Original Article

Design of a new magnesium-based anterior cruciate ligament interference screw using finite element analysis

Jonquil R. Mau\textsuperscript{a,b}, Kevin M. Hawkins\textsuperscript{a}, Savio L.-Y. Woo\textsuperscript{b}, Kwang E. Kim\textsuperscript{b}, Matthew B.A. McCullough\textsuperscript{a,*}

\textsuperscript{a} Department of Chemical, Biological, and Bioengineering, North Carolina A&T State University, Greensboro, NC, USA
\textsuperscript{b} Musculoskeletal Research Center, Department of Bioengineering, Swanson School of Engineering, University of Pittsburgh, Pittsburgh, PA, USA

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ABSTRACT

Background/objective: In anterior cruciate ligament reconstruction, a tendon graft, anchored by interference screws (IFSs), is frequently used as a replacement for the damaged ligament. Generally, IFSs are classified as being either metallic or polymeric. Metallic screws have sharp threads that lacerate the graft, preventing solid fixation. These constructs are difficult to image and can limit bone–screw integration because of the higher stiffness of the screw. Polymeric materials are often a better match to bone's material properties, but lack the strength needed to hold grafts in place. Magnesium (Mg) is a material of great promise for orthopaedic applications. Mg has mechanical properties similar to bone, ability to be seen on magnetic resonance imagings, and promotes bone healing. However, questions still remain regarding the strength of Mg-based screws. Previous \textit{ex vivo} animal experiments found stripping of the screw drive when the full torque was applied to Mg screws during surgery, preventing full insertion and poor graft fixation. The similar design of the Mg screw led to questions regarding the relationship between material properties and design, and the ultimate impact on mechanical behaviour. Thus, the objective of this study was to analyze the stresses in the screw head, a key factor in the stripping mechanism of IFS, then use that information to improve screw design, for this material.

Methods: Using finite element analysis, a comparison study of six drive designs (hexagonal, quadrangle, torx, trigonal, trilobe, and turbine) was performed. This was followed by a parametric analysis to determine appropriate drive depth and drive width.

Results: It was observed that with a typical torque (2 Nm) used for screw insertion during anterior cruciate ligament reconstruction, the maximum von Mises and shear stress values were concentrated in the corners or turns of the drive, which could lead to stripping if the values were greater than the yield stress of Mg (193 MPa). With a four-time increase in drive depth to be fully driven and a 30\% greater drive width, these maximum stress values were significantly decreased by more than 75\%.

Conclusion: It was concluded that improving the design of a Mg-based screw may increase surgical success rates, by decreasing device failure at insertion.

The translational potential of this article: The results of this work have the potential to improve designs of degradable IFSs, allowing for greater torque to be applied and thus greater screw fixation between host bone and the graft. Such a fixation will allow greater integration, better patient healing, and ultimately improved patient outcomes.

Introduction

Following an anterior cruciate ligament (ACL) tear, surgical reconstruction using tendon autografts or allografts as a replacement can stabilize the knee [1]. These grafts are held in place by means of interference screws (IFSs) in the bone tunnel [2]. Two classes of materials, metallic (i.e., titanium) and polymeric (i.e., poly乳酸 acid), are commonly used for the IFSs. Titanium IFSs can provide good initial fixation strength because of its high strength and an elastic modulus on the order of 100 GPa [3,4]. However, there are shortcomings that include magnetic resonance imaging interference, graft laceration resulting from their sharp threads, and the difficulty of removal during revision surgery [5].
As a result, polymeric IFSs were developed and gained popularity. Their potential to be bioabsorbable is also an attractive feature. Over time, the screw can be replaced by the bone—soft tissue interface. However, the actual degradation after implantation of these screws was slow, inconsistent, and often incomplete even after two years [6]. In addition, problems with screw breakage during insertion can be frequent [7,8]. Efforts have been made to understand screw-graft performance under postoperative conditions. Chizari et al [9] simulated cyclical loading on the graph-screw construct, using finite element analysis (FEA). Chizari concluded that finite element (FE) models were accurate when compared with experimental values. Additional work, particularly in the area of orthodontics has used FEA to examine the impact of various design factors [10].

