A Thesis

entitled


by

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

Master of Science Degree in

Mechanical Engineering

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An Abstract of


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Mandibular reconstruction surgery is a part of treatment for cancer, tumor, and all the cases that involve segmental defects. One of the most common approaches for the reconstruction surgery is to resect the segmental defect and use a double barrel fibula graft to fill the resected region and recover the mandible’s normal functions, such as chewing. The grafted bone is connected to the host mandible, using the standard of the care Ti-6Al-4V fixation plates. The fixation plates are available in the form of prefabricated plates and also patient-specific plates in the market. Due to the high stiffness of the Ti-6Al-4V plates in comparison with the mandible bone and the grafted bone, the loading distribution on the whole reconstructed mandible will be different from a healthy mandible. The high stiffness fixation hardware carries a great portion of the loading and causes stress shielding on the grafted bone and the surrounding host bone. Based on the bone remodeling theory, the stress shielding on the cortical bone causes bone resorption and may lead to implant failure.
A solution to reduce the risk of implant failure is to use a low stiffness biocompatible material for the mandibular fixation plates. We have proposed the use of stiffness-matched, porous NiTi fixation plates either in the form of patient-specific or prefabricated, instead of the standard of the care Ti-6Al-4V plates. NiTi is a biocompatible material that has a low stiffness in comparison with Ti-6Al-4V and also benefits from the superelastic feature. Superelasticity, which can also be found in bone tissues, allows the material to recover large strains (up to 8%) and increases the shock absorption.

In this thesis, we have evaluated the use of proposed fixation hardware by comparing it with a healthy mandible and a reconstructed mandible using the standard method. To this end, first different models including a healthy mandible, a reconstructed mandible using patient-specific Ti-6Al-4V fixation hardware, a reconstructed mandible using stiffness-match patient-specific hardware, and several prefabricated fixation plates were prepared. After verification of the models, the cases of reconstructed mandibles were used to simulate different periods, including during healing, and post-healing periods. Also, different loading conditions including highest bite force on the first molar tooth, rest condition, and also highest bite force on a dental implant right in the grafted bone were simulated. Also, the theory of applying pretention to the fixation plates was evaluated using the finite element method. We also designed and evaluated a set of prefabricated fixation kits with various stiffness option. After all these finite element simulations and having the CAD files of the porous fixation plates, the possibility of fabrication of the proposed hardware, in both forms of patient-specific, and prefabricated plates was evaluated using selective laser melting.
To my parents who always supported me...
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Chapter 1

1. Introduction

1.1. Mandibular Segmental Defect Surgery

Cancer, radiochemistry, tumor resection, trauma, or chronic inflammation can cause mandibular segmental defects. Mandibular segmental defects cause aesthetic and functional issues for the patient and must be treated as soon as possible to prevent bone deformity, airway obstruction, loss of speech/swallowing, and impairment of mastication [1, 2]. Using mandibular reconstruction surgery, surgeons try to restore the aesthetic and normal function of the mandible including bone continuity, muscle attachment sites, and stable dentition [3]. There are different approaches, which can be used for mandibular reconstruction surgery, but none of the currently available techniques can completely restore mandible function [4, 5]. Based on the patient condition, including the type of segmental defect (i.e. tumor, cancer, trauma, etc.), the financial issues, availability and also the surgeon’s skill, a specific technique is used by the surgeon. Each approach has its
own advantages and disadvantages and is defined by the type of implant, which is going
to be used to fill the segment(s) and also the connections, which are used to connect the
implant to the host mandible. To fill the defected section of the mandible, bone grafts (i.e.
dead piece of bone, either from the patient or from an external source), artificial
bones/scaffolds, and free flaps (vascularized lived piece of bone) are the available options [6-8]. Bone grafts and artificial scaffolds just prepare a bed for the surrounding bones to
grow into that section [9]. Free flaps need an extra micro vascularized surgery, but on the
other hand, the healing time will be reduced significantly in comparison with the other
two approaches [10]. After choosing the proper implant, one or more bone fixation plates
are used to immobilize whole structure and help the healing procedure. So far one of the
most common approaches for the reconstruction of a mandible is the use of a
vascularized free flap (usually from fibula) in combination with one or more surgical
grade 5 titanium (Ti-6Al-4V) fixation plates [11-13]. After healing, the newly grafted
bone also provides seating for dental implant posts and improves chewing process for the
patient. Figure 1 shows a case of mandibular reconstruction surgery using fibula graft and
standard of the care Ti-6Al-4V fixation plates.
For a microvascularized free flap reconstruction surgery, iliac crest and fibula could be two good candidates. For smaller defects (e.g., less than six millimeters) iliac crest could be a better option and for the larger defects, (e.g., greater than six millimeters) fibula is a common site for bone harvesting. While iliac crest could provide sufficient mandibular height to support dental implants, fibula graft does not have the sufficient height and width for reliable dental implantation and also may cause loss of facial contour [3, 16]. On the other hand, the fibula can cover the larger defects up to 24 cm, and also its removal causes
minimal donor site morbidity [10]. However, using a double barrel fibula graft, which is created by cutting a fibula into two segments, while preserving the blood supply, and then folding the segments on top of each other could solve the height issue and provides enough height for dental implantation [17, 18]. The maximum length of the defect that can be treated by a double barrel fibula graft cannot exceed 10 cm (if taken from one calf). In some cases, two additional mini plates are required to immobilize the upper barrel and connect that to the surrounding host mandible [19].

1.2. Different Type of Mandibular Fixation Plates for Reconstruction Surgery

As it is mentioned in the previous section, after harvesting the free flap, one or more mandibular bone fixation plates are required to immobilize the newly grafted bone. Currently, Titanium grade 5 (Ti-6Al-4V) is the most common material, which is used for mandibular fixation plates [17]. The mandibular bone fixation plates for reconstruction surgery can be categorized as the following:

1.2.1. Prefabricated Mandibular Reconstruction Plates (Emergency Kits)

These are the most basic and also the most common bone fixation plates that are used by surgeons around the world. The prefabricated plates are provided in standard kits, which include different geometries (shapes) for the fixation plates and also different thicknesses (1 to 3.5 mm) for each geometry. The surgeon chooses the proper fixation
plate(s) during the surgery, cut it to get to the desired length, and then bend the plate in a way that approximately fits the outer surface of the resected region. Several different bending and cutting tools are used by the surgeon to help him reach to the desired shape. The bending procedure could be the most challenging part of the surgery in some cases of reconstruction surgery due to the complexity of the defective region [9]. The prefabricated fixation plates contain several screw holes on the surface, and the surgeon chose some of them to screw the plate to the host mandible and the grafted bone. Since this kind of plates are provided in mass produced fixation kits, they are the most affordable while challenging method for the immobilization and reconstruction surgery. Also, this method could be a good choice for the cases of emergency surgeries. Figure 2 shows a summary of the reconstruction surgery using prefabricated fixation plates from Depuy Synthes Company.

Figure 2 Prefabricated fixation plates for reconstruction surgery, A) a standard kit including different fixation plates, B) Some of the different fixation plates available in a fixation kit, C) Some of the cutting and bending tools required during the surgery, and D) Final shaped fixation plate mounted on the mandible using screws
1.2.2. Custom-Bend Mandibular Fixation Plates for Reconstruction

Surgery

One of the problems associated with the use of prefabricated fixation kits is the bending process. The procedure is not straightforward and takes much effort. To solve this issue, commercial companies provided the solution to cut and bend the prefabricated fixation plates based on the CT-scan data of the patient, prior to the surgery. The process of requesting specific shape for the fixation plates takes time but significantly reduce the time of the surgery. Figure 3 shows a pre-bent fixation plate prior to the surgery.

