A Thesis

entitled

Finite Element Study of a Shape Memory Alloy Bone Implant

by

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Submitted to the Graduate Faculty as partial fulfillment for the requirements of the

Master of Science Degree in Mechanical Engineering

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An Abstract of

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Shape memory alloys have been used in several biomedical devices in recent years. Their special thermo-mechanical behavior in recovering a certain shape upon heating and being able to tolerate large deformations without undergoing the plastic transformations make them a good choice for different applications. Biocompatibility of nitinol as a widely used shape memory alloy material is the other main property for biomedical devices.

Osteoporosis is a common bone disease especially in elderly people. Bone degradation as the result of osteoporosis causes loosing of screws implanted in the bone during or after surgery. A new nitinol-based device which is designed to mitigate this adverse effect has been studied. This thesis analyzes the functionality of this novel nitinol-based expandable-retractable pedicle screw. The unique feature of this screw is
that it is removable as needed. The functionality of the screw is verified by experiment and compared to the results of the numerical simulation in Abaqus. This simulation tool is the combination of the numerical implementation of shape memory alloy constitutive thermo-mechanical modeling into the Abaqus UMAT Fortran subroutine and the Abaqus finite element solver. The verification of this tool in several experiments has been carried out to establish validity of the numerical approach.

The effect of the designed pedicle screw in mitigating the loosing effect has also been studied. Pullout test is a common way of evaluating a bone implant. The pullout force of a normal screw out of a normal bone was simulated with finite element in Abaqus. Consequently, performance of the new design in improving pull-out strength in osteoporosis bones has been studied.

This thesis presents the design of the novel pedicle screw and paves the way of evaluating various medical devices with enhanced functionality.
Acknowledgements

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List of Symbols

\[ T_{\text{body}} \] \quad \text{Body temperature}

\[ T_{\text{low}} \] \quad \text{Outside body temperature}

\[ A_f^{SE} \] \quad \text{Austenite final temperature of the supereleastic element}

\[ M_f^{SM} \] \quad \text{Martensite final temperature of the shape memory element}

\[ A_f^{SM} \] \quad \text{Austenite final temperature of the shape memory element}

\[ T_0 \] \quad \text{Reference temperature}

\[ s_0 \] \quad \text{Reference entropy state}

\[ M_s \] \quad \text{Martensite start temperature}

\[ A_s \] \quad \text{Austenite start temperature}

\[ A_f \] \quad \text{Austenite finish temperature}

\[ M_f \] \quad \text{Martensite finish temperature}

\[ C_M \] \quad \text{Stress influence coefficient for transformation into martensite}

\[ C_A \] \quad \text{Stress influence coefficient for transformation into austenite}

\[ \sigma_{MS} \] \quad \text{Stress at the start of transformation to martensite}

\[ \sigma_{mf} \] \quad \text{Stress at the finish of transformation to martensite}

\[ \sigma_{As} \] \quad \text{Stress at the start of transformation to austenite}
\( \sigma_{Af} \) ................. Stress at the finish of transformation to austenite

\( c^M \) ................. Specific heat coefficient in martensite

\( c^A \) ................. Specific heat coefficient in austenite

\( \sigma \) ................. Stress Tensor

\( u_0 \) ................. Reference internal energy state

\( f(\xi) \) ................. Hardening function

\( S^A \) ................. Compliance tensor in austenite

\( S^M \) ................. Compliance tensor in martensite

\( \alpha^A \) ................. Thermal expansion in austenite

\( \alpha^M \) ................. Thermal expansion in martensite

\( s_0^A \) ................. Reference entropy state in austenite

\( s_0^M \) ................. Reference entropy state in martensite

\( u_0^M \) ................. Reference internal energy state in austenite

\( u_0^A \) ................. Reference internal energy state in austenite

\( \dot{\varepsilon} \) ................. Derivative of strain

\( \Lambda \) ................. Transformation tensor

\( \dot{\xi} \) ................. Derivative of martensitic volume fraction

\( H \) ................. Maximum transformation strain in 3D

\( \varepsilon^{t-r} \) ................. Strain at the reversal point

\( \phi \) ................. Transformation function

\( \pi \) ................. Thermodynamic force

\( Y^* \) ................. Internal dissipation due to phase transformation

\( E_A \) ................. Austenite modulus of elasticity
$E_M$ ................. Marteniste modulus of elasticity

$\varepsilon_t$ ................. Maximum transformation strain in 1D

$\nu_M$ .................. Poisson’s ratio of martensite

$\nu_A$ .................. Poisson’s ratio of austeni

$\xi$ ..................... Martensitic volume fraction

$\varepsilon^t$ ................. Transformation strain

$G$ ..................... Gibbs free energy

$R$ ..................... Resistivity

$I$ ..................... Electrical current

$T$ ..................... Temperature

$S$ ..................... Compliance tensor

$c$ ..................... Specific heat coefficient

$\rho$ ..................... Density

$\alpha$ .................. Thermal expansion coefficient

$h_c$ ...................... Heat convection coefficient

$A_c$ ...................... Area of heat exchange

$T_{inf}$ .................. Ambient temperature

$C_p$ ..................... Specific heat capacity

$\sigma_Y$ ................. Yield stress
Chapter One

Introduction

1.1. Shape memory alloys

Shape memory alloys belongs to a group of materials called active materials [1]. Active materials are resulted from the extensive research over the past few decades on technologies in engineering the mechanical, thermal and electrical properties of materials. Recently, active materials have been used in different applications. Sensing is one of the applications in which the material can convert the mechanical variation into a non-mechanical output. In actuation applications, the material converts the non-mechanical input into the mechanical output. A group of active materials including shape memory alloys and piezoceramics show direct coupling behavior. In contrast, other active materials such as electo-rheological fluids (ERF) show indirect coupling. This indirect coupling usually eliminates the reciprocity of the coupling behavior that exists in other materials. For the actuation applications, two parameters play the most important roles in the suitability of the active materials: actuation energy density, which is defined as the available work output per unit volume, and the actuation frequency of the material. An
ideal actuator material is the one which has maximum actuation energy density and actuation frequency. In Figure 1-1 these two parameters are shown for different materials.

Figure 1-1: Actuation stress and Specific actuation energy density of different actuators [1]
Shape memory alloys are a specific type of smart material, which can recover their strain upon heating. Increasing the temperature of the material results in recovery of the introduced strain into the material even when the applied force is relatively large in a process known as shape memory effect. This property makes the energy density high in shape memory alloys. Also, under specific conditions, the material undergoes a hysteresis reversible transformation which enables the material to dissipate energy for energy absorption applications. These properties make shape memory alloys a good candidate for a variety of applications from aerospace and automotive to biomedical. However, low frequency response of the material is a disadvantage which restricts its applications.

1.1.1. Phase diagram and transformation

Phase diagram is a schematic representation of the transformation regions for shape memory alloys [2]. The lines in the phase diagram show the phase boundaries that separate the two solid phases of the shape memory alloy. Usually the phase diagram for shape memory alloys has temperature shown along the abscissa axis and the other variable is stress and is shown along the ordinate axis. SMAs have two solid states in typical operating temperatures: the high temperature phase, which is known as austenite (A), and the low temperature phase, or martensite (M). The mechanism in which the crystalline structure of the austenite phase transforms to the martensite phase is called lattice distortion and the transformation is called martensitic transformation. The martensite crystal can also be formed as twinned or detwinned or as reoriented. The reversible transformation of the material from austenite, which is known as the parent phase, to martensite makes the special thermo-mechanical behavior of shape memory alloys. The well-known phase diagram of shape memory alloy materials is shown in
The pseudoelasticity and shape memory effect as the special thermo-mechanical properties of shape memory alloys are described in the following sections.

Figure 1-2: Phase diagram of a shape memory alloy material [2]. The austenite and martensite transformation bands are shown. The critical stresses and temperatures of the material are placed on the temperature and stress axes.

1.1.2. Shape memory effect

Shape memory effect is the ability of the alloy to recover a certain amount of strain upon heating [3]. This phenomenon happens when the material is loaded such that the structure reaches the detwinned martensite phase and then unloaded while the temperature is below the austenite final temperature ($A_f$). Heating the material at this stage will lead to strain recovery of the material and the material will regain its original shape. This phenomenon can be better understood in the combined stress-strain
temperature diagram as shown in Figure 1-3. This diagram shows the typical thermomechanical behavior of shape memory alloys.

