic transformation as a result of a cyclic temperature test in TiNi [157].
Preliminary test 6:

A superelastic tensile-compressive test is introduced in this section in order to demonstrate the ability of the current model in capturing the tension-compression asymmetry effects in shape memory alloys. Figure 98 depicts the absolute stress-strain plot for the case of a SMA material with a coefficient of asymmetry \( \tau = 1.5 \). It is worth mentioning that the critical stress for the start of transformation increases in compression however the material demonstrates lower total transformation strain.

![Stress versus strain](image.png)

**Figure 98** Stress-strain results of a compressive-tensile loading on a superelastic SMA specimen indicating the tension-compression asymmetry.

Gall et al. [156] performed a series of tension and compression axial tests on polycrystalline as well as single crystal NiTi specimens. The results of the experiments on polycrystalline NiTi are shown in Figure 99. The material demonstrated tension-compression asymmetry in terms of the critical stress for the start of transformation (maximum 35%) as well as the maximum transformation strain (Maximum 68%). The
level of asymmetry, as implied from Figure 99, is dependent on the heat treatment of the alloy; peak-aged or over-aged. The aging treatment resulted in the precipitation of Ti$_3$Ni$_4$. The precipitates act as nucleation sites for the start of Martensite transformation and obstacles for the motion of dislocations leading to an increase in the critical stress for the dislocation motion and a decrease in the critical stress for the phase transformation. Another fact from Figure 99 is that the specimens could sustain very large compressive stresses without undergoing plasticity. The aforementioned asymmetry in single crystal SMAs (which is much stronger than that of polycrystalline SMAs and actually underpins it) roots back in the Martensite habit planes having very low symmetry with respect to the parent phase.
Figure 99 Compressive and tensile stress-strain plots of a polycrystalline NiTi specimen tested at 22 °C; (a) aged at 400 °C for 1.5 h (peak-aged), (b) aged at 500 °C for 15 h (over-aged) [156].

Preliminary test 7: SMA-spring antagonistic actuation

The NiTi rod, showed schematically in Figure 100, is acting against a linear spring. Before engagement with the spring, the rod experiences a cyclic loading and unloading which yields in a full compressive transformation residual strain remained in
it. The shrunk rod is then attached to the free spring with a coefficient of \( k = 10000 \) N/mm. Finally, a temperature load of what is plotted in Figure 101 is applied to the rod.

The cross sectional area of the rod is considered to be 1 mm\(^2\).

\[ F = -k \times u \]

\[ u = 0, \quad T = \text{temp inc} \]

**Figure 100** SMA rod in an antagonistic actuation condition against a linear spring.

**Figure 101** Temperature profile for the problem shown in Figure 100.

The resultant forces on the loaded end of the rod as well as the stress-temperature loading path for this actuation history are plotted in Figure 102 and Figure 103 respectively. The spring acts against the rod with a compressive force as the SMA rod is going through recovery and expansion due to the reverse transformation to Austenite (Seconds 5 to 6). In the second stage as the temperature of the rod drops (seconds 6 to 7),
the compression force lessens. This is because of the fact that the modulus of NiTi in Martensite phase is about a third of its modulus in Austenite [164]. The equilibrium stress level is such that the material ends in both detwinned and twinned Martensite state; as implied form Figure 104.

![Resultant force](image1)

**Figure 102** The force brought upon the loaded end of the NiTi rod in preliminary test #7.

![Stress-temperature loading history](image2)

**Figure 103** The thermomechanical loading history as superposed on the NiTi stress-temperature phase diagram.
Figure 104: Variation of Martensite fractions in the NiTi rod in response to the thermomechanical loading in Figure 103.

The stress-strain plot is the concluding result for this section (See Figure 105).

Figure 105: Stress-strain plot for the preliminary test #7.
The results of the foregone baseline examples in this section are qualitatively comparable to the outcomes of the numerous models developed by other researchers. Figure 106 shows the typical modeling results of SMA behavior found in the literature.
Figure 106 Typical simulation results representing the behavior of shape memory alloys: (a) cyclic loading with gradually decreasing stress [158], (b) Martensite fraction evolution in a cyclic temperature simulation [159], (c) stress-strain response in an isothermal cyclic loading test [142], (d) compressive-tensile loading and unloading of Nitinol [160], (e) Tension-compression test on an SMA material at a T<As followed by strain recovery [161], (f) superelastic stress-strain behavior including tension-compression asymmetry effects [162].
4.2. Validation of the model:

The current model developed in COMSOL Multiphysics® was evaluated against experimental results. Two cases of experimental data were attained from the published literature and reworked using the current model.