Figure 3 a pre-bent fixation plate prior to the main surgery.
1.2.3. Custom-Made (or Patient-Specific) Mandibular Fixation Plates for Reconstruction Surgery

Although the previous solution reduces the time of the surgery, still does not allow surgeons to cover every type of defective regions. Patient-specific fixation plates have been recently introduced to the market by some of the pioneers in the market, such as KLS Martin, and Depuy Synthes. In this method, a specific fixation plate(s) is designed based on the geometry of the patient's mandible. The exact geometry of the mandible can be obtained using a set of CT-scan images. The designed fixation plate may have various thicknesses in different regions of the mandible based on the patient's need. Also, the position, type, and angle of the screws can be determined in the designed process. After creating a computer aided file (CAD file), the final product can be fabricated using 3D-printing or machining process. The process of requesting, design, verification of the design, fabrication, and delivery of the final product take about ten days for Depuy Synthes. This solution costs about 7 to 10 times more than the prefabricated fixation plates but significantly enhance the surgery. Table 1 shows the commercial names for the patient-specific solutions from some pioneer companies, and Figure 2 indicates a schematic of the patient-specific plates.
Table 1 Commercial names for the patient specific fixation plates from different providers

<table>
<thead>
<tr>
<th>Provider</th>
<th>The commercial name for the custom-made fixation plates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stryker</td>
<td>Stryker’s Customized Mandible Reconstruction Plate (CMRP)</td>
</tr>
<tr>
<td>Depuy Synthes</td>
<td>Patient Specific Plates for Mandible</td>
</tr>
<tr>
<td>KLS Martin</td>
<td>Individual STL model with pre-shaped reconstruction plate</td>
</tr>
</tbody>
</table>

Figure 4 Commercial patient-specific fixation plates, A) Depuy Synthes, B) KLS Martin, and C) Stryker

1.3. The Principal Risks of a Mandibular Reconstruction Surgery

In all of the current standard of the care methods for mandibular reconstruction surgery, the fixation plates are made of titanium surgical grade 5 (Ti-6Al-4V) [9, 20]. While these fixation plates provide sufficient immobilization between the host mandible and the newly grafted bone following the surgery, after bone healing they might cause some serious complexities. The complexities are due to the relatively high stiffness of the
Ti-6Al-4V plates (112-120GPa) in comparison with the surrounding bone (10-37 GPa) [21]. After the bone healing, the loading and boundary conditions on the mandible are similar to a healthy mandible, but the existence of a very high stiffness fixation plate attached to the mandible's bone disturbs the stress distribution all over the mandible, especially around the fixation plates. Based on the bone remodeling theory, bone as a live tissue is sensitive to the loading conditions [22, 23]. If a bone tolerates a higher level of loading than the normal condition, it becomes stronger and on the other hand, if the same piece of bone does not carry the required loading scenario, it gets weaker and starts to absorb [24]. The bone remodeling theory could help us to justify why a right handed tennis player will have a stronger and greater right hand bone (even in comparison with his own left hand), and also why astronauts cannot walk on their own foot right after coming back to the earth (the reason is that while they are in space due to the lack of gravity their foot’s muscles and bone do not carry normal loads (their own weight) for a period of time and so get weaker). Therefore the existence of a high stiffness fixation hardware in contact with the cortical bone, cause the surrounding bone to carry a smaller portion of the loading conditions and cause stress shielding in that regions. Based on the bone remodeling theory, the resultant stress shielding on the bone weaken those specific regions and may lead to bone resorption and even implant failure [21]. Although the fixation plates can be extracted after the healing period, the surgeons prefer not to extract the hardware due to the risk of harming the soft tissues and surrounding bone, unless in emergency and special conditions [25]. Infection due to the use of fixation plates, failure of the fixation plates or creation of more room for insertion of the dental implants is considered as the emergency and special cases [26].
In order to study the mandible's performance, knowing the type and source of the applied forces is the first step. The mandible is subjected to two types of loading including muscle forces and the bite force. The masseter, temporalis, and pterygoid are the three most important muscles, which are effective on the mandible. The muscle forces vary in different conditions depending on the occlusion state (rest or chewing), bite loading conditions (balanced or unbalanced loading, bilateral or unilateral loading, grinding, or clenching), and the teeth, which are involved. Even at rest condition, those muscles are not inactive, and still mandible is under loading [27, 28]. So stress shielding could potentially cause bone resorption almost in every loading condition and event at the rest condition. Strain-adaptive bone remodeling theory can predict the amount of bone loss [29]. For the case of using Ti-6Al-4V fixation plates, the hardware carries a great portion of the loading condition and reduces the load previously exposed on the grafted bone, and those affected areas would remodel in response, both externally in the form of reduced thickness, and internally in the form of increased porosity, which we call that bone resorption in general [30]. Resorption resulting from stress shielding and/or the damage resulting from abnormal stress concentrations can contribute to the failure of an implant [31]. Beside stiffness of the fixation plates, the geometrical factors of the device including thickness, the contact area between fixation plate and mandible and/or grafted bone, and also type, diameter and location of the screws might affect the stress shielding of the mandible [32].

1.4. **Suggested Solution for Mandibular Reconstruction Surgery**

To overcome problems associated with stress shielding without extracting the hardware, one solution could be the use of a bioresorbable material, which automatically
resorbs after the bone healing process. When the hardware or at least specific parts of the hardware resorbs, the loading condition of the reconstructed mandible goes back to the case of a healthy mandible with no additional fixation hardware. There has been some research done on the field of bio resorbable materials but still more researches are required [33]. Other solution could be the use of a lower stiffness material, which does not disturb the stress distribution after bone healing, meanwhile provides sufficient immobilization during the healing period. The theory of using a low stiffness patient specific material has been previously studied by Shayesteh et al. [11]. In that work, they have simulated a case of a reconstructed mandible using patient-specific fixation plate. The authors assumed the patient specific fixation plates have a lower young's modulus close to that of cortical bone and using these new material properties they have simulated a case of reconstruction surgery for the post-healing period. The results showed that using a lower stiffness material for the fixation plates could significantly reduce the stress shielding effect on the mandible. One of the possible approaches to reduce the stiffness could be applying porosity to the bulk structure of a part [34, 35]. Introducing engineering porosity to the dense Ti-6Al-4V fixation plates can significantly reduce the stiffness [35]. Furthermore using another low stiffness biocompatible material, such as NiTi not only could reduce the stiffness but also can add some other great features to the device [36]. In the next section, we have talked about some of the advantages of porous Nitinol implants and the fabrication methods.
1.5. Porous Nitinol Implants

In comparison with other biocompatible metals, such as cobalt-chromium alloys, Titanium alloys fuse more quickly to the bone structure [37]. Ti-6Al-4V is a biocompatible well-known titanium alloy, which has numerous medical applications. Having a high strength, besides a low density, high biocompatibility, and a passive oxide biofilm at the surface of the material, which resists corrosion after implantation are the nice features of this titanium alloy [38, 39].

On the other hand nickel-titanium (nitinol, NiTi) is biocompatible shape memory alloy (SMA) that is currently used in some medical applications, such as orthodontic wires and stents [40-44]. Since NiTi is SMA that is sensitive to heat and changing temperature, could not be fabricated by conventional methods, such as casting and forging and also machining this material is a challenging task [45, 46]. Recently selective laser melting (SLM) approach has been developed in a way that allows fabrication of NiTi parts using powder bed technique [47-49]. Using SLM, complex parts, such as scaffolds and porous structures with different level and type of porosities can be fabricated out of NiTi [50]. NiTi provides several interesting features, such as biocompatibility, low stiffness, superelasticity, high damping capacity, shock absorption, wear resistance, and fatigue resistance [51-54]. Porous Nitinol can be specifically used for mandibular fixation hardware because it additionally offers lower stiffness, stronger bone-implant integration, superelasticity behavior and energy absorption [36, 55].
1.5.1. Low Stiffness

NiTi has a relatively low stiffness in comparison with the Ti-6Al-4V. Also imposing engineered porosity, the equivalent young's modulus of a NiTi parts can be tuned to the level of cortical bone [56-58]. Having a fixation plate with a Young's modulus close to that of cortical bone reduce the stress shielding effect on the surrounding bone and decrease the risk of failure of the plate [59, 60]. The young's modulus of cortical bone of a mandible depends to the sex, and health condition of a patient [61]. Also in a single mandible, the Young's modulus varies in different regions. Table 2 shows the average young's modulus for different regions of a mandible. Based on the desired level of the stiffness the required level of porosity can be applied to fixation hardware.