![Shape memory effect path of a shape memory alloy material](image)

Figure 1-3: Shape memory effect path of a shape memory alloy material [1]

Starting from point A material is initially in the austenite phase. Cooling down the alloy to a temperature below its martensite final temperature (Mf) will make the twinned martensite crystal. At this point, loading the alloy at the same temperature will lead the crystal to transform to the detwinned martensite phase at point C. This path is nonlinear because of the transformation phenomenon. Unloading the applied stress of the material at the same temperature will be linear to point D and keeps the detwinned martensite phase. At this point the material keeps a residual strain. By heating the alloy, when the temperature passes the austenite start temperature (As) at point E, the transformation from detwinned martensite to the Austenite crystalline phase starts. This transformation recovers the residual strain of the alloy which will be fully recovered at point F where the
alloy passes the Austenite final temperature. Increasing temperature more, the material will reach the starting phase and temperature at point A.

This shape memory behavior is used for the actuation applications. The actuation behavior of shape memory alloys is shown in the Figure 1-4. In this figure, a constant dead weight is applied to one end of a SMA spring. From left to right, the SMA spring actuator starts from the detwinned martensite phase in which the material is stretched and has the maximum displacement. Upon heating, the SMA temperature is increased, which causes the gradual transformation to austenite while passing the martensite-to-austenite transformation region as can be seen in Figure 1-5. This transformation leads to recovery of the strain in the material which can be seen as the recovered displacement in the spring. Cooling down the spring will cause the temperature to pass the austenite-to-martensite band, which leads the forward transformation and generating transformation strain in the material and makes the material crystal convert to the detwinned martensite phase.
Figure 1-4: SMA spring in actuation

Figure 1-5: Actuation path in phase diagram
1.1.3. Pseudoelasticity

The pseudoelasticity or superelastic behavior is associated with the stress-induced transformation of the shape memory alloys, which generates strain in the material and recovery of this strain upon unloading at temperatures above $A_f$ (Figure 1-6). The superelastic thermo-mechanical behavior starts from temperatures above austenite final temperature ($A_f$) where stable austenite exists. Alloy is loaded to make the detwinned martensite crystal form. During the transformation from austenite to martensite, the forward transformation happens and the transformation strain is generated. Upon unloading, the generated strain in forward transformation is fully recovered in the backward transformation and the original form is achieved. As shown in Figure 1-7, the pseudoelasticity effect involves recovering large deformations. The stress-strain cycle of such behavior is shown in Figure 1-8.

![Figure 1-6: Pseudoelasticity path in phase diagram](image)
Figure 1-7: Large deformation and recovery of strain in SMA wire above Af

Figure 1-8: Stress against strain in pseudoelasticity effect [1]
1.2. Shape memory alloys applications

In recent years, active materials including shape memory alloys are gaining special attention particularly in aerospace and biomedical applications. A recent well-known project in the aerospace applications of shape memory alloys involves bending in the variable-geometry chevron (VGC) (Figure 1-9) designed to decrease the airplane noise during the takeoff [4].

Biomedical applications of shape memory alloys especially in the form of nitinol alloy have been increased during the past few decades because of the special thermo-mechanical behaviors along with the biocompatibility of the material. These behaviors gave the researchers special abilities to develop devices which were impossible to develop before with other titanium alloys or stainless steel.

Figure 1-9: Configuration of the BOEING variable-geometry chevron (VGC) [5]
A famous commercial application of shape memory alloys in biomedical devices is in the self-expanding stent [6]-[8]. The name stent comes from the name of Dr. C.T. Stent who developed a device for dental applications in the late 1800’s [9]. Today, the name “stent” is known as a group of biomedical devices which are used to scaffold tubular passages like the esophagus or, more importantly, for blood vessels. Nowadays, most of the stents are made out of stainless steel. They are expanded to the vessel diameter with the inflation balloon by plastic deformations to keep them to the vessel diameter. On the other types, nitinol stents use shape memory effect behavior which makes them self-expanding. They are shaped set to the vessel diameter and then compressed in a low temperature to keep a smaller diameter. Usually the outer diameter of the shape set form is set 10% larger to assure that the stent cannot move. These stents are usually made by laser cutting a tube to make the latticed wall. But more than the shape memory effect, the superelasticity of the nitinol stents inside the body is another strong point for them. This gives them the flexibility of 10 to 20 times more than stainless steel. This flexibility is an important property in some superficial applications where the stent may be subjected to outside deformation or pressure. These deformations in stainless steel stents can cause permanent deformations and serious consequences for the patients while the superelasticity effect in nitinol stents makes them a much better option in superficial applications.

The reasons that nitinol has been widely used in medical applications are listed as below [6].

- Elastic deployment
- Thermal deployment
• Kink resistance
• Biocompatibility
• Constant unloading stresses
• Biomechanical compatibility
• Dynamic interference
• Hysteresis
• MR compatibility
• Fatigue resistance
• Uniform Plastic deformation

Elastic deployment or the extra flexibility of nitinol, which is the reason of the super-elasticity effect, can be used for different medical devices. Some devices need an instrument that can move through sharp curvatures and then elastically deploy to the desired shape. In these applications clearly nitinol can outperform other metals. Among the devices that benefits from elastic deployment of nitinol, the RITA tissue ablation device is shown in Figure 1-10. In this device, the curved tubular needles can be deployed from the straight shape upon insertion [10].
The shape memory effect of the material is the reason for another unique property of nitinol called thermal deployment. The Simon Vena filter, as shown in Figure 1-11, takes the advantage of this attribute. This device is designed to filter large embolized blood clots in the vein. The device is shape into the catheter form while the material is in the martensite phase outside the body so it keeps the shape. During the movement of the device through the vessel, the flushing chilled saline solution keeps the catheter in the martensite phase. Once the device reaches the desired position, the blood flow warms it up and the device recovers its original form. The same procedure is valid for stents.
Figure 1-11: Simon vena cava filter to prevent mobilized thrombus [6]

Stents, like the *Simon Vena* filter, have an austenite finish temperature above room temperature. This makes them superelastic at body temperature and in the martensite phase while in the sheath. Insertion of a stent into a vessel is shown in Figure 1-12. When the stent is in martensite it can be deformed into the required low temperature form and it will keep the form while it is in the sheath. Once the warm blood increases the temperature of the nitinol stent, it will recover the introduced deformation and it will regain the original shape, which is larger and keeps this form. At this phase the superelasticity effect of nitinol is helpful to keep the vessel open.
The superelasticity effect of the material can be used in another application in the angioplasty guide-wires. These wires are very long when used to access the brain. Also the paths in the body are so circuitous and have branches that need the wires to be very flexible and steerable [12]. The ability of nitinol to tolerate large deformations without permanent deformations, which can decrease the steer-ability of the device, makes it a good choice for the wire material. These wires are often coated with Teflon to increase the lubricity of the guide wires. Other devices have also been developed based on the kink resistance of nitinol which are shown in Figure 1-13.
The amount of body reaction when an external material is placed inside the body defines the biocompatibility of a material. Researchers have reported an extremely good
biocompatibility for the nitinol material because of formation of $TiO_2$ layer and very similar to $Ti$ alloy inside the body [13]-[17]. Another aspect of the biocompatibility of nitinol is shown in Figure 1-14. As can be seen, the Ptentiodynamics results show that the biocompatibility of nitinol is between Ti6-6-4 AND 316l.

Figure 1-14: Nitinol potential is between Ti-6-4 and 316L [6]

By looking into the stress strain plot of Titanium and Stainless Steel, it is understood clearly that they are stiffer and not similar to the plots for biological materials. Unlike these metals, nitinol has a very similar mechanical behavior to the
biological materials. The stress-strain plots as shown in Figure 1-15 have similar hysteresis.

![Stress-Strain Curve](image)

Figure 1-15: Stress-Strain curve of a few biological materials and comparison to nitinol [6]

This property gives nitinol the ability to distribute the load with the surrounding tissue and promote the growth of the surrounding bone. A group of orthopedic devices like the bone staples and hip implants take advantage of this property.

One other property of nitinol is the MR compatibility. Researchers have reported that nitinol shows a clear image better than stainless steel and similar to pure titanium [6].
A MR image of a stent is shown in Figure 1-16. As can be seen, the stent shape is very clear in the MR image.

Figure 1-16: MRI compatibility nitinol in stent [6]

1.3. Pedicle screw in osteoporotic bone

1.3.1. Spinal bone

The spinal bone has both the cortical and trabecular parts. The cortical bone is compact with about 1.8 g/cm$^3$ density. Dissimilarly, the trabecular bone is cancellous with 0.01-0.9 g/cm$^3$ density. The cortical bone has mechanical properties which have been listed in Table 1.1.
Table 1.1: Mechanical properties of bone [18]

<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>

The Trabecular bone has a cancellous structure with vertical and horizontal fibers. According to the experiments, depending on the direction of the applied load, the mechanical properties of the bone change. Also the researchers have reported that the strength of the cancellous bone is 60%-70% more in compression in comparison to tension [18]. The differences of the Trabecular bone and Cortical bone are illustrated in Figure 1-17.