In this study, we explored the use of a magnesium (Mg)-based IFS. Mg has several advantages compared with traditional materials including the following: a modulus and tensile strength closer to cortical bone; higher ductility compared with polymers; and high levels of biocompatibility, biodegradability, and osteoconductivity. Mg-based alloys do not interfere with magnetic resonance imaging, allowing better imaging for postoperative assessments [11,12]. Previous work compared the biomechanical characteristics of Mg-based IFS to polymeric screws in cadaveric specimen, and found similar mechanical stability between the two [13]. Such findings suggest that using a degradable Mg-based screw would create similar postoperative outcomes as what is seen in polymeric screws. Initially, a Mg-based IFS of similar design to commercially available titanium screws was tested. ACL reconstruction via graft fixation of a patellar-tendon bone graft was attempted in an ex vivo goat model. It was found that stripping and breakage of the screw drive or head occurred during insertion. Previous efforts sought to improve screw drive design in hopes of better performance. Weiler et al compared six bioabsorbable polymer IFSs of similar size with differing drive designs. These authors found that resistance to breakage during insertion was highly dependent on the drive design; specifically, the drive diameter and drive shape [7,8,14–17]. Unfortunately, material properties of the screws were not altered as part of the analysis.

Using the finite element method, the stress distribution within the screw drive was analyzed [18,19]. From these findings, the research question formulated was what are the factors of the screw drive that could be modified to preserve the integrity of the screw? It was hypothesized that an increase in the drive surface area would allow for better distribution of the stresses during screw insertion; and thus, would reduce stripping of the screw drive. To do this, a parametric analysis of drive depth and drive width was performed on a total of six different drive designs. The success criterion was that the level of stress within the screw drive design in response to an applied torque must be 50% lower than the yield strength of the Mg alloy (193 MPa). To the authors’ knowledge, this study is the first to examine Mg-based IFS.

Materials and methods

The Mg-based IFS used for this study had a 15 mm length, 5 mm diameter, an inner diameter of 1.73 mm (cannulation), and a 2.51 mm hexagonal drive with a 3.10 mm drive depth (Figure 1). Three-dimensional computer models of the screws were developed using SolidWorks 2010 (SolidWorks Corp., Waltham, MA, USA) computer-aided design software. Finite element analyses were conducted on the models of the screw using ANSYS Workbench 14.0 (ANSYS, Inc., Canonsburg, PA, USA). A convergence study was conducted to determine appropriate number of elements in a model consisting of the titanium screw embedded in the polyurethane foam cylinder. This specific model was used for validation and converged at an element size of 0.80 mm (14,298 tetrahedral elements). Hence, the pullout simulation of screw pullout was run with 14,298 elements.

In lieu of a physical/experimental validation, an algebraic validation of the screw model was conducted using a relationship between pullout strength, thread geometry, and material shear strength [20,21].

Particularly, Chapman et al determined an algebraic relationship between design parameters and shear failure force in polyurethane foam (Equation 1) [20]. The predicted shear failure force ($F_s$) is the product of the ultimate shear stress of the material into which the screw is placed ($S$), length of screw insertion ($L$), screw circumference ($\pi D_{\text{major}}$, where $D_{\text{major}}$ is the major diameter), and the thread shape factor (TSF = 0.5 + 0.57735 $d/p$, where $d$ is thread depth and $p$ is thread pitch) [20]. Verification of this relationship determined that the aforementioned parameters can be used as predictors of screw pullout force [20].

$$F_s = S* L \times \pi D_{\text{major}} \times \text{TSF}$$

(1)

For validation purposes, $S$ was set to 1.40 MPa, $L$ to 13.36 mm, $D_{\text{major}}$ to 5.21 mm, and TSF to 0.75, where $d$ was 0.85 mm and $p$ was 2 mm. Thus, the predicted pullout force as determined from Equation 1 was