Table 2 Young's modulus for different regions of a mandible

<table>
<thead>
<tr>
<th>Mandible</th>
<th>Cortical bone</th>
<th>Cancellous bone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symphysis</td>
<td>18.9-22.3</td>
<td>2.3-3.6</td>
</tr>
<tr>
<td>Parasympysis</td>
<td>17.6-23.5</td>
<td>1.5-2.6</td>
</tr>
<tr>
<td>Angle</td>
<td>21.3-25.7</td>
<td>2.5-4.5</td>
</tr>
<tr>
<td>Ramus</td>
<td>20.8-28.7</td>
<td>2.8-3.5</td>
</tr>
<tr>
<td>Condyle</td>
<td>21.9-26.4</td>
<td>1.8-2.6</td>
</tr>
<tr>
<td>Coronoid</td>
<td>25.6-31.2</td>
<td>2.6-3.3</td>
</tr>
</tbody>
</table>
1.5.2. **Implant Integration:**

Although the main goal of adding porosity to the structure of the fixation plates is to reduce the equivalent Young’s modulus of the hardware, porosity can also improve the bone-implant incorporation [62]. Based on the literature, cellular and vascular activities, and thereby blood clot formation, would increase within the porous implants in comparison with the solid implants [63]. The reason is that having interconnecting pores within the implant would provide more space for bone ingrowth, more surfaces for bone-implant integration, and interlocking between the implant and surrounding bone. It is worth noting that the optimal pore size for bone tissue ingrowth is 50-500 micrometers [64]. Bone apposition and osseointegration are the two important factors, which affect the bone ingrowth into the porous implants [65, 66]. Osseointegration can be defined as forming an interface between the implant and bone without intervening with any soft tissue [67]. An in vivo study on sheep lumbar spine implants show that osseointegration of porous Nitinol is better than Ti-6Al-4V over the recovery time [68]. Also, another similar study on the femurs of rabbits confirms the excellent osseointegration of porous Niti implants[69].

Bone apposition, which is defined as the capacity of the bone tissue to set itself to surface material is another important factor in implant integration [70]. Based on the literature, textured and porous NiTi has shown more bone apposition due to more contact points and more surface area [71].

In addition porous Niti implants benefit from the implant pump-like and capillary-like properties, which cause the implant to absorb more fluid required for bone ingrowth
from the surrounding area. Also, porous NiTi's wettability affects the fluid velocity
through the pores. Overall, capillary force and wettability of the porous Nitinol implants
increase the bone ingrowth throughout the implant [68, 72].

1.5.3. Superelastic Feature

NiTi is a shape memory alloy with two interesting features, superelasticity and
shape memory effect. The shape memory effect is used in some medical devices, in
which by applying heat (usually in the form of electricity current) the shape of the
devices changes to a preset shape [73]. This feature is devices, such as heart stents [74].
The other interesting feature of NiTi is the superelasticity effect, which allows the
material to tolerate up to 8% elastic strain is a hysteresis loop [75]. Bone tissues have the
same superelastic feature, which is shown in Figure 5 [76]. Because of this similarity,
reduced stiffness superelastic NiTi could behave similar to bone tissues in mechanical
loading and therefore could be a good candidate for implant's material. It is worth noting
that NiTi can have Superelastic or shape memory feature depending on the performing
temperature and its composition. Recently both superelastic and shape memory NiTi in
room and body temperature have been successfully fabricated using selective laser
melting (SLM) [77].
1.5.4. Energy Absorption

The superelastic feature increases the damping capacity and energy absorption of the material. In addition, adding well-adjusted porosity could increase the shock absorption further more [53]. Therefore porous NiTi implants provide good protection against the propagation of shock waves if it will be subjected to shock loading. According to the literature Absorbed energy would increase as the porosity increase within the implant. It is shown the amount of energy absorption of porous NiTi is more than Ti and Ti-6Al-4V at a certain amount of stress [53].
1.6. Safety and Efficiency of Using NiTi

Different metals have been used for medical devices and implants including stainless steel, CoCr alloys, Titanium alloys and degradable metals, such as pure iron and magnesium alloy. The fine surface, mechanical, biological, and physical properties made them a good choice for these purposes. However there are some important factors, which restrict the use of metals including corrosion, toxicity, infection, and muscle re-attachment [78, 79].

1.6.1. Corrosion and Toxicity Risks

Although corrosion is unavoidable for metals, but the level of corrosion can be controlled and minimized for some metals. About the NiTi implants, corrosion is more important because it may cause Nickel release. Nickel is one of the human carcinogenic metals and may cause serious problems, such as allergic response, cytotoxicity, and genotoxicity due to the formation of a membrane around the implant caused by ion release [80]. The created membrane prevents implant integration surrounding bone and may cause failure [81]. The cytotoxicity, allergic or genotoxic response of solid NiTi have been studied, and it was acceptable for using in biomedical devices [82]. The formation of a passive oxide film (TiO2) on the surface of the NiTi devices prevents the Nickel release and corrosion [83, 84]. It is worth nothing that the amount of Ni release for porous NiTi parts is higher than solid NiTi implants due to an increase in the contact surface with the same external dimensions [85, 86], but even for the porous NiTi the amount of Ni release is below cytotoxic concentrations [87, 88].
Mechanical loading may damage the passive oxide film and cause Ni release, and so additional surface modifications would be required. Usually, a thick layer of TiO2-x film up to 30 micrometers is added on all external surfaces in order to minimize the risk of damage to the oxide layer under mechanical loading [89]. The common approach for adding this extra layer is thermal annealing, plasma ion immersion implantation (PIII), vapor deposition (PVD), chemical treatments, PIII method followed by chemical treatment, and in-situ nitriding [90-92]. For the porous structures, chemical surface modifications are more preferable due to the limitations of using other methods to reach all pore surfaces. The amount of Ni release for NiTi is determined by immersing NiTi sample in simulated body fluid (SBF) solutions before and after the surface modifications [36].

1.6.2. Infection

The formation of a membrane around the implant could also cause infection due to the colonization of planktonic bacteria, such as staphylococci on the surface of an implant. Planktonic bacteria may prevent the host cells from colonization and by its own colonization forms a protective biofilm that resists bacterial clearance by the host’s natural defenses and antibiotics [93]. Since the bacteria can grow slowly or even remain dormant on metallic implants for several months to years to reach sufficient levels to begin to invade the surrounding bone, the infection often occurs not immediately after implantation [94].

Adding porosity increases the level of colonization and infection for NiTi implants and because of that, the removal of the implant is recommended by some
references [95]. The removal of an implant, especially a porous implant after bone integration could be a challenging task due to connective tissue growth within the implant, and it may be associated with adverse consequences of unfavorable facial contour alterations and vascular supply interruption.

Based on all these facts it is important to control the key factors and prevent bacterial adhesion to the surface of metallic implants to reduce infection as much as possible. Some of the most important factors are surface topography, intermolecular forces, hydrophobic properties, and local environment variables [96].

1.6.3. Muscle Re-Attachment

Muscle re-attachment is another important factor for metallic biocompatible materials. In some of the cases of reconstruction surgery especially when angle or coronoid process are involved the muscles are detached either due to the bone loss before or during the surgery. In these cases, it is crucial to re-attach muscles to the grafted bone or the metallic implants to provide the chewing and speech ability and to restore the full functional of mandible [97, 98].