Figure 1-17: Trabecular and Cortical bone [19]
1.3.2. Pedicle screw

Bone screws for various spinal treatments and fixations have been used for about 70 years [20]. Pedicle screws are used in vertebral column fixation and treatments. Pedicle is the small bony area, on either side of the vertebral body. Pedicles are the connection member of the vertebral body to the arch (Figure 1-18). Pedicle screws are used as bone anchoring elements to firmly grip the bone to facilitate attachment to the spinal implants.

![Vertebral anatomy](image)

**Figure 1-18: Vertebrae anatomy [21]**

Pedicle screws themselves don’t fix the spine in one place. Usually a connection rod is used to firmly connect these screws, which are inserted into two or three spinal segments (Figure 1-19). Using the pedicle screws and the connection rod, surgeons can fix the spinal segments together for spinal fusion. Due to the pedicle’s high density in healthy bones and its special structure, it makes it a good place for screw placement. The pedicular fixation system (which consists of a minimum of four pedicle screws and the rods) can resist against large loads and stabilize a fractured spine. These loads require the pedicle screws to be tightly fixed to the pedicle bone. Medical applications of pedicle screws show that tolerating the applied forces is possible for pedicle screws inside a
healthy bone. When the bone is not healthy, poor screw purchase becomes the main concern [25].

Figure 1-19: Pedicle screw fixation. a) Pedicle screws implanted into the pedicle area. b) pedicle screw and the connection rod and c),d) pedicle screw and the connection rod implanted into the pedicle bone to fixate the spine and correct deformity [23], [24]
1.3.3. Osteoporosis and its adverse effect in bone fixations

Osteoporosis is a very common bone disease in elderly people and especially in females which increases the risk of fracture in the bones of the patients. In this disease, the bone mineral density (BMD), which is related to the amount of the minerals in a certain volume, decreases drastically. The occurrence of this disease in elderly people steeply increases with age.

The National Osteoporosis Foundation (NOF) estimates that there are approximately 10 million people living in the United States who suffer from osteoporosis [27]. Approximately 80% of them are women. An additional 34 million U.S. citizens are considered at risk of developing osteoporosis due to having low bone mass. Statistical information regarding the prevalence and risk of osteoporosis among different demographics is presented in Table 1.2. The statistics pertain to individuals who are over the age of 50 years.

<table>
<thead>
<tr>
<th>Table 1.2: Osteoporosis statistical information [27]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Women</strong></td>
</tr>
<tr>
<td><strong>% with osteoporosis</strong></td>
</tr>
<tr>
<td>non-Hispanic Caucasian and Asian</td>
</tr>
<tr>
<td>non-hispanic African-American</td>
</tr>
<tr>
<td>Hispanic</td>
</tr>
</tbody>
</table>

There are some methods to measure the level of osteoporosis in patients. One of them is the *Jikei osteoporosis Grading Scale* which is based on radiographic images [28], [29]. Figure 1-20 shows the radiographic images of the patient’s spine from healthy bone to osteoporosis Grade 3. The image of the Grade 3 osteoporosis clearly shows that the bone is disappeared and the density is reduced.
For the surgeon, when deciding on the use of bone fixations for patients, the main concern is patients’ bone quality. Poor bone quality will cause loosening of the bone fixation during or after surgery. The bone’s poor quality in osteoporosis for the pedicle bone is shown in Figure 1-21.
The axial pullout test is a common way of evaluating the bone screw fixation strength. As shown in Figure 1-22, the pedicle screw is implanted inside the pedicle bone. In the pullout test, the screw is being pulled out of the bone in the axial direction of the screw. There is an ASTM standard (ASTM F543-02) available for this test.

![Axial pull-out test of pedicle screw fixation](image)

Figure 1-22: Axial pull-out test of pedicle screw fixation [54]

To overcome the drawbacks of osteoporosis in pedicle screw fixations, several methods have been used. Researchers have shown that strength of the screw inside the bone is related to the geometry of the screw. Increasing the major diameter of the screw
leads to stronger engagement of screw and bone. Chapman et al. [55] also showed that thread geometry has a significant effect on the pullout force of pedicle screws. The procedure of fitting the screw to the bone also has an effect on the pullout force. Battula et al [56] developed a parameter based on the pilot-hole size drilled into the bone before pedicle screw insertion. They showed that holes with a diameter larger than 72% of the screw’s outer diameter had an adverse effect on the pullout test.

One of the methods that showed successful treatment in mitigating the osteoporosis adverse effect was to inject a special kind of bio-compatible cement through the screw in order to glue the screw to the surrounding bone [57], [58], [59]. Even though this method has shown good performance in pullout tests, it poses several disadvantages which restrict its application. The hardening process of one common type of these cements (called Poly methyl methacrylate or PMMA), is an exothermic reaction releasing unwanted heat to the surrounding areas. This heat can be dangerous since the areas in question are so close to the neural elements of the spine. Also, the cement poses the threat of causing an infection around the pedicle bone. Lastly, applying the cement makes it much more difficult to remove the pedicle screw in the future, which may be necessary in the case of revision surgery. Another method is to use Hydroxyapatite coated implants. Both experimental and clinical research have shown higher bone screw purchase than the uncoated pedicle screws [60].

Recent research has shown novel methods that take advantage of expandable elements that increase the strength of the connection between screw and bone [61], [62]. The expandable form of dental implants is the other application of the expandable screws [63]. The elements in these screws are only expandable (and not retractable) so
that the removal of the screw becomes a much more challenging problem.

1.4. Smart pedicle screw design

In this section, the concept of a novel pedicle screw, developed previously in Dynamic and Smart Systems Laboratory, is discussed [31]. In this thesis, the design has been revised for improved functionality. The presented pedicle screw uses nitinol’s superior thermo-mechanical behavior to serve as the expandable elements of the pedicle screw. Another nitinol element serves to make the design retractable too.

1.4.1. Expandable-retractable nitinol elements

The presented pedicle screw consists of a typical pedicle screw and a few additional nitinol assemblies around the screw designed to produce two stable forms. One of the stable forms is the low temperature form that is achieved outside the body, and the other stable form is the high temperature form which is achieved when the screw is exposed to body temperature. In the low temperature form, the nitinol assemblies retract on the pedicle screw as shown in Figure 1-23. At the high temperature, the second stable form, which is the expanded form of the screw, is achieved as shown in Figure 1-24. The explained expansion-retraction procedure is repeatable so that nitinol assemblies can be retracted again to the original form by cooling down to the low temperature. This feature can be used to remove the screw as needed.
The assembly consists of two nitinol elements. These two elements are assembled in an antagonistic fashion such that they force each other in the opposite directions. One of the two elements is super-elastic (SE) in both low temperature ($T_{low}$) outside body and body temperature ($T_{body}$) cases. This means that the SE material’s austenite final temperature ($A_f^{SE}$) is lower than both low temperature and body temperature ($T_{low} > A_f^{SE}$ and $T_{body} > A_f^{SE}$). The other element remains a shape memory (SM) element at low temperature and transforms to its austenite phase at body temperature. To this end, the SM material should be selected such that its martensite final temperature ($M_f^{SM}$) be higher
than the low temperature and its austenite final temperature \( (A_{f}^{SM}) \) be lower than body temperature \( (T_{\text{low}} < M_{f}^{SM} \text{ and } T_{\text{body}} > A_{f}^{SM}) \). This design causes the tendency of the SM element to be more toward its original shape at body temperature. The SE and SM elements’ original shape is set such that in low temperature, the SE element is stronger and the assembly stays toward the SE element, which is set to be the retracted form of the screw. When the screw is inserted inside the bone, both the screw’s and its nitinol elements’ temperature will reach body temperature. At body temperature, the SM element passes its austenite temperature and moves the assembly toward its original shape that is set to be the expanded form. The described temperature relationships of the SM wire and SE tube are shown in the phase diagram in Figure 1-25. If for any reason a surgeon decides to remove the pedicle screw, he/she can cool down the screw in order to achieve the retracted form again and unscrew the pedicle screw out of the bone. The expanded and retracted form of the nitinol assembly with the shape memory (SM) and superelastic (SE) elements is shown in Figure 1-26.
Figure 1-25: States of the SM and SE elements in their phase plot at inside and outside body temperature. The SM element is in martensite at outside body temperature and transforms to austenite phase in body temperature while the SE element is in austenite at inside body and outside body temperatures.