4.2.1. 3 point bending test:

Trochu et al. [163] and Jaber et al. [151] used the experimental work reported in [152] for comparison with their developed model. A 3 point bending test was performed on a Cu-Al-Be SMA alloy with 11.4 wt% Al and 0.6 wt% Be at a temperature of T=20°C. The dimensions of the beam are depicted in Figure 107.

![3 point bending test setup](image)

Figure 107 The 3 point bending test setup.

This experiment was simulated with the current model through a plane-stress approach. Half of the beam was modeled and meshed with conventional Quadratic Lagrange square elements. The material properties used for the SMA beam can be found in Table 4.
Table 4 Material properties of the SMA beam in the 3 point bending test.

<table>
<thead>
<tr>
<th>Moduli</th>
<th>Transformation temperatures (°C)</th>
<th>Transformation constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>D_a = 73.2 × 10³ MPa</td>
<td>M_f = -100</td>
<td>C_M = 5 MPa/°C</td>
</tr>
<tr>
<td>D_m = 73.2 × 10³ MPa</td>
<td>M_s = -54.2</td>
<td>C_A = 10 MPa/°C</td>
</tr>
<tr>
<td>ε_{L_p} = 1.66 %,</td>
<td>A_s = -35</td>
<td>σ_s^{cr} = 0.0 MPa</td>
</tr>
<tr>
<td>\upsilon_A = \upsilon_M = 0.3, \tau = 1</td>
<td>A_f = -5</td>
<td>σ_f^{cr} = 242.3 MPa</td>
</tr>
</tbody>
</table>

Jaber et al. [151] material properties

\( D_a = D_m = 73.2 \times 10^3 \) MPa,
\( \sigma_s^{AM} = 371, \quad \sigma_f^{AM} = 613.3, \quad \sigma_s^{MA} = 548, \quad \sigma_f^{MA} = 305.7 \)
\( \varepsilon_{\text{Max}}^{irr} = 1.66\%, \quad \upsilon_A = \upsilon_M = 0.3, \tau = 1 \)

The properties for the current model were derived based on a fit with the stress-strain results of the uniaxial response of the same material. Figure 108 depicts the experimental stress-strain results as well as 1D modeling outcomes with the material properties stated in [151] and the properties obtained for this study.
The uniaxial stress-strain plots, experimental [152] as well as current 1D model.

The maximum deflection of the SMA beam under a point load acting on its mid-span is shown in Figure 109. The result of the modeling in the large deformation framework with 20 elements on the length and 100 elements on the height of the beam is also included in this figure. The good agreement between the experimental and modeling results is obvious from the mentioned figures.

Mesh optimization is a necessary step in general modeling via Finite Element Method. Too many elements unnecessarily consume valuable time and computer resources and on the other hand not enough elements leads to poor prediction estimates. Figure 110 illustrates the comparison between meshing the beam with different number of elements. The difference between 10 or 100 layers of quadratic square elements on the height is negligible. Also the mesh of 10 and 20 elements on the beam span do not yield much dissimilar results. The acceptable minimum is apparently a 10x5 mesh.
As recalled from the previous section, the model was developed in both small displacement and large deformation frameworks. Typically the strains of more than 5% in a structural analysis problem call for the large deformation approach to be used. With small deformation, the linear strain tensor and Cauchy stress tensor are used. Once the deformation exceeds 5%, the small displacement formulation is not exact anymore and large deformation stress/strain tensors and formulations should be used. The difference of these approaches in predicting the displacement of the beam can be seen in Figure 111. As it is obvious, the small displacement method with even a very fine mesh can only predict the deflection up to 4.5 mm, i.e. 20% of the length of the beam.

Another discussion in this section concerns the use of Cauchy stress for the stress-temperature phase diagram. The stress used in the stress-temperature phase diagram is the Cauchy stress which represents the loading on the current deformed configuration. As
inferred from Figure 112, using the 2nd Piola-Kirchoff stress in the stress-phase diagram, instead of Cauchy stress for the sake of simplicity for solving the nonlinear equations incurs minor error.