1.7. Manufacturing of Porous of NiTi

Porous materials have been used widely in surgical implants whether as coatings on the prosthesis for biological fixations or as a scaffold to improve regeneration of tissues. Porous materials were first presented by Sosnik in 1943 when he added mercury to the melt to make pores in aluminum [99]. Later, the effect of using porous materials on
osseointegration for biomedical application was investigated [100]. Different approaches were used for fabrication of porous structures. Porous metals can be categorized as closed-cell and open-cell. Each unit cell in the close-cell material is enclosed by thin walls, while open-cell materials and foams are created by overlapping interconnected cells. The size, shape, location and level of porosity depend on the fabrication approach [101]. Adding porosity to medical implants increases the possibility of bone ingrowth through the pores. Also adding porosity reduces the equivalent stiffness of the parts. The second effect may be used to reduce and adjust the stiffness of the porous implant to the level of the cortical bone to reduce and prevent the stress shielding effect.

Due to the sensitive structural and functional properties of NiTi a considerable effort is required for fabrication of this alloy. Usually alloying is the first step for fabrication of the NiTi parts except for special powder metallurgical processing methods where alloying and shaping are combined in one processing step. Because of the high reactivity of the melt NiTi, production is under vacuum conditions. Vacuum induction melting (VIM) or vacuum arc remelting (VAR) of elemental Nickel and Titanium are the common approaches. Electron beam or plasma melting are considered as the less financially viable methods. In case of using cast for fabrication of NiTi parts, multistage thermal and thermo-mechanical treatments (solution annealing and/or homogenization, hot forging, cold forming followed by recrystallization annealing, aging treatment) have to follow the casting process, due to the inadequate structural and very low functional properties of cast NiTi. Subtractive methods, such as welding and forming are used for shaping and fabrication of finished NiTi. Furthermore machining of NiTi is a challenging
task and other conventional processing routes do not allow the fabrication of porous NiTi [102-105].

Liquid phase processing can also be used for fabrication of porous NiTi parts. This method is restricted because of the high melting temperature of NiTi (~1583K) and also due to the high density of NiTi (6.45 g/cm³), injecting a gas into a NiTi melt that is used for other metallic foams (e.g. Aluminum foams) is challenging [105]. Only two liquid phase melting procedures have been used for fabrication of porous NiTi or NiTiCu. A zone melting method for NiTi rods under a Hydrogen/Helium atmosphere was introduced by Sugiyama et al. [106]. In this method first hydrogen is dissolved in the melt NiTi, and then the dissolved hydrogen rejected, which results in creating aligned and elongated pores during directional solidification. Pre-sintered SrF2 salt foams were used by Young et al. as space holders in a replica cast method. In this approach first, the alloy is molten under vacuum followed by applying gas pressure (Ar, 1 atm) to infiltrate the foam with liquid. Then the space holder is removed by ultra-sonicating in a solution of distilled water and 20 \% HNO3 after solidification and cooling down. Using this method, porous NiTiCu with about 60\% porosity can be achieved. Based on the references, transformation temperatures changes due to the presence of secondary phases (Oxygen stabilized Ti2 (Ni, Cu)). The authors also reported a very low level of stiffness for the porous parts (<3GPa), and a high deformation recovery in mechanical testing [106].

Powder metallurgical methods are more common for fabrication of porous NiTi. A near-net-shape product is provided by powder metallurgy (PM) methods, which could significantly simplify the manufacturing process [105]. One of the main issues about NiTi parts produced by powder metallurgy methods is the high contaminant levels [107]. This
level of contaminant is because of the large surface area of the powder particles and due to at least two additional high-temperatures processing steps (powder production, PM process). For instance, Schetky and Wu report Oxygen content from 1500 to 3000 ppm [107]. Increasing impurity level considerably degrades the structural and functional properties of NiTi. A precisely controlled process (e.g., sintering temperature) is crucial to control the level of the impurity for the porous NiTi parts. Otherwise, Ni or Ti-rich precipitates may form in addition to NiTi, and also, some areas may consist of pure Nickel or Titanium due to different diffusion behavior and diffusion velocities [108, 109].

Recently, additive manufacturing (AM) has been applied for fabrication of solid and porous NiTi implants [108, 110]. In general, all of the AM processes use a Computer aided design (CAD) file in creating physical parts based on that. First, the CAD file of the part is sliced into different layers with specific thicknesses. The thickness of the layers is based on the required resolution and the powder size. Then the data of the sliced CAD file are transferred into the manufacturing machine, and each layer is created on the top of the previous layer. These layers can be fabricated using different raw materials but for the metallic parts these layers are usually provided in powders and molten by a laser. Other energy resources, such as electron beam can be used instead of the laser but so far for AM of NiTi parts only laser has been used. The most common powder-bed AM technologies for fabrication of NiTi parts are Selective Laser Melting (SLM), Selective Laser Sintering (SLS), and Direct Metal Laser Sintering (DMLS). Also, some flow-based techniques, such as Laser Engineered Net Shaping (LENS) and Direct Metal Deposition (DMD), where a nozzle directly delivers the powder into the laser focus area can be used for fabrication of
NiTi, which is less common than the powder-bed methods. Figure 6 shows a schematic of a powder-bed AM process [88, 111, 112].

![Schematic of powder bed selective laser melting process](https://sculpteo.com)

**Figure 6** a schematic of powder bed selective laser melting process, image credit: sculpteo.com

1.8. **Objective of Study**

The main purpose of this thesis is to introduce a new generation of stiffness-matched mandibular fixation plates for reconstruction surgery to reduce the risk of the surgery. In order to do that, first, we have studied and modeled the biomechanical
behavior of a healthy mandible including stress distribution, displacements, and strains. The results of the first section of the project are used as a baseline for the next levels. Then we have designed and introduced two type of mandibular fixation plates for reconstruction surgery. As the first phase of the project, stiffness-matched, patient-specific fixation plates are introduced, simulated and fabricated. In the second phase of the project an upgraded emergency kit for mandibular reconstruction surgery fixation plates is designed, simulated and fabricated.

1.8.1. **Stiffness-Matched Patient-Specific Fixation Plates**

As it is mentioned in the section 1.2.3, patient specific or custom made fixation plates are considered as the best possible approach for mandibular reconstruction surgery. In this approach, a set of required fixation plates is designed based on the geometry of patient’s mandible. The design is highly precise thanks to the CT-scan data of patient mandible. Using this approach the location and direction of the screws can be chosen prior to the surgery in a way that prevents any intersection with nerves, tooth roots, and other screws. In a case study, we have designed a set of patient-specific fixation plates for a dried mandible. First, the general geometry of the fixation plates was designed based on the common approaches. Then the required stiffness is applied to the patient-specific fixation plates in order to reduce the equivalent stiffness to the level of surrounding cortical bone. Using finite element simulations, we have compared the efficiency of using stiffness-matched, patient specific fixation plates in comparison with the use of a common standard of the care Ti-6Al-4V custom made fixation plates.
1.8.2. Pre-Fabricated or Emergency Kit for Mandibular Reconstruction Surgery with Various Stiffness

Although patient-specific solutions provide noticeably improved results, but they cost about seven to ten times more than other conventional methods, and also several days (7 to 14 days) are required before the surgery. Because of the time limitation, lack of required facilities or sometimes financial issues, the patient specific solutions cannot be applied to some patients. Thus it is important to consider and improve emergency kits beside patient-specific solutions. To make an improvement on the standard mandibular fixation kits, we have added the various stiffness feature to the fixation kit. To this end, we have applied a different level of porosity to the current emergency kits and fabricated them using NiTi instead of Ti-6Al-4V. Similar to the first phase of the project, reduced-stiffness fixation kits were designed, simulated and fabricated in the end.

1.9. Publications

1.9.1. Journals


**1.9.2. Conference Papers**


Chapter 2

2. Materials and Methods

In this chapter we have created different models including a healthy mandible, a reconstructed mandible using the standard of the care Ti-6Al-4V plates and using the stiffness-matched fixation plates. Also, different porous fixation plates in the form of patient specific and emergency kits were designed and modeled. All CAD models were simulated using finite element simulations under different boundary conditions and loading scenarios. Finally, the proposed stiffness matched fixation plates were fabricated using selective laser melting method.