Figure 1-26: Expandable-retractable nitinol assembly with SM and SE elements in a) retracted form and b) expanded form.
1.5. Objectives

The main objective of the research is to verify the concept of the new pedicle screw. To be able to verify the concept of the designed expandable and retractable elements, a framework is needed to numerically simulate the behavior. Like other numerical tools, the results of the simulation need to be verified before being used in design and optimization. To this end a set of experiments are required to verify the model.

The other objective is to evaluate the performance of the expandable elements in mitigating the osteoporosis adverse effect in the bone fixation. Similarly finite element software can be used to evaluate the performance.

1.6. Approach

To achieve the desired objectives, the first step is to be able to numerically simulate the performance of the designed shape memory alloy expandable-retractable attached to the pedicle screw to mitigate osteoporosis effect in bone fixation. To this end, the numerical form of a three dimensional thermo-mechanical model of shape memory alloys, which is coded in Abaqus UMAT subroutine, is used. The numerical tool is able to capture the shape memory effect and pseudoelasticity in three dimensional geometries. This simulation tool is used to verify the concept of the designed elements which can expand and retract around the shaft of a pedicle screw. The model for this actuation system in larger scales is made in Abaqus and validated through the experiment to verify the concept.

The other objective was to verify the effect of the expanded element around the pedicle screw and show the higher purchase of the bone fixation. Another model is
prepared in Abaqus to numerically simulate the bone screw strength and verify the performance.

1.7. Contributions

The contribution of the work was to be able to successfully simulate the three dimensional thermo-mechanical behaviors of the shape memory alloys in the biomedical device. The performance of the finite element numerical code in Abaqus UMAT subroutine is verified for the biomedical devices applications with experiments. More than that, another model is developed in Abaqus finite element software to predict the performance of the designed novel pedicle screw in pullout test. The following publications are the results of the efforts during this research.

1.8. Publications

Journal:


Proceeding:


6. A. Eshghinejad, M. Elahinia,"Functionality analysis of nitinol elements in expandable pedicle screw to mitigate osteoporosis”, Midwest Graduate research symposium, the University of Toledo, 2011 Report
Business plan report: “SMArt pedicle screw production and marketing analysis”, Annual UTIE Business Plan Competition at the University of Toledo, OH, October 2011
Chapter Two

Mathematical modeling of shape memory alloys and the numerical implementation

2.1. Introduction

In order to completely understand the thermo-mechanical behavior of shape memory alloys in any application, developing mathematical models is inevitable. During the recent years the area of constitutive modeling of shape memory alloys has been the point of interest of many researchers. The developed models can be classified into two groups: Micromechanical-based models and phenomenological models [32].

The micromechanical models use the polycrystalline behavior of SMAs in martensite and austenite. These models develop the mathematical thermo-mechanical models in the microscopic viewpoint.

The phenomenological models assume the mixture of two solid state phases to represent the behavior of the material. Preisach models [33] and the irreversible thermodynamics principles [34] can be listed among these models. These modeling use different energy conservation principles. Most of the parameters along with the state
variables in the phenomenological models are easy to measure. This makes these models 
easier to use in application and the numerical implementations.

Tanaka and Nagaki [35] model was among the first phenomenological models 
presented. The state variables in this model were strain (\( \varepsilon \)) and temperature (T) and the 
martensite volume fraction which has a value between zero and one (0 < \( \xi \) < 1). The 
internal variables were assumed be time and space averaged on the material domain. The 
model developed by Liang and Rogers [36] in later years and followed by Brinson 
models [37][38][39] and added the twinned and detwinned Martensite as another internal 
variable to model the behavior based on an experimentally defined phase diagram. It was 
shown that various one dimensional phenomenological models are similar but they are 
different in formulations of the transformation functions [38]. Later Gao et al.[39] 
improved the previous works by developing a one dimensional finite element method for 
truss elements, utilized to model shape memory alloys behavior in several models.

Modeling and analysis of SMA beams in bending has been the subject of several 
investigations. Gillet et al. [40] developed a numerical method to predict the behavior of 
a SMA beam in a three-point bending test. They conducted experiments for validating the 
numerical results. M. Jaber et al. [41] used finite element analysis to predict SMA beam 
behavior in a nitinol staple. Hartl et al. [42], [43] addressed the training, characterization, 
and derivation of the material properties of their shape memory alloy actuator. They also 
assessed the actuation properties of their active beam actuator and analyzed it accurately 
using finite element analysis. They developed a numerical tool in Abaqus to simulate the 
actuator's thermo- mechanical behavior. Tabesh et al. [44] used a combined SMA rod and 
tube assembly in bending. They used the shape memory effect and superelastic behavior
of nitinol alloy to develop a bi-stable actuator. In their actuator the tube and rod apply bending force in an antagonistic manner as a result of temperature variation. Mineta et al. [45] used a SMA bending beam to develop a micro-actuator. Zbiciak performed dynamic analysis for superelastic beams [46].

While numerical methods are widely used and accepted for analyzing SMA devices, they have certain limitations. Validity of the results is always a concern, which necessitates experimental validation. It is a known fact that experimentation with these alloys, even for simple tests, is difficult and could be expensive. It is desirable that the numerical solutions can be validated against closed-form solutions [47]. Exact solutions are less expensive computationally and as a result they provide faster simulations. Additionally, exact models are more readily applicable in real time simulations and control of SMA actuators. Mirzaefar et al. [47] have conducted a study to find the exact solution for torsional behavior of shape memory alloy bars. They simplified a three dimensional model [67] to a one-dimensional shear form. This way, they developed an exact form for the relationship between the applied torque and the angular displacement. Two studies [48], [49] proposed an analytical solution for solving the moment due to stress distribution of a superelastic material versus the curvature of a SMA Euler-Bernoulli beam. The limitation of these solutions is due to assuming equal elastic moduli for austenite and martensite phases of the material. The other limitation is assuming equal initial and final stresses for the phase transformation values. This assumption is not exactly what we usually observe in tensile tests of SMA specimens.
In the next section one of the famous phenomenological constitutive models of shape memory alloys which were used in this work will be described. The numerical implementation of the model in Abaqus as the finite element software is also described.

### 2.2. Boyd-Lagoudas constitutive model for shape memory alloys

The model presents a three dimensional thermo-mechanical constitutive model for shape memory alloys. The model has been extensively explained in Lagoudas et al. [66]. In this section the model is briefly described which will be used for the following simulations.

The model is based on the Gibbs free energy as given by:

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

where \( \sigma, \xi, \varepsilon^t, T \) and \( T_0 \) are defined as the Cauchy stress tensor, martensitic volume fraction, transformation strain tensor, current temperature and reference temperature, respectively. Other material constants \( \alpha, S, \rho, c, u_0 \) and \( s_0 \) are the effective thermal expansion tensor, effective compliance tensor, density, effective specific heat, and effective specific internal energy at reference state and effective entropy at reference state. The hardening function was shown in the equation as \( f(\xi) \). As described in Lagoudas [1], by setting the hardening function in the available models different hardening curves can be achieved. These material constants are defined with rule of mixture in the material.

\[
S = S^A + \xi(S^M - S^A)
\]
The variables with superscripts A and M show the values in austenite and martensite phases respectively. Based on the continuum mechanics equations to find the strain derived by the energy, the total strain will be found as:

\[ \varepsilon = S: \sigma + \alpha(T - T_0) + \varepsilon^t \]  

(8)

The first term is related to the strain due to the applied stress and the second term is the strain due to thermal expansion and the last term is the strain due to transformation. This equation requires a relationship between the transformation strain tensor \( \varepsilon^t \) and the martensite volume fraction. This relationship is expressed by:

\[ \dot{\varepsilon} = \Lambda \dot{\xi} \]  

(9)

In this equation, the transformation tensor is \( \Lambda \) which defines the direction of transformation. Two different forms are proposed for the transformation tensor. The first one is:

\[ \Lambda = \begin{cases} 
\frac{3}{2} H \frac{\sigma'}{\bar{\sigma}} , & \xi > 0 \\
H \varepsilon^{t-r} / \bar{\varepsilon}^{t-r} , & \xi < 0
\end{cases} \]  

(10)

where \( H \) is the maximum axial transformation strain, and \( \varepsilon^{t-r} \) is the transformation strain at the reversal point. Other parameters are defined as:
This transformation tensor is suitable for proportional loading cases. For more complicated cases a transformation tensor independent of the loading direction is defined as below for loading and unloading cases:

\[
\Lambda = \frac{3}{2} H \frac{\sigma'}{\bar{\sigma}}
\]  

(14)

A new parameter named as thermodynamic force is defined on the second thermodynamic law inequality in order to later recognize the transformation happening recognition.

\[
\pi = \sigma: \Lambda + \frac{1}{2} \sigma: \Delta S: \sigma + \Delta \alpha: \sigma(T - T_0) - \rho \Delta c[(T - T_0) - T \ln \left(\frac{T}{T_0}\right)]
\]  

(15)

where prefix \(\Delta\) shows difference of the parameter value in martensite and austenite.