![3 point bending test](image)

Figure 110 The mesh optimization for the 3 point bending model.
Figure 111 The distinction between large deformation and small displacement approaches.

Figure 112 The effect of using the 2nd Piola-Kirchoff stress in the stress-phase diagram as an approximation for Cauchy stress.
The Cauchy stress in the axial direction $\sigma_x$ is plotted on the deformed beam in Figure 113. The beam is under the peak load at the instant shown.

The fraction of stress-induced Martensite variants, $\xi_{sp}$ and $\xi_{sn}$, at this instance are plotted in Figure 114 and Figure 115 respectively. It is obvious that some layers close to the top and bottom edges, where the stress state is high enough, go under transformation during the loading. Ergo, there is a coexistence of untransformed, transforming and transformed material. The positive and negative stress-induced Martensite is formed in the tensile and compressive layers respectively and there is a clear symmetry with respect to the centre line as expected.

![Figure 113 Axial stress $\sigma_x$ in the 3 point bending test.](image-url)
Figure 114 Distribution of the positive stress induced Martensite in the beam.

Figure 115 Distribution of the negative stress induced Martensite in the beam.
4.2.2. Pure bending test:

Rejzner et al. [145] performed a series of testing to study the behavior of SMA in pure bending. Figure 116 shows a typical axial stress-strain diagram from a tensioning superelastic NiTi wire. The outcome of the current model in COMSOL Multiphysics® is also included in this figure.

The pure bending test conducted at 30°C on an equiatomic NiTi rod with a diameter of 1.2 mm was modeled using the current model. The SMA alloy in this test showed asymmetry in tension and compression which was considered in the modeling. The material properties used for this model is listed in Table 5.

![Figure 116 Superelastic axial stress-strain plot.](image)
Table 5 Material properties of the SMA beam in the pure bending test.

<table>
<thead>
<tr>
<th>Current model</th>
<th>Moduli</th>
<th>Transformation temperatures (°C)</th>
<th>Transformation constants</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$D_a = 44.7 \times 10^3$ MPa</td>
<td>$M_f = -91$</td>
<td>$C_M = 5$ MPa/°C</td>
</tr>
<tr>
<td>$D_m = 52.0 \times 10^3$ MPa</td>
<td>$M_s = -87$</td>
<td>$C_A = 5$ MPa/°C</td>
<td></td>
</tr>
<tr>
<td>$\varepsilon_{Lp} = 5.85%,$</td>
<td>$A_s = -75$</td>
<td>$\sigma_s^{cr} = 0.0$ MPa</td>
<td></td>
</tr>
<tr>
<td>$\nu_A = \nu_M = 0.42, \tau = 1.2$</td>
<td>$A_f = -54$</td>
<td>$\sigma_f^{cr} = 80$ MPa</td>
<td></td>
</tr>
</tbody>
</table>

The moment applied to both ends of the rod is plotted in Figure 117. The discretized domain for the pure bending test, containing 1800 elements and 55500 degrees of freedom (DOF), is shown in Figure 118. Quadratic Lagrange brick elements were used for the meshing.

![Figure 117 The moment applied to the rod in the pure bending test.](image)
The distribution of the normal stress on the vertical axis of the beam cross section is plotted in Figure 119 with respect to time. The stresses are completely vanished after unloading indicating the recovery of the transformation strains.

The experimental moment-curvature plot as well as the one attained from the FEA model are compared in Figure 120. The model could successfully predict the loading/unloading hysteresis in the pure bending of the NiTi beam.
Figure 119 Variation of the normal stress on the cross section of the beam.

Figure 120 Moment-curvature plots in the pure bending test (experimental data from [145]).
4.2.3. FEA modeling and parametric analysis of the SMArt™ pedicle screw:

It was shown in Chapter 3 that the design of the smart expandable pedicle screw can approximately be modeled as an assembly of a wire and a tube. The model consists of a wire which has a circular deformation upwards and a tube which has a circular deformation downwards (See Figure 121).

![Figure 121 The assembly of the wire and tube in the free (memorized) configuration.](image)

The diameters for the wire and tube that match the configuration of the base screw were singled out from the commercial sizes acquirable form Memry Corporation (See Table 6).
Table 6 Commercial sizes of NiTi wires and tubes.