![Image](https://example.com/image.png)
230.12 N. The computational simulation used for validation included a 5 × 15 mm screw embedded in a cylinder with a 20 mm diameter and 20 mm length (Figure 2). The screw was assigned the material properties of titanium alloy as defined by ANSYS 14.0 ($E = 9.60 \times 10^5$ MPa, $\nu = 0.36$) [20]. The surrounding cylinder was assigned the material properties of 10 pcf polyurethane foam ($E = 57.0$ MPa, $\nu = 0.24$), which is used as a bone substitute for screw pullout testing. Boundary conditions for validation included fixing the bottom surface of the bone block eliminating all movement. The screw was displaced 0.30 mm axially, the displacement at which internal threading of the polyurethane foam cylinder failed. This displacement was determined from initial studies in the authors’ laboratory. The coefficient of friction between the screw and the cylinder was 0.42, which is the coefficient of friction between metal and bone [22]. The force resulting from the 0.30 mm displacement of the screw was reported as the pullout force predicted by the computational simulation. The computational pullout force was compared with the predicted pullout force determined by Equation 1 ($230.12$ N) and the percent difference was calculated.

A comparison study of six different drive designs was performed using the finite element method simulating the loading on the screw drive during insertion. Each model was modified to have each of the following drive designs: hexagonal, quadrangle, torx, trilobe, and turbine (Figure 3). The screws were assigned Mg alloy material properties as defined by ANSYS 14.0 ($E = 4.5 \times 10^4$ MPa, $\nu = 0.35$). The screw models were meshed with a 0.1 mm element size (~80,000 tetrahedral elements) as determined from an additional convergence study of the screw model alone. Boundary conditions included fixing the outer threaded surface of the screw, thus restricting translation and rotation in all directions. A 2 Nm torque was applied to the inner surface of the drive of the screw. This torque is within the range of published insertion torques reported for ACL IFSS [8,23–25]. The maximum von Mises stress and maximum shear stress were recorded for each model as well as the stress distribution within the drive design. Also, the surface area of the screw was recorded for each screw model.

Lastly, a parametric study of drive depth and drive width was conducted on all six of the drive designs. A $2^2$ factorial design determined the impact of drive depth and drive width on the stress values experienced within the screw drive (Figures 4 and 5). The two levels for drive depth were 3.10 mm, a drive depth of the Mg-based screw that is similar to that of traditional metal screws; and 13.10 mm, a fully driven design as seen with many polymer screws [8]. The drive width was defined as the diameter of the circle in which the drive design is circumscribed. The levels for drive width were 2.30 and 2.90 mm. The drive width of 2.30 mm was half the distance between the cannulation (1.73 mm) and the outer width of the initial Mg-based screw, 2.90 mm. Thus, there were four combinations of drive depth and drive width: (1) 3.1 mm drive depth and 2.3 mm drive width; (2) 3.1 mm drive depth and 2.9 mm drive width; (3) 13.1 mm drive depth and 2.3 mm drive width; and (4) 13.1 mm drive depth and 2.9 mm drive width. As described above, a 2 Nm torque was again applied in the drive of the screw models whose outer threaded surface was fixed. The maximum von Mises stress values were recorded. This was done for a total of 24 combinations of drive design, drive depth, and drive width. The statistical significance of these factors was determined by performing an analysis of variance, where $p < 0.05$ is significant, using SAS version 9.2 (SAS Institute Inc., Cary, NC, USA).

Results

The corresponding stress distributions of the six drive designs (hexagonal, quadrangle, torx, trilobal, trilobe, and turbine) were compared. The maximum von Mises stresses were 196, 209, 212, 197, 245, and 280 MPa, respectively. The maximum shear stresses were 112, 120, 122, 113, 140, and 131 MPa, respectively. Figure 6 shows the von Mises stress concentrations for the screw with a hexagonal drive design with warmer colours (i.e., yellow, orange, red) indicating higher stress values. The maximum stress concentrations were seen in the corners or turns of the drive. The maximum von Mises stress of 196 MPa was greater than the yield strength of the Mg alloy (193 MPa). Thus, failure of the material at the corners of the screw, because of the applied force is highly likely. Von Mises stresses at the corners of the drive exceeded the yield strength of the Mg in all six drive designs with the same drive width (2.9 mm) and drive depth (3.1 mm).