Based on the thermodynamic force the transformation function can also be defined as:

\[
\phi = \begin{cases} 
\pi - Y^* & \dot{\xi} \geq 0 \\
-\pi - Y^* & \dot{\xi} \leq 0
\end{cases}
\]  

(16)

In this equation \(Y^*\) is a constant and mentioned as the internal dissipation due to the phase transformation. Using the second thermodynamic law from the Gibbs free energy, the following inequalities can be derived:

\[
\phi(\sigma, T, \xi) \leq 0 \rightarrow \begin{cases} 
\phi = 0 & \text{if } \dot{\xi} \neq 0 \\
\phi < 0 & \text{if } \dot{\xi} = 0
\end{cases}
\]  

(17)
This means that when the transformation is happening the $\phi$ function needs to be equal to zero and when there is no transformation in the material the $\phi$ function needs to be less than zero. The hardening functions which were mentioned in Equation 1 can be defined in several forms. The Tanaka [50] form of the hardening function is selected as:

$$f(\xi) = \begin{cases} \frac{\Delta s_0}{a_\phi^M} [(1 - \xi) \ln (1 - \xi) + \xi] + (\mu_1^c + \mu_2^c) \dot{\xi} & \dot{\xi} > 0 \\ -\frac{\Delta s_0}{a_\phi^A} \xi [\ln(\xi) - 1] + (\mu_1^c + \mu_2^c) \dot{\xi} & \dot{\xi} < 0 \end{cases} \tag{18}$$

and the Liang and Rogers form of the function can be selected as:

$$f(\xi) = \begin{cases} -\frac{\Delta s_0}{a_\phi^A} \int_0^\xi [\pi - \cos^{-1}(2\xi - 1)] d\xi + (\mu_1^c + \mu_2^c) \dot{\xi} & \dot{\xi} > 0 \\ -\frac{\Delta s_0}{a_\phi^M} \int_0^\xi [\pi - \cos^{-1}(2\xi - 1)] d\xi + (\mu_1^c + \mu_2^c) \dot{\xi} & \dot{\xi} < 0 \end{cases} \tag{19}$$

The Boyd-Lagoudas [66] form is a polynomial form as:

$$f(\xi) = \begin{cases} \frac{1}{2} \rho b^M \xi^2 + (\mu_1^p + \mu_2^p) \dot{\xi} & \dot{\xi} > 0 \\ \frac{1}{2} \rho b^A \dot{\xi}^2 + (\mu_1^p + \mu_2^p) \dot{\xi} & \dot{\xi} < 0 \end{cases} \tag{20}$$

where the constants can be achieved to enforce the continuity of the function during forward and backward transformation. Another hardening function is developed by Hartl [5] known as smooth hardening function.

$$\dot{g}^t = \begin{cases} \frac{1}{2} a_1 (1 + \xi^{n_1} - (1 - \xi)^{n_2}) + a_3 & \dot{\xi} > 0 \\ \frac{1}{2} a_2 (1 + \xi^{n_3} - (1 - \xi)^{n_4}) + a_3 & \dot{\xi} < 0 \end{cases} = \begin{cases} f^t_{fwd} & \dot{\xi} > 0 \\ f^t_{rev} & \dot{\xi} < 0 \end{cases} \tag{21}$$

In this form of the hardening function, the parameters $n_i$ define the degrees of smoothness.
2.3. Numerical implementation of the model in Abaqus

The described constitutive model to predict the behavior of shape memory alloy materials cannot be used to model various geometries and conditions without implementation into a numerical environment. To be able to have the capability of analyzing complex problems, a previously developed code into the Abaqus finite Framework [51] as a user material subroutine (UMAT) is used. This code is the numerical implementation of the described constitutive model. The method in which the global Abaqus solver uses the UMAT subroutine to model a nonlinear material like shape memory alloys is described in Figure 2-1. As shown, the model uses displacement based FEA, which is known as the more popular method. Based on the thermo-mechanical loading pass, solver begins by guessing the appropriate initial deformation over the domain nodes by solving the linear problem (elastic stiffness matrix). These strains are fed into the user material subroutine. The UMAT subroutine updates the stresses based on the shape memory alloys constitutive model. Other than the updated stresses, the local tangent stiffness over the material point domain is also calculated. These stresses are used to calculate the forces on the elements by integration over the element. The resultant force applied on all nodes is calculated which needs to be zero to satisfy the static equilibrium. The residual forces on these nodes are calculated and if the magnitude is less than a certain tolerance the solution is valid and the solver moves forward to the next loading path. If the magnitude is large, Newton-Raphson method is used to guess new values for the deformations where the calculated tangent stiffness in the UMAT relates the residual force to the new guessed displacements.
Figure 2-1: Schematic illustration of the problem solving in Abaqus with UMAT subroutine [5]

Inside the previously developed UMAT subroutine, as described before, for each node the strain is the input from the Abaqus global solver and the stress and the stress tangent stiffness are the outputs. The UMAT algorithm assumes no transformation at the beginning of each step. If with the elastic assumption, $\phi < 0$ happens then the UMAT can return the result as the stress of the node. But if violation of the inequality happens with the elastic assumption, it means that transformation is taking place. As described in Qidwai and Lagoudas [65] using the return mapping algorithm the required stress and tangent stiffness can be found in the transformation condition. In this case, the increment of the martensite volume fraction evolves and based on the described constitutive equations the resultant stress is calculated. Each time the transformation function is recalculated and once $\phi = 0$ condition is achieved the results will be returned to the global solver.
Chapter Three

Results: Evaluation and discussion

3.1. Preliminary simulations

Now that we have the numerical tool implemented into the Abaqus solver to analyze shape memory alloys behavior, we are able to observe the results for some preliminary tests. These two preliminary simulations were conducted to observe the specific thermo-mechanical behaviors of shape memory alloys in tension.

In the following sections, a block out of shape memory alloy material with the material properties reported in Table 3.1 is used for the simulations. The block model is made in Abaqus GUI as shown in Figure 3-1. The left side nodes of the block are fixed and equal forces are applied to the right end nodes.
**Table 3.1: Material properties used for preliminary simulations**

<table>
<thead>
<tr>
<th>Material properties</th>
<th>Value</th>
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<tbody>
<tr>
<td>$E_M$ (Gpa)</td>
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</tr>
<tr>
<td>$E_A$ (Gpa)</td>
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<td>$Mf$ (C)</td>
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<td>Cm (Mpa/C)</td>
<td>7</td>
</tr>
<tr>
<td>Ca (Mpa/C)</td>
<td>7</td>
</tr>
</tbody>
</table>

**Figure 3-1: Prepared block model in Abaqus for preliminary simulations**
3.1.1. Simulation of a superelastic case

In the first simulation, we want to observe the superelasticity behavior of the material in tension. For this reason, the temperature of the block is set to 52°C to be above the austenite final temperature (Af). The resulted stress against strain on the block due to the applied force is plotted in Figure 3-2. As can be seen, the generated strain due to transformation in loading is fully recovered in the unloading path. This simulation showed the ability of the numerical tool in modeling the superelasticity thermo-mechanical behavior of shape memory alloys.

![Figure 3-2: Preliminary simulation of the superelastic behavior](image)

3.1.2. Simulation of a shape memory case
To simulate the shape memory effect, the temperature of the block needs to be below the austenite start temperature. To this end, the temperature is set to 20 \textdegree C and the initial state is in austenite phase. The result of loading and unloading the block is shown in Figure 3-3. As can be seen, the transformation strain in loading is generated, but this strain has not been recovered during the unloading. This simulation showed the ability of the numerical tool in modeling the shape memory effect behavior of shape memory alloy materials.

![Figure 3-3: Preliminary simulation of shape memory effect](image_url)
3.2. Validation of the numerical tool

To be able to use the developed numerical tool in Abaqus to analyze shape memory alloys thermo-mechanical behavior, the generated output results should be verified against some experimental results. To this end, in the following sections, the numerical tool’s results are compared in two general cases of bending and torsion.