<table>
<thead>
<tr>
<th>Case No.</th>
<th>1</th>
<th>2*</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>A OD (mm)</td>
<td>0.762</td>
<td>1.189</td>
<td>0.889</td>
<td>1.016</td>
<td>1.016</td>
</tr>
<tr>
<td>A ID (mm)</td>
<td>0.762</td>
<td>1.189</td>
<td>0.902</td>
<td>1.021</td>
<td>1.021</td>
</tr>
<tr>
<td>A OD (mm)</td>
<td>1.31</td>
<td>1.321</td>
<td>1.290</td>
<td>1.250</td>
<td>1.321</td>
</tr>
</tbody>
</table>

The modeling procedure for the first case, as an example, is described hereafter. The wire has an OD of 0.762 mm, length of 11 mm, and is deformed along a path with the equation of:

\[ y_A = -\sqrt{613.55 - x^2} + 24.77 \]  \( (39) \)

The equation represents a helix with a diameter of 5.13 mm and a pitch of 3.63 mm opened in a plane. The wire is made of NiTi shape memory alloy with Austenite finish temperature (Af) of 70°C. The offset of the tip from an axis crossing the center of the fixed end of the wire (See Figure 121) is 2.44 mm.

On the other hand, the tube has an OD of 1.31 mm and length of 11.74 mm with an inner diameter that fits the OD of the wire. The deformation of the tube is based on:

\[ y_B = +\sqrt{424.36 - x^2} - 20.6 \]  \( (40) \)

This equation also represents a helix with a diameter of 4 mm and a pitch of 3.63 mm opened in a plane. Therefore based on this equation, the offset of the tip from an axis crossing the center of the fixed end of the tube is 3.26 mm. It is made of another composition of NiTi shape memory alloy that has an Af of 35°C. It is worth mentioning that a change of composition in the order of 0.01% wt in the binary NiTi alloy will lead to a shift in transformation temperatures in the range of ±10°C. Thus, it is possible to
achieve the desired window of transformation temperatures by selecting the proper composition in the alloy and applying necessary thermomechanical treatments [165]. The assumed mechanical and transformation properties of NiTi alloys used for the modeling of the wire and tube are listed in Table 7.

<table>
<thead>
<tr>
<th>Material properties for NiTi alloy A (wire) and B (tube)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Moduli</strong></td>
</tr>
<tr>
<td>NiTi: Ni 55.6%wt</td>
</tr>
<tr>
<td>$D_a = 67 \times 10^3$ MPa</td>
</tr>
<tr>
<td>$D_m = 26.3 \times 10^3$ MPa</td>
</tr>
<tr>
<td>$\varepsilon_{Lp} = 6.7%$ , $\nu_A = \nu_M = 0.33 , \tau = 1.0$</td>
</tr>
<tr>
<td>$A_f = 70$</td>
</tr>
<tr>
<td>NiTi: Ni 55.1%wt</td>
</tr>
<tr>
<td>$D_a = 67 \times 10^3$ MPa</td>
</tr>
<tr>
<td>$D_m = 26.3 \times 10^3$ MPa</td>
</tr>
<tr>
<td>$\varepsilon_{Lp} = 6.7%$ , $\nu_A = \nu_M = 0.33 , \tau = 1.0$</td>
</tr>
<tr>
<td>$A_f = 35$</td>
</tr>
</tbody>
</table>

With this configuration, the assembly after engagement can assume three different deflection modes. One is at a relatively low temperature where both the wire and the tube are in the Martensite state. It is possible to engage the wire into the tube at this situation and fixate the assembly to the body of the smart screw. Figure 121 shows the model of the wire and the tube in the original configuration. The straight dashed line represents the surface of the screw. This is a situation where the SMA protrusions are in the collapsed form at the time of implanting the screw in the bone. Secondly, at a temperature around
37°C (body temperature), the tube will transform into Austenite state and tend to bend the whole assembly in favor of its initial deformed state. This represents the situation where the SMA protrusions of the smart screw are expanded. Finally, the third configuration is reached at a temperature above 70°C. It is the retraction condition for the SMA protrusion at the time of removing the screw. The smart screw can be removed or revised by heating it up to the Af of the retractor wires. In that case, the wire activates and tends to deflect the assembly back to the collapsed condition. The operation stages are summarized in Figure 122.