2.1. Modeling and Design

2.1.1. Modeling Healthy Mandible

As the first step, a dried healthy human mandible was prepared to be used for the modeling purposes. The mandible belongs to a female about 18 years old and looks healthy. Using high-resolution CT-scan imaging, the CAD file of the dried mandible was
created. This CAD file was considered as a geometry for a healthy mandible. The teeth and periodontal ligaments were separated for improving finite element simulations. Also, the cortical and cancellous bone regions were distinguished using the CT-scan data. Finally, the CAD file of the complete healthy mandible including teeth, periodontal ligaments, cancellous bones and cortical bone was created and assembled together.

2.1.2. Modeling the Mandible Including Segmental Defects

In order to simulate a common mandibular reconstruction surgery, a segmental defect bearing first to third molar teeth with 40 mm length was resected from the healthy mandible model. In this study, we have focused on mandibular reconstruction surgery using double barrel fibula graft. So a CAD file of double barrel fibula was created based on anatomical data in Solidworks. The double barrel fibula graft was designed in a way that fills the segmental defect on the mandible. So far we have modeled a mandible that requires a reconstruction surgery, and a double barrel fibula graft is going to be used as filling implant.

2.1.3. Metallic Fixation Hardware and Screws

In this step of modeling, we have focused on the fixation plates, which are going to immobilize the double barrel fibula graft with respect to the host mandible. A lower fixation hardware or mandible bar with a dimension of 1.5 mm × 78 mm × 4 mm including 9 threaded holes was created in Solidworks. The geometry of the mandible bar was designed in a way that exactly fit on the defected region of the mandible. In addition
to the mandible bar, two miniplates with a dimension of 1 mm × 18 mm × 2.8 mm, each one including 3 threaded holes was designed to connect to the upper section of the double barrel fibula graft and immobilize that section. Also, the location of the screws was selected in a way that prevents any interaction with teeth roots and nerves. This method is same as the procedure, which is done by commercial companies, such as Synthes and KLS martin for the design of the patient specific fixation hardware. The mandible bar is fastened to the host bone using bicortical screws, which are long enough to pass through both the lingual and buccal sections of the bone. All threaded screws have a diameter of 2 mm. 6 screws were used on the mandible bar, and 2 screws were used on each miniplate. Unicortical screws that only pass through the cortex of the bone were used for the miniplates.

At this stage, we have modeled a reconstructed mandible with double barrel fibula graft using patient-specific fixation plates. Now we need to apply required level of porosity to the fixation plates to adjust the equivalent stiffness of the implants to the level of the surrounding cortical bone. Using the CT-scan data, it was concluded that average stiffness for the surrounding cortical bone, in this case, is 12 GPa. Using finite element simulation and trial and error approach one can calculate the required level of porosity that is required to be applied to adjust the stiffness [57]. For this case, 53% porosity was required to be applied to the solid NiTi fixation hardware to reduce the equivalent stiffness of the parts to 12 GPa. Also, 80 percent of porosity is required to apply to solid Ti-6Al-4V fixation plates to create the same effect. Figure 7 shows a schematic of the whole process of creating a patient-specific fixation plate, starting from the CAD file that is created by the CT-scan data, to the porous patient specific plate.
Figure 7 the whole process of the design of a stiffness-matched, porous fixation plate, starting from the CAD file to the final plate.

2.1.4. Design of the Emergency Kit's Fixation Plates

As it is mentioned earlier in the text, for some cases of reconstruction surgery due to different factors, such as time, skill, equipment, and financial issues, using prefabricated reconstruction plates is necessary. Nowadays different pioneers companies, such as Depuy Synthes, KLS Martin, and Stryker provide prefabricated fixation kits. These kits usually contain several plates, which have different shapes, and different thicknesses. Different shapes can be used for different parts of the mandible and surgeon choose proper thickness from the available options in the kit. Each manufacturer provides its own standard kits for reconstruction surgery. The shape of some of the plates may differ for different companies, and some shapes are exclusive for some manufacturers. On the other hand, there are some standard prefabricated reconstruction plates that can be
found in almost every prefabricated kit. Two types of these standard shapes were selected as the elements of our proposed kit (Figure 8). The CAD file of the selected geometries with different length and thicknesses were created in the Solidworks software. In the next step by applying porosity to the designed fixation plates, various stiffness option is added to the kit.

![Figure 8 Selected standard fixation plates and their CAD files](image)

### 2.1.5. Applying Porosity to the Fixation Plates

Adding porosity increase the bone ingrowth effect and also reduce the equivalent stiffness of the part. The type and level of the porosity greatly affect the mechanical properties of the part. Since we plan to fabricate, the proposed fixation plates using selective laser melting approach first the CAD file of the porous parts need to be created. If the CAD model of the porous part is not available some theories, such as Gibsan and Ashby [113, 114] approach should be used for modeling the mechanical response of the porous part. Having the CAD file of a porous structure has advantages and disadvantages. The advantages of having the CAD file of a porous part is that the modeling and finite element simulation of the part are more precise in comparison with the cases of using
porous material theories. On the other hand creating the CAD file of a porous structure is not as easy as creating the CAD file of the solid parts. Due to the complexes geometries and fine details, other approaches are required to create porous CAD files. Also applying proper mesh to the porous parts is a challenging task. In this project, 3-Matic software by Materialise was used to create the CAD file of porous fixation plates. In this approach first the CAD file is divided into surfaces (STL file), and then all of the modifications including adding porosity are applied to the surfaces. In the end, the surfaces are transferred into solid parts. Figure 9 shows the whole procedure for creating a homogeneous porous part. First, the CAD file is converted to an STL file. The STL file is imported to the 3-matic software. A single unit cell is required to consider for imposing porosity throughout the part. For this purpose, a simple cube with the dimension of 1 mm was considered. Different porous cells may be considered based on the application. Then the unit cell spreads through the STL part. At this stage, the porosity is in the form of graphs with no thickness. By assigning thickness to the graphs, the porous structure can be created. To create support for the screws and increase the strength of the porous part, a shell can be designed and added to the porous structure. By assigning different thicknesses to the porous graphs, different level of porosity can be created. This procedure was applied to the patient specific plates, which were designed for the dried mandible, and also on all of the plates for the emergency kit.
2.1.6. Modeling a Case of Reconstructed Mandible Including Dental Implants Added to the Implanted Section of the Mandible

In order to study the efficiency of the proposed fixation plates, different conditions were simulated and compared to the case of the healthy mandible as a reference. The goal is to create a stress distribution more close to the case of the healthy mandible for different loading condition. In addition to the case of a reconstructed mandible with the proposed fixation plates, the case of adding dental implants on the grafted bone was also simulated. To this end, several sets of dental implants, each including three similar dental implants were designed. Then the dental implants with different diameters were added to the reconstructed mandible. We have also studied the optimal diameter for the dental implant. We assume that the bite force is applied to the
crown of the first dental implant and then applied to the root. In the simulations, we focused on the root.

2.2. Meshing and Adding Finite Element Constrains

After modeling, all parts including different fixation plates, screws, mandible and its components need to get mesh. Hypermesh (Hyperworks, Troy, MI, USA) were used to mesh the models with 4-node tetrahedral elements (C3D4). The mesh convergence study was done all every part and based on that the optimized number of elements is reported in Table 3.

Table 3 the number of elements for the Finite Element Analysis model components. The number of tetrahedral elements was determined by convergence analysis.