3.2.1. Validation in bending

To validate the numerical tool in Abaqus and modeling shape memory alloy material behavior in bending, the model was confirmed in bending against a previously published experiment. This exercise was conducted to verify the model accuracy. For all simulations presented, implicit Abaqus solver was utilized.

The first step is to find the material properties of the shape memory alloy which is tested. The material properties needed in this model were found from the reported tensile test data in Gillet et al. [40]. The material properties that are used are reported in Table 3.2. The tensile simulations match the experimental tensile test plot as shown in Figure 3-4.

<table>
<thead>
<tr>
<th>$E_M$ (Gpa)</th>
<th>$E_A$ (Gpa)</th>
<th>$\sigma_{MS}$ (Mpa)</th>
<th>$\sigma_{MF}$ (Mpa)</th>
<th>$\sigma_{AS}$ (Mpa)</th>
<th>$\sigma_{Af}$ (Mpa)</th>
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<td>73.2</td>
<td>371</td>
<td>613.3</td>
<td>548</td>
<td>305.7</td>
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<td>0.3</td>
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</tbody>
</table>
Figure 3-4: Simulation results of tensile test in Abaqus against experiments by Gillet et al. [40]

The bending prediction of the model was validated using a three point bending experiment conducted by Gillet et al. [40]. The length of the beam is 49.92mm and the cross section is a 2.9mm by 0.95mm rectangle Figure 3-5.

Figure 3-5: Three point bending test beam dimensions

The simulation is performed in Abaqus using 20 node elements with reduced integration (C3D20R). It is worth noting that for bending, the shear locking phenomenon occurs with full integration 8 node brick elements in bending and, as a result, the
Simulation predicts overly stiff behavior of the beam. Shear locking is a numerical phenomenon found in bending analysis and modal analysis. This phenomenon can be seen when observing the difference between first-order and second-order brick elements. In first-order brick elements, the deformed shape will cause an unreal shear stress which will cause the material to be stiffer than in a real case. This problem can be solved by using a 20 node reduced integration element. Sixty, thirteen and ten elements were used to mesh the beam's length, height and width, respectively. A 6.5mm ramp displacement (from the presented experimental force-displacement plot) is applied on the middle section of the beam in the loading step and the reaction forces are measured. The same method is applied for the unloading part of the simulation. The stress distribution in the middle of the beam is shown in Figure 3-6. The simulation results for the loading and unloading force versus displacement are superimposed with the experiment results by Gillet et al. [40] as illustrated in Figure 3-7. As can be seen, there is good agreement between the simulation and experiment.

Figure 3-6: Stress distribution on the beam
3.2.2. Validation of the model in torsion

To validate the combination of the Abaqus solver and the developed numerical tool in modeling shape memory alloy rod in torsion, the results of the simulation were compared to the experimental data.

To obtain the material properties of the wire samples, three tensile tests were done using a mechanical testing machine (BOSE ElectroForce 3330) equipped with a temperature controlled environmental chamber (Applied Test Systems environmental chamber) as shown in Figure 3-8.

Figure 3-7: Force versus displacement of the three point bending test in simulation against experimental results by Gillet et al. [40]
The tests were conducted at the following four different temperatures: 36 C, 40 C, 50 C, and 60 C. Each of the samples underwent 5 complete cycles of loading and unloading to ensure that a stable plateau was reached at each temperature. The displacement rate for the tensile tests was 0.5 mm/sec for a 188 mm long wire which is equivalent to a strain rate of 0.2660 %. Results of this tensile testing for each of the temperatures can be seen in Figure 3-9. The data obtained from these tests was used for comparison of the model to the lowest loading rate of the torsional samples.
Figure 3-9: Tensile test experiment

Transformation stresses were found from the stress-strain diagram for each temperature. From this, a line between the three critical points of the temperatures was fit to obtain the slopes of martensite and austenite in the stress-temperature phase diagram (CM and CA). To find the transformation temperatures, the equation of the related transformation line was set equal to zero and the transformation temperatures were found. Young’s Moduli were also calculated from the stress-strain curves by calculating the slopes of the linear, fully transformed, regions of martensite and austenite. These material properties are summarized in Table 3.3.
Table 3.3: Material properties of the nitinol rod

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
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<td>°C</td>
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</tr>
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<td>$C_A$</td>
<td>8.6</td>
<td>Mpa/°C</td>
</tr>
<tr>
<td>$\varepsilon_L$</td>
<td>0.039</td>
<td>-</td>
</tr>
</tbody>
</table>

To simulate the behavior in pure torsion an axisymmetric element with a rotational degree of freedom around its center axis (element CGAX8 from the Abaqus element library) was used (Figure 3-10). Similar to the experimental testing, the length of the wires was 0.4 inches while the diameters were 0.018, 0.020 and 0.023 inches. The number of elements in the radial direction from the center to the maximum radius was 30. To get an appropriate aspect ratio, 300 elements were used within the length of the part. The bottom surface of the specimen was held fixed in the vertical direction. The rotational displacement is applied to the top surface of the specimen (the maximum applied rotational displacement was chosen from the experimental results in the rotational displacement). While increasing and decreasing the applied rotation angle in loading and unloading, the produced reaction torque in the wire was computed by summing each of the reaction torques at the nodes of the clamped end. All of the simulations were held at 23°C.

As shown in Figure 3-11, the 3-D model accurately predicts the loading curve of the material, but shows a lower level of stress in the unloading plateau, which leads to a
wider hysteresis. The same behavior is exhibited in the torque-angle plots for the various wire diameters. The 3-D model, however, predicts the behavior of the material more accurately. Figure 3-12 shows how the model predicts the torque-angle behavior of the material for each of the three wire diameters.

Figure 3-10: Axisymmetric elements in the torsion model of a rod
Figure 3-11: Comparison of the 3-D model (developed in Abaqus) with the experimental axial stress-strain curve of 0.020" wire.

Figure 3-12: Comparison of torque-angle results of the model (developed in Abaqus) with the experimental data for various wire diameters (d=0.023, 0.020, 0.018 inch).
3.3. Evaluation of the concept of antagonistic SM and SE expandable-retractable elements

To evaluate the functionality of the designed antagonistic concept for the nitinol assembly to expand and retract around the pedicle screw, some experiments were required. The experimental method and its results are described in the next section. The finite element (FE) analysis tool in Abaqus software was also validated with the experimental results.

3.3.1. Experiments

Shape setting the elements was performed first. For this experiment, the SE element was a nitinol flat wire with the cross section of 0.8mm × 9mm and the SM element was a nitinol round wire with the diameter of 2mm. The shape set curve geometry is presented in Figure 3-13. Note that these sizes and geometries are used as a proof-of-concept for the expandable-retractable assembly. The size, geometry of the curves and the method of attachment should be modified in the next designs of the elements.
The actuator device was made up by assembling the two nitinol elements in an antagonistic fashion placed inside the notches designed in the aluminum fixture (Figure 3-16). The SE element’s original curve was upward and the SM element’s original curve was downward. To heat the SM wire, Joule heating was used by applying electric current through the wire. The electric wires to heat the SM element were connected to the ends and both were connected to a programmable power supply (Agilent 6543A). To control the input current to the SM wire, the power supply was controlled by the input signal coming from a software/hardware control package (dSPACE 1104).

The dSPACE package consists of hardware to connect devices and a software to program the function called ControlDesk. The hardware, as shown in Figure 3-14, has several input ports to connect to a wide range of sensors and output ports to connect to devices such as actuators and controllable amplifiers. In the software part, the Matlab Simulink models can be imported to receive the input signals and prepare the required output signals to the output ports.
Figure 3-14: dSPACE hardware. The input and output ports are shown in the board.

The whole experimental setup can be seen in Figure 3-16. To measure the tip displacement of the actuator, a laser distance sensor (optoNCDT 1401) was used (Figure 3-15). The output signal of the sensor was fed into the dSPACE hardware to be captured in its specific computer software (ControlDesk).

Figure 3-15: Laser distance sensor device (optoNCDT 1401)
Figure 3-16: Actuator assembly with the antagonistic SE and SM elements. The wire is connected to the two sides of the SM wire.

A Matlab Simulink model was prepared to be implemented into the dSPACE software. The first aspect of the model was to convert the laser transducer voltage signal into a displacement. The required gain for this conversion was calibrated experimentally. The next portion of the model was developed to generate the appropriate signal to the dSPACE output port. This port gives the required signal for the power supply to generate the current output to heat the SM wire. For this experiment, a Joule heating differential equation was simulated to predict the wire temperature.