1st stage
- T<10°C
- Both the wire and tube are in Martensite state.

2nd stage
- T=37°C
- The tube becomes Austenite.

3rd stage
- T=70°C
- The wire becomes austenite.

Figure 122 Different stages of the wire-tube assembly operation.

The behavior of the assembly in Figure 71 is approximated by the simplified model in Figure 121.

This assembly is transferred to COMSOL Multiphysics® to be simulated via the SMA capability developed in the framework of this software. Figure 123 shows the
meshing of the assembly with quadratic hexahedral elements. 15 elements were used along the axis of both the wire and the tube. The model consists of a total of 8000 elements and 243000 DOFs.

Furthermore, the variation of temperature at different stages of the simulation is shown in Figure 124. For further simplicity and in order to avoid complications of contact modeling, the following approach in modeling is adopted. The wire and the tube are deformed at the 1st stage temperature level under a distributed tip loading. The loading causes Martensite transformation in top and bottom layers of the tube and wire that sustain the highest amount of stress. Therefore upon unloading, there will be some residual deformation in the structure. The type of loading and boundary conditions (B.C.) used for this model are shown in Figure 125. In this case, a symmetry B.C. is considered at the end of the cantilever tube and wire for achieving a better convergence.

Figure 123 Discretization of the wire-tube assembly with quadratic Lagrange brick elements.
The behavior of the system in terms of tip load versus tip displacement is evaluated to determine the equilibrium condition, i.e. the same equal loading acted on the tube and the wire which results in a total tip displacement equal to the initial gap between the tips of the two structures (detailed explanation in section 3.5.3.) This procedure is repeated for the system while in the body temperature as well as high temperature. As noted before, this is an approximated estimation of the behavior of the actual system in which the wire is inserted into the tube.

![Graph showing temperature variation at different stages](image)

Figure 124 Temperature at the three stages of the simulation.
The typical distribution of detwinned Martensite in the wire-tube assembly is illustrated in Figure 126. The figure belongs to a solution instance at the second stage (See Figure 122) and shows the consumption of detwinned Martensite in transformation to stress-induced Martensite at the layers of the beams with higher stress levels.
Figure 126 Typical Martensite distribution in the assembly ($\zeta_d$ shown here).

The load-deflection plots for the wire and tube of size #1 at the low temperature level (first stage) are depicted in Figure 127 and Figure 128. As mentioned earlier, both the wire and tube are loaded from 100% detwinned Martensite and retain the transformation strain after unloading.
Figure 127 The deflection of the wire under a tip load at the first stage (low temperature).

Figure 128 The deflection of the tube under a tip load at the first stage (low temperature).
The state of equilibrium is noted in Figure 129 where the sum of the deflections of the wire and the tube at the tip under a load of 1.2 N equals the initial gap. The initial gap between the wire and the tube at the tip is $2.44 + 3.26 = 5.7$ mm.

Figure 129 Load-displacement plots for the wire-tube assembly at the first stage. The equilibrium is reached at a common level of force where the sum of displacements is equal to the initial gap.

Figure 130 and Figure 131 show the deflection behavior at the second (body temperature) stage. While the system is at body temperature, the tube transforms to Austenite state which is a stiffer and stronger phase than Martensite. Therefore the behavior of the tube denotes a closed hysteresis.
Figure 130 The deflection of the wire under a tip load at the second stage (body temperature).

Figure 131 The deflection of the tube under a tip load at the second stage (body temperature).
Figure 132 contains the results of the equilibrium analysis for the second stage. $\Delta L$ can be determined form this figure.

Finally, the load displacement plots for the third stage are brought in Figure 133 and Figure 134. Because both the wire and the tube are in the Austenitic phase at this level of temperature, they show pseudoelastic hysteresis in their deflection behavior. The results of the equilibrium analysis for the third stage are shown in Figure 135. $\Delta H$ can be determined form this figure.
Figure 133 The deflection of the wire under a tip load at the third stage (high temperature).

Figure 134 The deflection of the tube under a tip load at the third stage (high temperature).
Figure 135 Load-displacement plots for the wire-tube assembly at the third stage.