The parametric study was performed to determine the effects of drive depth and drive width on the maximum von Mises stress values. The corresponding surface areas (mm²) and maximum von Mises stresses (MPa) for each combination with the differing drive designs are listed in Tables 1 and 2, respectively. Combinations 3 and 4 for each of the drive designs yielded maximum von Mises stresses that were below 50% of the yield stress of Mg alloy except combination 3 of the turbine design. Combination 4 of the quadrangle drive design yielded the lowest von Mises stress of 47 MPa closely followed by combination 4 of hexagonal and torx drive designs with maximum von Mises stresses of 48 MPa and 49 MPa, respectively.

![Figure 3](image-url) (A) Top view of the hexagonal screw (B) quadrangle screw (C) torx screw (D) trilobal screw and (E) trilobe screw and (F) turbine screw models.
For each of the six drive design groups, the maximum von Mises stress decreased approximately 80%. The greatest decrease of 88% was with the trigonal drive design. The parametric study determined that both drive depth and drive width are statistically significant factors having an impact on the maximum stress observed in the model, with p values < 0.0001 and 0.0028, respectively. Overall, there was an inverse relationship between surface area and von Mises stress. Figure 7 shows the relationship of surface area versus maximum von Mises stress for each of the 24 combinations (6 drive designs and 4 combinations of drive depth and drive width) and a greater surface area within the drive of the screw yielded smaller stress values. Using this validated model, a torque applied within the screw drive of the six differing drive designs consistently showed that the concentration of the stress were in the corners and turns of the drive (Figure 6). Because of the applied torque, it was found that the hexagonal drive design had the lowest maximum von Mises stress. It was followed by the trigonal, quadrangle, torx, turbine, and trilobe designs.

![Figure 4](image_url)

**Figure 4.** (A) 2.30 mm drive width and (B) 2.90 mm drive width for parametric analysis.

![Figure 5](image_url)

**Figure 5.** (A) 3.10 mm drive depth and (B) 13.10 mm depth for screw parametric analysis.

![Figure 6](image_url)

**Figure 6.** (A) The boundary and loading conditions from the isometric view, (B) Location of the maximal von Mises Stress, (C) A cross section of the location of the maximum von Mises stress (D) Top view of the von Mises plot of the screw model with the hexagonal drive design. The maximum von Mises stress is signified by a red flag, in the corners of the screw drive.

### Table 1

| Screw drive designs | 3.1 mm depth | 3.1 mm depth | 13.1 mm depth | 13.1 mm depth |
|---------------------|--------------|--------------|---------------|---------------|
|                     | 2.3 mm width | 2.9 mm width | 2.3 mm width  | 2.9 mm width  |
| Hexagonal           | 21           | 27           | 90            | 114           |
| Quadrangle          | 20           | 26           | 86            | 111           |
| Torx                | 23           | 31           | 95            | 130           |
| Trigonal            | 9            | 25           | 40            | 104           |
| Trilobe             | 23           | 32           | 96            | 134           |
| Turbine             | 31           | 40           | 129           | 171           |