The simulated differential equation to predict temperature can be found in Equation 22.

\[ RI^2 - h_c A_c (T - T_{\text{inf}}) = m C_p \frac{dT}{dt} \]  \hspace{1cm} (22)

Where the input current to the wire has the following form:

\[ I = D(-\cos\left(\frac{\pi t}{300}\right) + 1) \]  \hspace{1cm} (23)
where $D$ is the amplitude of the current signal. The constant parameters used in the differential equation are listed in Table 3.4. The resistivity of shape memory alloys is known to change from martensite to austenite because of different crystals in these phases. But for temperature predictions in this work, resistivity is assumed to be constant during the transformation and is achieved by dividing voltage and current in room temperature. The input signal during the experiment is plotted in Figure 3-18.

<table>
<thead>
<tr>
<th>Table 3.4: Implemented constants for prediction of temperature.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resistivity ($R$)</td>
</tr>
<tr>
<td>0.27 Ohm</td>
</tr>
<tr>
<td>Specific heat ($C_p$)</td>
</tr>
<tr>
<td>836 J/Kg.C</td>
</tr>
<tr>
<td>Density ($\rho$)</td>
</tr>
<tr>
<td>6.5 g/cm$^3$</td>
</tr>
<tr>
<td>Heat convection coefficient ($h$)</td>
</tr>
<tr>
<td>120 J/(m$^2$.C.sec)</td>
</tr>
</tbody>
</table>

Figure 3-17: SIMULINK model to predict temperature. The model consist of the block to read from dSPACE input port (ADC) and the block to send signal to the output port (DAC)
We can solve the differential equation using analytical method for the first order differential equation. The equation can be rearranged to the following form:

$$\frac{dT}{dt} + AT = B \left( \frac{1}{2} \cos \left( \frac{\pi t}{155} \right) - 2 \cos \left( \frac{\pi t}{310} \right) + \frac{3}{2} \right)$$  \hspace{1cm} (24)

where:

$$A = \frac{h_e A_e}{mc_p}$$

$$B = \frac{RD^2}{mc_p}$$

If we solve the nonhomogeneous part of this first order differential equation separately and add up the solution, the following general equation can be achieved:

$$T - T_0 = Ce^{-At} + C_1 \cos \left( \frac{\pi t}{155} \right) + C_2 \cos \left( \frac{\pi t}{310} \right) + \frac{3B}{2A}$$  \hspace{1cm} (25)

where:

$$C_1 = \frac{155A}{pi} D_1$$

$$D_1 = \frac{B}{2} \left( \frac{155\pi}{\pi^2 + 155^2 A^2} \right)$$

$$C_2 = \frac{310A}{pi} D_2$$

$$D_2 = -2B \left( \frac{310\pi}{\pi^2 + 155^2 A^2} \right)$$

$$C = -C_1 - C_2 - \frac{3B}{2A}$$
Figure 3-18: Input signals to heat the SM wire and the predicted temperature of the SM element due to the current input signals. The prediction was done Simulink® model by numerically solving the Joule heating differential equation.

Two sine wave currents with the amplitude of 3A and 2.5A are generated by the required input signal to the amplifier. The electricity connection wire connects the generated current to the two sides of the SM wire. The predicted temperatures according to each current input are illustrated in the same figure. When the temperature of the assembly is at its low temperature, the SE wire is strong enough to keep the assembly toward its original shape, as shown in Figure 3-19. Gradually, by heating the SM wire above its austenite finish temperature, motion at the tip of the actuator is observed. After appropriate heating, no further displacement can be observed with increasing temperature (Figure 3-20). The reason is that the SM element will completely pass its transformation band at a certain temperature (although the transformation is not the same for the points along the length and height of the beam). The described heating and cooling process was
repeated several times and a repetitive motion of the wires can be observed.

Figure 3-19: Actuator setup in room temperature.

The observed behavior in low and high temperatures from the actuator is desirable for evaluating the concept. As shown in Figure 3-21, by heating the assembly, the tip will
move toward a stable form and, by cooling it down, it will achieve the other stable form and the procedure is repeatable. Obviously, to achieve the final design of the antagonistic nitinol assembly for the pedicle screw, the material properties, shape set form, cross section, and length of the wires should be optimized for that case.

Figure 3-21: Measured displacement of the tip versus the temperature of the beam

3.3.2. Finite element simulation

To better optimize the device, a simulation tool was used to avoid the time consuming process of making several prototypes. For the finite element analysis, Abaqus software suite [64] was used. Because of the unique thermo-mechanical behavior of shape memory alloy materials, a previously developed user-defined material (UMAT) subroutine is used [65]. The UMAT subroutine is based on a numerically implemented full 3D SMA constitutive model, which is in term based on the Boyd-Lagoudas model [66]. The UMAT subroutine is used to model the behavior of the SM wire, which is a function of the variation in temperature. The SE element is modeled with an elastic
material which can obviously undergo large deformations without variation in its modulus of elasticity. The constant superelastic modulus of elasticity was found by experiment to be 52 GPa. But it can have large strains without reaching the plastic region. The material properties which were used for the SM wire in the simulation are shown in Table 3.5.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_A$</td>
<td>32 Gpa</td>
</tr>
<tr>
<td>$E_M$</td>
<td>22 Gpa</td>
</tr>
<tr>
<td>$M_s$</td>
<td>62 C</td>
</tr>
<tr>
<td>$M_f$</td>
<td>27 C</td>
</tr>
<tr>
<td>$A_s$</td>
<td>60 C</td>
</tr>
<tr>
<td>$A_f$</td>
<td>92 C</td>
</tr>
<tr>
<td>$\varepsilon_L$</td>
<td>0.02</td>
</tr>
</tbody>
</table>

The Abaqus model was prepared in a few steps. Initially the SE and SM parts were drawn in their shape set form. Next, a rotation displacement was applied to the tip surface of the nitinol parts to make both straight while the assembly was in the low temperature. The next step applied the required contact between the surfaces of the SE and SM elements. In the same step, SM wire was heated up to achieve the temperature from experiment. The wire was cooled down to the low temperature and then again heated to the high temperature. Since the nitinol wires are used in bending here and as described in the validation of the subroutine in bending, C3D20R elements were used to avoid the shear locking phenomenon. The contact was chosen to be surface to surface with contact overclosure removal. The predicted shapes of the assembly in high and low temperatures are depicted in Figure 3-22. These pictures show a striking resemblance to
those of the experimental results in Figure 3-19, Figure 3-20.

Figure 3-22: Simulated mises stress distribution of the SM and SE elements in a) high temperature and b) low temperature form.

The results of tip displacement against temperature of the assembly are plotted in Figure 3-23 and Figure 3-24 for the two sets of experiments with different input signals. The expected behavior for the concept of the antagonistic SM and SE assembly is achieved. The tip position of the assembly moves between the two stable positions in low temperature and high temperature. Also the FE analysis tool in Abaqus can predict the SMA behavior in this experiment. The maximum displacement of the actuator is very well predicted by the simulations. The displacement of the SM wire begins to increase with a steep slope after the temperature is increased beyond its austenite start temperature (60°C). After adequate heating of the assembly, the actuator will reach its stable displacement at high temperature. Cooling the wire assembly below its martensite start temperature (62°C) causes the tip position to move toward its low temperature position.
After cooling below the marten-site final temperature (27°C) the assembly reaches the low temperature stable position. It should be noted that the final tip displacement (agreeing well) was of interest, not the path the sample takes to get there.

Figure 3-23: Temperature-displacement path of the actuator with the 5A current profile as the input.
3.4. Pullout test

In this section the performance of the designed pedicle screw is evaluated in a pullout test. A pullout test is regarded as a common way of evaluating the mechanical effectiveness of bone screw implants. There is an ASTM standard (ASTM F543-02) available for this test (Figure 3-25). As can be seen in the figure the screw is being pulled out of a fixed block in the normal direction to the block surface and the required force is recorded. The test relies on the fact that the major mode of clinical failure of bone implants is due to normal forces that are pulling the implant out of the bone. During the test, the implanted bone screw resists against a pulling out force. The ultimate pullout force of the screw is defined as the amount of force whereby the material force-displacement relation finishes the linear region. This force determines the strength of the
Figure 3-25: Schematic of test apparatus for pullout strength test from ASTM F543-02 standard

3.4.1. Finite element simulation

In order to simulate the pullout test of the SMArt pedicle screw in the FEA software and evaluate the benefit of the expandable elements, the problem is divided into three sections. First, the pullout test was simulated in Abaqus using a normal screw and healthy bone material properties which were previously simulated and validated by Zhang et al. [67]. By comparing the result of the performed simulation with the presented pullout force in the paper, the FEA simulation procedure was confirmed. The second step was dedicated to the pullout test modeling of the pedicle screw in osteoporotic bone and the effect of the expandable elements. The last step was to simulate the effect of the expanded elements in the pullout test. At last the result of the simulation in the normal fixation.
bone is compared to the result in osteoporotic bone with the expanded elements.