4.2.4. Selection of the optimum geometry:

It should be mentioned that the higher $\Delta_L$, the more engagement of the smart pedicle screw with its surrounding bone and hence the higher the pull-out resistance of the screw. $\Delta_H$ should be as low as possible so that the screw becomes revisable. Therefore, the goal is to find a configuration of diameters - outer diameter of the tube $d_B$ and the outer diameter of the wire $d_A$ - by which $\Delta_L$ maximizes and $\Delta_H$ minimizes. Investigation of load-deflection behavior for different commercial wire-tube sizes in Table 6, as earlier described step by step for case #1, elucidated that case #2 yields the most desirable performance. The performance of Case #3 to #5 was not significantly different from case #1.
For case #2, with the lowest ratio of the tube thickness to the wire diameter, the following results were obtained:

\[ \Delta_L = 3.01 \text{ and } \Delta_H = 1.26 \text{ mm} \]

The positive \( \Delta_H \) indicates that the assembly does not close completely at high temperature. Decreasing the tube thickness and increasing the diameter of the wire will help to improve this issue; however the manufacturing conditions and ductility of the NiTi material limit the smallest thickness achievable for this purpose.

This configuration sizes will be used for manufacturing the first sample of the SMArt\textsuperscript{TM} pedicle screw.

Another engineering point in the design of NiTi components is the strain the material sustains. If the application entails cyclic loading, the strain should not surpass 3\% to keep the fatigue properties of NiTi in a safe margin.

The current application is a one-time operating one, although fatigue external loadings might act upon the screw. Figure 136 illustrates the first principle strain plots of the wire and the tube at the instance of their maximum deformation. The 8 \% maximum level, which pertains to the superelastic tube, is in the normal operating range for NiTi alloys.
Figure 136 First principle strain (plotted on the undeformed beams for more clarity).

4.3. **Pilot testing of the SMArt™ pedicle screw:**

The performance of the SMA smart bone screw was tested in the course of a pilot pull-out experiment.

Standard Hex head lag screws with ¼” thread size; 3-1/2” total length and 2-3/4” threaded length were enhanced with Nitinol superelastic wires. Wires with a diameter of 0.5 mm and a length of 16 mm were attached to the screw through cross drilled holes in the minor diameter of it. The holes were drilled such that their beginning and end would be on different levels of the thread without damaging the thread profile (See Figure 137-a).
Figure 137 (a) \textit{SMART} screw: lag screw enhanced with Nitinol wires. (b) Control screw. (c) Experimental setup showing the screw inserted in the foam block and mounted on a tensile testing machine.

The superelastic wire protrusions close at the time of screw insertion and re-open when placed in the receiving material. Thanks to super-elasticity, this bending and unbending would not introduce any permanent plastic deformation in the Nitinol wires.

The lag screw enhanced with the SMA wires was inserted in a $43 \times 43 \times 90$ mm block of foam with the density of 15 lb/ft$^3$ (comparable to normal bone; 5-10 lb/ft$^3$ for osteoporotic bone) to make the specimen for the axial pull-out test. Prior to insertion, a hole was drilled and tapped into the block with a diameter of $\frac{1}{4}$”. The size of the whole was selected a little larger with respect to the thread size of the lag screw in order to represent osteoporotic bone. As shown in Figure 138, the cancellous bone surrounding a pedicle screw inserted into human vertebrae will degrade due to osteoporosis, hence the
screw will lose its purchase with the bone which ultimately will lead to screw loosening or back-out.

![Image](image1.jpg)

Figure 138 Pedicle screw: bone degradation due to osteoporosis.

The primary objective of the design of the bone screw enhanced with SMA wires is to overcome this drawback by further opening the wires which could maintain the contact with the receded bone. The screw insertion depth in the foam block was 53 mm. A control specimen was also prepared with exact same specifications but using an original lag screw.

The specimens were evaluated on a testing machine with a tensile pull-out load applied to the head of the screws; as illustrated in Figure 137-c. The pulling rate was set to 5 mm/min in accordance with ASTM F543-02.

The results are depicted in Figure 139 as tensile load versus displacement graphs. The mode of failure was rupturing of the material surrounding the screw thread. The load at the instance where the displacement reached equal to the screw pitch (2.85 mm) was chosen as the strengths of the screw. The improvement in the pull-out strength of the screw via enhancing it with superelastic SMA wires is obvious from this figure.