<table>
<thead>
<tr>
<th>Model Component</th>
<th>Type of element</th>
<th>Number of elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resected mandible</td>
<td>3D, Solid, Tetrahedral, Deformable</td>
<td>218,328</td>
</tr>
<tr>
<td>Teeth (13 Total)</td>
<td>3D, Solid, Tetrahedral, Deformable</td>
<td>65,179</td>
</tr>
<tr>
<td>Ligaments (13 Total)</td>
<td>3D, Solid, Tetrahedral, Deformable</td>
<td>21,053</td>
</tr>
<tr>
<td>Top Graft</td>
<td>3D, Solid, Tetrahedral, Deformable</td>
<td>42,065</td>
</tr>
<tr>
<td>Lower Graft</td>
<td>3D, Solid, Tetrahedral, Deformable</td>
<td>45,037</td>
</tr>
<tr>
<td>Fixation hardware(s)</td>
<td>3D, Solid, Tetrahedral, Deformable</td>
<td>58,327</td>
</tr>
<tr>
<td>Screws (10 Total)</td>
<td>3D, Solid, Tetrahedral, Deformable</td>
<td>67,027</td>
</tr>
</tbody>
</table>
All meshed parts were then assembled together, and constraints were defined. The constraints between screw-fixation plate, screw-host mandible, screw-fibular graft, teeth-ligaments and host mandible-ligaments were defined as tie. In addition, the friction factors of 0 (simulation of the reconstructed mandible during the initial healing period) and 1 (simulation of the reconstructed mandible after the gaps between the grafted and host bone fragments had healed) are considered for the simulation of the surface to surface contact between host mandible and the fibular graft.

2.3. Material Properties

Table 4 summarizes the material properties of the FEA model components including fixation hardware, bone, teeth, and periodontal ligament [50, 115, 116]. Cortical and cancellous bones were modeled as anisotropic material, and the other components were assumed to be linear elastic materials. It should be noted that Ti-6Al-4V material properties were assigned to the screws for all models.
Table 4 Material properties of the Finite Element Analysis mandible components

<table>
<thead>
<tr>
<th>Material</th>
<th>$E_x$ (MPa)</th>
<th>$E_y$ (MPa)</th>
<th>$E_z$ (MPa)</th>
<th>$v_{xy}$</th>
<th>$v_{yz}$</th>
<th>$v_{xz}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cortical Bone- Symphysis region</td>
<td>23,000</td>
<td>15,000</td>
<td>10,000</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Cortical Bone- Angle region</td>
<td>20,000</td>
<td>12,000</td>
<td>11,000</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Cortical Bone- Rest of mandible</td>
<td>17,000</td>
<td>8,200</td>
<td>6,900</td>
<td>0.32</td>
<td>0.325</td>
<td>0.31</td>
</tr>
<tr>
<td>Cancellous Bone</td>
<td>960</td>
<td>390</td>
<td>320</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Cortical- fibular graft</td>
<td>26,800</td>
<td>26,800</td>
<td>26,800</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Cancellous- fibular graft</td>
<td>1,650</td>
<td>1,650</td>
<td>1,650</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Teeth</td>
<td>17,600</td>
<td>17,600</td>
<td>17,600</td>
<td>0.25</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>Periodontal Ligament</td>
<td>2.7</td>
<td>2.7</td>
<td>2.7</td>
<td>0.45</td>
<td>0.45</td>
<td>0.45</td>
</tr>
<tr>
<td>Ti-6Al-4V</td>
<td>112,000</td>
<td>112,000</td>
<td>112,000</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
</tbody>
</table>

For modeling the mechanical properties of NiTi, a user defined material (UMAT), which was developed using micro plane theory, was used. The mentioned UMAT was developed by Dr. Kadkhodaei et al. group [117-119], and is capable of simulating the superelastic and shape-memory effect of NiTi. This UMAT was verified in several studies [41, 120, 121]. We have also verified and calibrated the UMAT as the first step. For calibration of the UMAT transformation temperatures of the NiTi samples are required that can be obtained using DSC test. In addition, the Young's modulus for the two phases of austenite and martensite, Poisson's ratio, and some constant are required that can be obtained using compression and tensile test [118].
2.4. Applying Boundary Conditions and Loading Scenarios

The bite force created by masticatory muscles is the greatest source of stress that is usually applied to the mandible. Our FEA models the peak masticatory load. Muscles are active even when the mandible is at rest. The amount of muscle forces depend on many factors including occlusion state (maximal chewing or soft food chewing) and bite loading conditions (balanced or unbalanced loading, bilateral or unilateral loading, grinding, or clenching) [27]. In this study, muscle forces related to a maximal bite force on the first right molar was considered as the loading input for the healthy mandible model (model 1) (i.e., a 526N bite force based on Korioth et al. [122]). Three different fixation hardware scenarios (cases A, B, and C) were considered for the models 2 and 3.

Case A) the simulation the highest bite force after surgery (without applying any pretension to the fixation hardware). Since the reconstruction surgery causes a reduction in chewing power, all the muscle force values in this study were assumed to be of 60% of Korioth et al.’s [122] values for a normal healthy mandible [115]. This is the force applied in all three FEA models. Case B) The simulation of used NiTi fixation hardware that had received 100 N of pretension load (i.e., on both superior and the inferior plates). This value for the pretension load was obtained from the FEA model in a way that increased contact pressure of the lower section of the graft bone by 50%. Case C) This simulation used NiTi hardware that had undergone 100 N pretension load on both superior and the inferior fixation plates.
2.5. Fabrication

Selective laser melting has been used for all of the fabrication purposes in this thesis [50, 123-129]. We have used fabrications for three different purposes: calibration of the UMAT, patient specific fixation plates, and prefabricated kit.

In order to simulate the mechanical response of the porous fixation plates two main series of parameters are required: material properties of the bulk material and the geometry of the pores [130]. The geometry of the pores is included in the CAD files. For the material properties of the bulk material, calibration procedure is required. The reason is that based on the literature, the mechanical properties of SLM fabricated parts, especially made of NiTi, significantly differ from the raw material's properties, which are used for fabrication [131, 132]. To face this issue, some dense samples with the same processing parameter as those used for fabrication of porous fixation plates were fabricated. The fabricated dense samples were used for compression and DSC test in order to measure the mechanical properties and transformation temperatures of the SLM fabricated parts. This information was used for the calibration of the UMAT. This procedure has been done prior to the finite element simulations.

After simulating the patient-specific stiffness-matched fixation hardware and creating the final design, again SLM method was used to fabricate the final plates. These plates were mounted on the dried mandible, which was used as the reference for the design. Finally, SLM method was used to fabricate a set of different fixation plates for the emergency kit that offers various stiffness beside standard thicknesses and shapes.
2.5.1. Phenix PXM, SLM Machine

Phenix PXM machine from 3D systems was used for the selective laser melting processes in this thesis. The machine benefits from a 300 W Ytterbium fiber laser, with a Gaussian profile (TEM00) and the quality of is m²<1.2, and the diameter of the laser is approximately 80 µm. The machine uses a scraper and a roller mechanism to spread the powder and create the powder layer. First, the feeding piston moves upward and provides the required powder. After that, the metal scraper moves and collects powder from the feeding piston. Finally, the roller deposits the collected powder on the building surface (substrate). After preparing the powder bed, the laser turns on and selectively scans and melts the powder based on the geometric data of the part that is transferred to the machine prior to the fabrication process. The selective areas solidify and create a dense area or layer, which is surrounded by the loose powder. Then the building piston moves down as the thickness of a single layer, and the whole process is reaped until the final part is fabricated. Figure 10 shows a schematic of the machine and the fabrication process.

Figure 10 Phenix PXM, SLM machine
2.5.2. Powder Selection

Powder selection is one of the most important factors that widely affects the quality of the SLM fabricated parts. Powder size and shape, flowability, and impurity content are some of the key factors that need to be considered for the SLM fabrication of NiTi. Electrode Inert Gas Atomization (EIGA) method was used to atomize the NiTi ingots and create the powder. EIGA technique allows the production of spherical particles with high powder bed density and good followability. In general a fine particle size increases the resolution of the fabricated parts, but on the other hand decreases the followability of the powder. Haberland et al. showed that an effective compromise of the aforementioned factors is achieved by using medium-size particles (25-75 µm) [133].

In this study, Ni-rich NiTi ingots (Ni50.8Ti49.2) from Nitinol Devices & Components, Inc. (Fremont, CA), were atomized to powders using an Electrode Induction-melting Gas Atomization (EIGA) technique (by TLS Technique GmbH (Bitterfeld, Germany)).