3.4.2. Normal bone pullout

A pullout test of a normal pedicle screw out of a healthy bone was analyzed. This was done by simulating a 6.5mm outer diameter bone screw with spherical under-surface and asymmetrical thread. The thread profile dimensions of the screw were derived from British Standard Institution [68]. The dimensions of this thread profile are shown in Figure 3-26 and defined in Table 3.6. The bone material properties were derived from Goel et al. [69] and the screw was assumed to be stainless steel with the material properties presented in Tencer and Johnson [70]. These material properties are listed in Table 3.7.

Table 3.6: Employed pedicle screw dimensions in this study. All the dimensions are derived from [5]

<table>
<thead>
<tr>
<th>d1 (mm)</th>
<th>d2 (mm)</th>
<th>a1 (°)</th>
<th>a2(°)</th>
<th>r1(mm)</th>
<th>r2(mm)</th>
<th>e(mm)</th>
<th>p(mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.5</td>
<td>3.0</td>
<td>5</td>
<td>25</td>
<td>1.2</td>
<td>0.8</td>
<td>0.2</td>
<td>2.75</td>
</tr>
</tbody>
</table>

Table 3.7: Employed material properties for bone and screw.

<table>
<thead>
<tr>
<th>Material</th>
<th>E (Mpa)</th>
<th>ν</th>
<th>σ_y (Mpa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bone</td>
<td>100</td>
<td>0.2</td>
<td>2.0</td>
</tr>
<tr>
<td>Screw</td>
<td>193,000</td>
<td>0.3</td>
<td>250.0</td>
</tr>
</tbody>
</table>
Figure 3-26: Cross section profile of the employed 6:5mm cancellous bone screw with spherical under-surface and asymmetrical thread, derived from British Standard Institution [5]

In this simulation, all the posterior elements of the vertebra were ignored and the screw thread contacts were the focus. The vertebral body was modeled with a block with dimensions of 16mm width, 16mm height and 22mm length. The position of the pedicle screw was assumed to be in the middle of the block. The bone thread holes were assumed to have the same profile as the screw. For this model a pedicle screw with eight threads measuring 22mm in length was used. Because of the symmetry in geometry, one quarter of the screw and the surrounding bone were modeled. This simplification required more boundary conditions. The outside surfaces of the bone were fixed in all directions. The bone and screw symmetry surfaces were restricted to move only in the direction of the screw’s length. The screw and bone parts were meshed with 4-node linear tetrahedron (C3D4). A finite sliding, surface to surface contact with contact overclosure removal was used as the contact properties. Hard contact normal behavior was applied to the bone and screw thread surfaces. A friction coefficient of 0.2 was implemented for the contact between surfaces according to Lie et al. [71]. Finally, the top surface of the screw was
coupled to the center node of the screw and displacement was applied to this node. The graphics of the pullout simulation in this step is depicted in Figure 3-27. The ultimate pullout force of the screw was observed to happen in 0.2 mm displacement.

![Figure 3-27: Meshed quarter screw and the surrounding bone in pullout simulation.](image)

3.4.3. Osteoporotic bone pullout

To model the pullout test of a pedicle screw in an osteoporotic bone, the mechanical properties of the bone were changed to reflect osteoporosis around the pedicle screw. One of the adverse effects of osteoporosis on bone mechanical behaviors is in reduction of bone modulus of elasticity as expressed by Dickenson et al. [72]. For this study, the bone modulus of elasticity was assumed to reduce 20 percent of its strength due to osteoporosis. Another effect of osteoporosis is the degradation of bone material around the pedicle screw. In this study, half of the thread depth in the bone was
assumed to be degraded. Element type, boundary conditions, and displacement load were the same as the simulation for the normal bone test.

3.4.4. Expanded elements pullout test

The advantage of the expandable elements around the screw in pullout test was assessed in simulations, with the assumption of full expansion of the elements around the pedicle screw. This assumption requires full engagement of the expandable elements to the surrounding bony structure. The previously described pullout test simulation was repeated by adding the expanded elements around the screw and the resultant pullout force was recorded. The expanded element was a round wire with 0.4 mm diameter and 4.5 mm length. This element was added between two threads and placed tangential to the screw surface. The contact properties of the expandable elements to the bone surface was assumed to be the same as the properties declared for the pedicle screw surface with bone surface. In this simulation, the effect of other expanded elements was assumed to be the same. The meshed screw and the expanded wire element is depicted in Figure 3-28.

Figure 3-28: Meshed screw and the expanded wire in pullout test simulation.
3.4.5. Results of the pullout test simulation

The results of the performed simulations are illustrated in Figure 3-29. As shown in the plot, the six expandable elements around the pedicle screw increase pullout force from osteoporotic bone. The simulation results confirm the effect of the expandable elements which enhance the purchase of the pedicle screw in an osteoporotic bone.

![Figure 3-29: Results of pullout simulations of the pedicle screw in normal bone, osteoporotic bone, and with expanded wires.](image)

As shown in the plot, normal bone has its maximum pullout force in about 0.2 mm of screw displacement. At this displacement the pullout force is about 550 N as was expected based on the work by Zhang et al. [67]. The red line shows the Osteoporotic bone pullout test results. The pullout force in this case is about 150 N less than the normal bone strength. The results of adding the expanded elements on the screw are shown with the blue lines. By adding one element the strength of the screw is increased
by about 25 N. With this pattern in improvement of the screw pullout force, the performance of the pedicle screw will reach to the normal behavior with 6 expanded elements around the screw. The results of simulations show that the purchase of the pedicle screw in the bone is enhanced by the nitinol expanded elements.
Chapter Four

Conclusion and Future Work

4.1. Conclusion

Shape memory alloys are a unique kind of alloys which show a specific thermo-mechanical behavior. They have the ability to return to a certain predefined shape upon heating after deformation. The second specific property is the ability to tolerate large deformations without undergoing the plastic region. These specific properties along with the biocompatibility of nitinol are the reasons that this alloy has been used in recent years for biomedical devices applications.

To better design and analyze the nitinol devices which are used in biomedical applications, a simulation tool is required. To this end, the constitutive modeling of the thermo-mechanical behavior of the shape memory alloys has been implemented into the Abaqus UMAT subroutine and works in combination with the Abaqus finite element solver.

A novel pedicle screw design which has been proposed previously is analyzed in this study. The unique part of the design was the assemblies which were placed on the
pedicle screws shaft. The assemblies were made out of nitinol material which brought the capability of expanding and retracting (in certain temperatures) to the screw. The functionality of the described assembly was evaluated by making a prototype in larger scale and performing experiments. The result of the tip displacement of the assembly was recorded and reported as the function of temperature variation of the nitinol beam. The FEA modeling of SMA material thermo-mechanical behavior in Abaqus was also conducted and verified by comparing the results with the experimental ones. Pullout test as the standard method of evaluating the pedicle screws was also modeled in Abaqus as the FEA modeling software. In the modeling, the pullout test results of a regular screw were compared to the enhanced screw with expandable elements. In both experiment and modeling, the expandable screw showed much higher pullout force than a regular screw.

4.2. Future Work

This work can be continued in different aspects. First, the numerical thermo-mechanical modeling of the shape memory alloy material in Abaqus can be further improved. Shape memory alloys are known to have different behaviors in different rates of loading the material. The numerical UMAT subroutine can be developed to capture the rate dependency of the shape memory alloy behaviors based on the developed equations in literature. This capability enables the numerical tool to be able to be used in variety of applications. Other than that, the ability of modeling different material properties in one simulation which is not possible in the current version of the UMAT subroutine can be added.

Moreover, now that we have the capability of finite element simulating of the thermo-mechanical behavior of the devices made out of nitinol in Abaqus, there is the
possibility to modify, analyze and prototype other designs for the pedicle screw to better mitigate osteoporosis effect. In the future designs, the possibility of easy production of the device should be better considered. In the design procedure different capabilities in producing nitinol geometries should be considered.

Additionally, the pullout test finite element simulation can be improved in more realistic way and be compared to the experiments. The procedure of failure of the bone in the pullout test of pedicle screw should be studied in more medical aspects details and be considered in the modeling. After the production of a SMArt pedicle screw the pullout tests in a bone material can be performed and be compared to the result of a regular screw pullout test.
References


pull-out strength on human spine”, Journal of Biomechanics 37