It is worth noting that SMArt™ screw would gain resistance again after the displacement reached 3 mm which can be attributed to the repeated entanglement of the
SMA wires with the foam resulting in further resistance of the screw against the pull-out force; a behavior which could not be seen in the control specimen.

The outcomes of this experiment would demonstrate the effectiveness of the SMA Smart screw design.

![Graph showing the results of the axial tensile test: force versus displacement. The tensile strength is selected at the force required to displace the screw in the block as much as the screw thread pitch.](image)

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Figure 139 Results of the axial tensile test: force versus displacement. The tensile strength is selected at the force required to displace the screw in the block as much as the screw thread pitch.
Chapter Five

Conclusions and future work

5.1. Conclusions:

Shape memory alloys (SMA) have received widespread attention from researchers in various fields of engineering sciences due to their exceptional properties of shape memory and superelasticity. NiTi equiatomic alloys among other SMA, show acceptable biocompatibility to be implemented in biomedical applications. Applications of NiTi in biomedical areas specifically orthopedics demonstrate its unique performances not achievable with conventional materials.

Pedicle screws, which are used as an anchoring point for implanting spinal instrumentations in the spinal fracture and deformity treatments, entail a major drawback i.e. loosening and back-out. The strength of the screw contact with the surrounding bone diminishes as the bone degrades e.g. due to osteoporosis.

Two “Smart” pedicle screw designs were developed to address this issue. As the first embodiment, a screw was designed which has an exterior and an interior part. The exterior part resembles a conventional pedicle screw with cross-liked split legs. The
interior part opens up while reaching to the body temperature and expands the screw legs. This design was not pursued due to the manufacturing complications of Nitinol.

Another embodiment of the SMArt™ pedicle screw design uses NiTi superelastic-shape memory coils wrapped around it. The smart assembly consists of an external superelastic tube which is responsible for expanding the design protrusions when reached to body temperature; also an internal shape memory wire inserted into the tube is sought to retract the assembly while locally heated to above the body temperature. In this way the screw design becomes removable.

The whole assembly was modeled as a beam structure in COMSOL Multiphysics® finite element software. The behavior of shape memory alloy was defined in the software via its Partial Differential Equation (PDE) module. The SMA model is a Tanaka-based model and is capable of capturing shape memory effect, superelasticity and hysteresis behavior, and partial transformation in both positive and negative directions. This 1D model was further modified to be included in a 3D framework such that it makes possible the simulation of a beam under bending and was validated in comparison experimental results available from the literature.

The functionality of the smart screw design, an illustration of the applicability of novel SE and SM properties in orthopedics, was studied via this FEM model. The results of the FE simulation show that the wire-tube assembly is capable of performing the required expansion and retraction functions. Moreover, a parametric analysis was conducted over the effect of different sizes of the wire and the tube. The geometry sizes for the first sample of this innovative pedicle screw were determined based on the outcomes of this analysis.
5.2. *Future work:*

The work done thus far in this research looks appropriate to further in several directions.

First of all, the performance of the two different designs of the smart pedicle screw ought to be numerically simulated. In this case, a finite element model is required that takes into account the bone-screw interaction and is capable of simulating a pull-out test. The present model approximated the functioning of the helical wire-tube assembly in 2D. This limitation should be addressed by a more detailed 3D model that can capture the SMA behavior. In this way, the two pedicle screw designs can also be compared in terms of pull-out performance.

Moreover, the removal of the smart pedicle screw entails activating the retractor wires via an external heating source. This may cause damage to the surrounding bone and tissue. Therefore, a finite element heat transfer simulation is necessary to evaluate the heat interaction between the screw surface and the bone tissue and estimate the safe temperature required for activation.

Additionally, the first prototype of the *SMART*™ pedicle screw is being manufactured at the time of the composition of this thesis. It is necessary to modify the design of the screw according to the interpretations from the cadaveric experiments performed on the screw sample. The final commercialization of the *SMART*™ pedicle screw is the ultimate goal of this research. Moreover, the model developed in COMSOL Multiphysics has the potential to be completely expanded to 3D. To this end, the SMA constitutive and kinetics law must be modified accordingly.
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