2.5.3. Process Parameters and Post Processing

Based on a series of studies on part density, impurity pickup, transformation characteristics, and functional behavior of SLM fabricated parts, the optimized parameters have been obtained [123, 129, 134]. The processed parameter are summarized in Table 5 [129, 135, 136].
Table 5 Process parameters used in SLM manufacturing of NiTi parts

<table>
<thead>
<tr>
<th>Effective laser power (W)</th>
<th>Layer thickness (μm)</th>
<th>Scanning velocity (m/s)</th>
<th>Hatch distance (μm)</th>
<th>Energy input (J/mm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>250</td>
<td>30</td>
<td>1.25</td>
<td>120</td>
<td>55.5</td>
</tr>
</tbody>
</table>

After SLM fabrication, the parts were solution annealed at 1223 K for 5.5 hours in H2O. Then aging is performed at 623 K for 15, minutes and finally, the parts were water quenched.

2.6. Mechanical and Thermal Testing

A Perkin-Elmer Pyris 1 Differential Scanning Calorimetry (DSC) with the heating/cooling rate of 10ºC/min in a nitrogen atmosphere was used to determine the transformation temperatures (TTR’s). Solution annealing was done using a Lindberg/Blue M BF514541 Box furnace, and to avoid oxidation of the samples; they were placed in an argon-filled quartz ampules. The compression samples were loaded up to 800 MPa (before reaching to the critical stress for plastic deformation) and unloaded using a 100 kN MTS Landmark servo-hydraulic test platform (Minneapolis, MN). The strain rate of $10^{-4} \frac{1}{\text{sec}}$ was employed during loading, whereas unloading was performed under force control at a rate of $100 \frac{N}{\text{sec}}$. An MTS high-temperature extensometer was used to obtain strain measurements.

It is worth noting that the impurity limits for medical NiTi are prescribed in ASTM F2063-05 [137]. The impurity level for clinical applications must be below 0.05...
ppm. The impurity content was tested in three of the NiTi samples that we fabricated. We observed impurity levels of 0.035, 0.0500, and 0.007 ppm for Carbon, Oxygen, and Nitrogen, respectively.
Chapter 3

Results

3.1. Validation

The validation for the simulations was done in two different steps. First using the calibration data, the mechanical response of the compression samples is verified. Second, the finite element model of the mandible is verified based on a previous experimental study.

3.1.1. Validation of the ABAQUS UMAT

In order to calibrate the UMAT, the DSC test results, and the compression test results were used. Using the DSC test (Figure 11) transformation temperatures of the SLM fabricated parts were measured. The details of the measurement method can be found somewhere else [120]. Based on the literature, the compression test of the bulk
samples was used to extract the Young’s modulus (both for austenitic and martensitic phase) and other parameters of the UMAT [120]. Using these two tests, the material properties of SLM fabricated NiTi parts were extracted and are summarized in Table 6.

![Figure 11 DSC test for the 100% dense NiTi samples](image)

**Table 6** Material parameters of dense Ni-rich NiTi fabricated by SLM technique at 37℃. (E_A and E_M are the austenitic and martensitic modulus of elasticity). Transformation temperatures have been shown by $M_s$, $M_f$, $A_s$, and $A_f$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$E_A$ (GPa)</th>
<th>$E_M$ (GPa)</th>
<th>$v$ [130]</th>
<th>$M_s$ (K)</th>
<th>$M_f$ (K)</th>
<th>$A_s$ (K)</th>
<th>$A_f$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>37</td>
<td>42</td>
<td>0.33</td>
<td>230</td>
<td>253</td>
<td>270</td>
<td>280</td>
</tr>
</tbody>
</table>

Using the measured material properties, the ABAQUS UMAT was updated and calibrated in a way that could successfully simulate the compression results of the bulk samples. Figure 12 shows the simulation and experiment results of the compression test ($r>0.99$, $p<0.005$, RMSE=12.6 MPa and $r>0.98$, $p<0.005$, RMSE= 38.3 MPa for the simulation of loading and unloading responses, respectively). Using the calibrated UMAT, we can simulate the mechanical response of complex structures including the porous fixation plates.
3.1.2. Validation of the Mandible Model

To validate the created healthy mandible model, an experimental study by Ichim et al. group [138] was used as the reference. In the reference experimental study, two strain gauges were used to measure the buccal and lingual strains of mandibular cortical bone on a dried cadaver mandible. The loading condition on our model was updated based on the Ichim et al. work. Figure 13 demonstrate the simulation results of our model beside the experimental measurements of the reference work. As it is shown in the Figure 13, the two series of simulation results both on lingual and on buccal sides tracks the experimental results (r>0.99, P<0.0005, RMSE=2.8e-6(%) and r>0.99, P< 0.0005, RMSE<6.42e-6(%) for the Buccal and Lingual sides of mandible cortical bone in the molar region, respectively).
Figure 13 model Validation: a comparison between experimentally obtained data (EXP) with FEA-predicted model data on the buccally and lingually placed strain gauges.

3.2. Finite Element Results of the Patient Specific Case

First, using the calibrated UMAT the mechanical response of a porous sample with the same porosity type and level that is applied to the patient specific fixation plate is simulated. Based on the CT scan data Young's modulus of the surrounding cortical bone on our sample mandible was measured as 12 GPa. Then using simulation approach, it was concluded that imposing 45.7% porosity to the dense NiTi samples can tune the equivalent stiffness of the part to the desired level (here 12GPa). Figure 14 shows the compression results of a 45.7% porous NiTi in comparison with cortical bone. Also for comparison purposes, the mechanical response of solid Ti-6Al-4V, which is used in the standard of the care fixation plates, is demonstrated. As it is shown in the Figure 14, the
patient specific plate behave so close to the cortical bone and on the other hand the Ti-6Al-4V plates are much stiffer than the bone. This difference in Young's modulus causes a noticeable stress shielding effect on the cortical bone in case of using Ti-6Al-4V plates and can be prevented by replacing them with stiffness matched porous NiTi plates.

**Figure 14** the equivalent stress-strain plot under compression for NiTi cubic samples with 45.7% porosity, cubes of dense Ti-6Al-4V and samples of mandibular cortical bone.

The finite element simulations were done for two different periods: A) immediately following surgery or during the healing process, while the pieces of bone are not healed yet, and B) after healing period (post-healing) when the grafted bone and the host mandible are completely healed together and created a uniform part.
3.2.1. During Healing

During the healing period, the bone fracture healing is occurring, and the hardware (fixation plate) is bearing most of the strain from chewing and other mandibular activities. In this period one of the most important challenges is to immobilize the grafted bone and decrease the micromotions in the interfaces between the graft and the host bone as much as possible. The risk of graft unvascularization that is caused by micromotions decreases by providing a proper immobilization. In summary, if the fixation hardware can tolerate loading during the healing period and also immobilize the grafted bone, the graft bone at the interfaces is integrated into the host mandible, and they create an integrated bone.

Since the graft unvascularization is counted as one of the reasons for the mandibular reconstructive surgery failure we have proposed and studied the effect of adding a pretention on the fixation plates in order to increase the immobilization. By applying pretention (which can be done by stretching the fixation hardware prior to the installation), the contact pressure on the surfaces between the graft and the host bone increases and cause more immobilization. In order to study the effect of adding pretention, a pretention load of 100 N is applied to the both standard of the care Ti64 plates and porous NiTi plates and added to the simulations. Figure 15 shows the average contact pressure on the surrounding bone for the two cases of using patient-specific stiffness matched fixation plates, and standard of the care Ti64 plates. For the loading regime we have simulated the models under two conditions: 1) when the mandible is at rest and only the pretention force is working (since muscle forces at rest condition are
negligible in comparison with the pretension force, we have neglected the muscle forces in this condition), and 2) when the highest bite force is also applying besides the pretension load. For the two loading regimes, it can be seen that the stiffness matched porous NiTi fixation plates perform better than the Ti-6Al-4V plates.

![Graph showing effect of using NiTi and Ti-6Al-4V fixation plates on average contact pressure](image)

**Figure 15** the effect of using NiTi and Ti-6Al-4V fixation plates on the average contact pressure at the interface between the graft and host bone (i.e., fibular bone graft and host mandible) during the healing period (i.e., in the immediate post-operative period there no strength at the graft-host bone junction).

### 3.2.2. Post-Healing

For the post-healing period, the stiffness-matched fixation hardware is expected to increase the loading of the grafted bone over traditional, Ti-6Al-4V hardware and improve the remodeling process by decreasing the stress shielding effect.

In order to study the stress shielding effect after healing period, the two models of reconstructed mandible using the standard of the care Ti-6Al-4V hardware and using
stiffness matched porous NiTi hardware were simulated in three different loading scenarios. A) when the models are loaded due to the highest bite force (i.e., 60% of the maximum bite force on the healthy mandible), B) when the models are loaded due to the pretension load, which is applied to the fixation plates (prior to the installation on the mandible) and the mandible is at rest, C) when the models are loaded due to the highest bite force in combination with the pretension force that is applied on the fixation plates.

Figure 16 shows the average von Mises stress on the surrounding cortical bone for the two models under different loading conditions. For all of the loading conditions, the average von Mises stress on the cortical bone of the grafts is higher for the cases of using stiffness-matched fixation plate (by factors of 1.95, 1.82, and 2.14, respectively). In addition, the average von Mises stress in the same region of the healthy mandible is simulated and showed with a dashed line in the same figure for comparison. Similarly Figure 17 shows the maximum von Mises stress in the same regions, and again for the case of using stiffness matched fixation, maximum stress is higher and also is lower than the maximum allowable stress on mandible bone (<100 MPa). Based on these two figures we may conclude that by taking advantage of the superelasticity and applying pretension during the procedure the von Mises stress on the fibular grafts bone increases, which results in a better long-term outcome for the patients. This increased stress can reduce the stress shielding effects and the risk of implant failure.
Figure 16 the average Von Mises stress on the surrounding bone in two cases of using Ti-6Al-4V and porous NiTi fixation plates, with and without applying the pretension to the fixation plates.

Figure 17 the maximum von Mises stress on the surrounding bone in two cases of using Ti-6Al-4V and porous NiTi fixation plates.
3.3. The Case of Adding Dental Implants

After bone healing, one more step to improve the chewing and load distribution on mandible is adding dental implants to the grafted bone that is recently healed. Adding dental implants is not possible for all of the cases but, if it is possible, can significantly improve the mandible functions. We have designed four different sets of dental implants to be added to the reconstructed model after the bone healing period. The designed dental implants had different diameters of 3, 4, 5, and 6mm, and the length of all implants was 16mm. Figure 18.a shows the CAD model of the reconstructed mandible after adding the dental implants. The stress distribution on the mandible including dental implants is shown in Figure 18.b.

Figure 18 a) CAD model of the reconstructed mandible including dental implants. b) Stress distribution after FE simulations
Stress on dental implants does not depend on fixation hardware material, but on the dental implant diameter. As the diameter of the dental implant increases the stress on the dental implant decreases (Figure 19).

![Graph showing the effect of dental implant diameter and fixation hardware material on maximum von Misses stress of dental implant.](image)

**Figure 19** the effect of dental implant diameter and fixation hardware material on maximum von Misses stress of dental implant

The stress on surrounding bone of the dental implant depends on two parameters: a) fixation hardware material, the maximum stress on surrounding bone increases in case of using porous NiTi, and b) dental implant diameter, the larger diameter for dental implants results in a higher stress on surrounding bone (Figure 20).
The stress on the fixation hardware depends on the fixation hardware material. In the case of using Ti-6Al-4V, the maximum stress on the fixation hardware is about five times greater than the case of using porous NiTi fixation hardware. However the maximum stress on the fixation hardware does not depend on the dental implant diameter.

**Figure 20** the effect of dental implant diameter and fixation hardware material on maximum von Misses stress of surrounding bone

**Figure 21** the effect of dental implant diameter and fixation hardware material on maximum von Misses stress of fixation hardware
3.4. Simulation of Different Plates for the Emergency Kit

After creating the CAD files based on the standard fixation kits in the market, the different level of porosities is applied to the standard shapes. Also as a second solution, we studied the effect of adding porosities to the dense Ti-6Al-4V plates. Figure 22 shows the stress distribution on the Ti-6Al-4V fixation plates with different levels of porosities. Also, the mechanical response of the porous Ti-6Al-4V plates is shown in Figure 23.

Figure 22 comparison of the stress distribution on porous Ti-6Al-4V 4-hole straight plates under tension. (The parts include 0, 47, 58, 67, 75, and 82% porosity)
After doing the finite element simulations, as the final step to evaluate the use of porous NiTi stiffness matched fixation plates instead of the standard of the care Ti-6Al-4V plates, the possibility of fabrication was studied. SLM approach was used for fabrication of the patient specific fixation plates and also the emergency kit's plates [139].
3.5.1. Fabrication of Patient Specific Fixation Plates

Using the same parameters, which were used for fabrication of NiTi compression samples, the set of patient specific stiffness-matched fixation plates were fabricated. Since the CAD files were created based on the CT-scan data of the mandible, the fabricated patient-specific fixation plates were successfully mounted on the reference mandible as it is shown in Figure 24.

![Figure 24](image)

**Figure 24** reconstructed mandible using stiffness-matched, 3D printed, NiTi fixation devices

3.5.2. Fabrication of the Emergency Kit's Fixations with Different Porosities

For the second phase of this project, we have selected three different standard shapes from the emergency kit of the reconstruction surgery. The different level of porosities was applied to these standard shapes, and the final CAD files with different
thicknesses were finalized. In order to show the possibility of fabrication of these fixation plates, we have fabricated one of the standard shapes with the thickness of 3 mm and porosity levels of 40%. Figure 25 shows the fabricated sample.

**Figure 25** a sample fixation plate fabricated by SLM.
Chapter 4

4. Conclusion, Suggestions, and Future Works

In this thesis, we have proposed the use of stiffness matched fixation plates for reconstruction surgery instead of the standard of the care Ti-6Al-4V plates. The stiffness-matched fixation plates were introduced in two different forms: A) as patient specific plates, and B) as prefabricated emergency Kits. In order to evaluate the performance of the proposed fixation hardware a series of finite element, simulations were performed and compared with a healthy mandible and also the case of using traditional Ti-6Al-4V plates. These different finite element simulations include different loading conditions immediately following the surgery (during the healing period), and also after healing period. We have also studied the effect of applying pretention on the fixation plates prior to the installation in order to improve the immobilization and reduce the risk of the failure.

Dental implants can be added to the reconstructed mandible to improve the mandible functions, such as biting, chewing, and aesthetics aspects. Also, it is well-known that adding dental implants improve the loading distribution on the mandible and
reduces the risk of implant failure. We have also simulated the effect of adding dental implants to the reconstructed mandible using our proposed fixation plates. For all of the simulations, the results indicate a more similar stress distribution contour to the healthy mandible in the case of using stiffness-matched fixation plates [140].

For the second phase of the project, we focused on the emergency kits, which are used for some specific cases of reconstruction surgery. Sometimes due to the lack of enough time, required facilities, or even skills, it is necessary to use prefabricated fixation plates for the reconstruction surgery. These prefabricated fixation plates are provided in the form of emergency kits, and we have added the option of different stiffness to the prefabricated fixation kits. The surgeon can choose the required stiffness for the plates based on the CT-scan data beside the proper thickness and shape. The remaining part of the surgery is the same as the standard of the care fixation plates. He needs to bend the plates to create the desired contour and install them on the mandible.

Finally, we have studied the possibility of fabrication of these porous fixation plates using selective laser sintering. The fabrication process was successful, and we could show this fact by installing the patient specific fixation plates on the reference mandible.

Mechanical testing of the fabricated fixation plates under different loading conditions can be considered as the next step and our future works.

We have also participated in an I-Corps program and introduced these new stiffness-matched fixation plates to the potential market.
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