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|---------------------|--------------|--------------|---------------|---------------|
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| Trilobe             | 23           | 32           | 96            | 134           |
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Impact on maximum stress observed in the model, with p values < 0.0001 and 0.0028, respectively. Overall, there was an inverse relationship between surface area and von Mises stress. Figure 7 shows the relationship of surface area versus maximum von Mises stress for each of the 24 combinations (6 drive designs and 4 combinations of drive depth and drive width) and a greater surface area within the drive of the screw yielded smaller stress values. Using this validated model, a torque applied within the screw drive of the six differing drive designs consistently showed that the concentration of the stress were in the corners and turns of the drive (Figure 6). Because of the applied torque, it was found that the hexagonal drive design had the lowest maximum von Mises stress. It was followed by the trigonal, quadrangle, torx, turbine, and trilobe designs.
The objective of this research was to explore the stress distribution within the screw drive of a Mg-based IFS to better understand the stripping mechanism. An IFS using Mg-based materials has potential advantages over currently available metallic and polymeric screws while aiming to reduce their disadvantages. In this study, Mg-based IFSs were analyzed using a 3-D finite element model. The model was validated in an idealized condition, with a screw embedded in polyurethane foam. The force required to pull the screw out of the foam matched well with results determined from Equation 1. To our knowledge, this is the first study specifically evaluating stresses at the screw drive. This area (i.e., the screw drive) is an important area of study, as physical tests show insertion failure occurring in the head of the screw during implantation. It was hypothesized that increasing the area of the drive would better distribute stress within the screw. This was confirmed as evidenced by the decreasing values of maximum von Mises stress found in the models. It is worthy to note that in the new screw designs, the maximum stress values were below the level of failure for Mg alloys. There were differences in the stress according to the shape of the drive. This is expected, as different shapes would create different contact areas. Parametric analysis explored the impact of drive depth and drive width on screw performance. Specifically, increasing drive depth four times the current length and increasing drive width by 30%, led to maximum stresses decreasing by more than 75%. These results suggest that drive depth and drive width are factors that would have significant impact on maximum stresses in a screw. Both should be considered when designing a screw with a lower maximum stress and in turn resist drive failure as both yielded statistically significant changes in von Mises stress. In addition, increasing drive depth and width will result in a surface area up to five times greater than the original design. Other means of reducing stripping of the screw include a redesign of the surgical tools. However, it is not clear what the optimal design or material for surgical tools should be because of the variety of Mg alloys used.

This work successfully used FEA to estimate the performance of an IFS during insertion. Results from our study add to current screw design literature centred on what design factors affect the fixation strength of IFSs. The drive was changed to incorporate a fully driven quadrangle design, which has sharper angles to resist the load required for insertion as well as reduce the stress experienced within the drive of the screw. Other investigations of the effect of insertion torque on screw advancement support the methods used here. Multiple studies use a maximum insertion torque ranging from approximately 0.5 to 3.5 Nm [8,23,24,26]. More specifically, Weiler et al investigated how insertion torque affects insertion success, concluding that torque at failure is highly determined by the drive design. The turbine-like drive design had the highest maximum allowable torque followed by the trilobe, quadrangle, trigonal, hexagonal, and torx. For the present study, a similar trend was expected; however, drive designs ranked in the following order from least to greatest maximum von Mises stress: hexagonal, trigonal, quadrangle, torx, turbine, and trilobe. A possible explanation for the difference in results is that Weiler et al used six commercially available polymer screws with different drive designs. These screws were of similar length, but varied in diameter, material properties, thread profile, cannulation, and drive depth. The variability of these factors may have influenced the reported maximum allowable force. For the present study, all the screws had the same material properties, thread design, length, width, cannulation, and drive depth.

There are some limitations to the present study. First, we conducted an algebraic validation of the computation model. For future studies, a physical validation protocol will compare the results obtained from the FEA to the results of an experimental pullout test. Still, the percent difference between the pullout force determined from the computational simulation and the predicted pullout forces was only 5%, which is adequate for validation. Second, the boundary conditions aimed to mimic the experimental protocol do not represent the actually surgical application that includes a soft tissue graft and the surrounding bone. As the external surface of the screw was held fixed, this boundary condition provided more constraints on the screw compared with what is seen clinically. In this analysis, we did not account for the surgical tools nor methods associated with screw insertion. However, the boundary and loading conditions in this study generated the effects of the applied torque in the screw drive. This allowed the model to reasonably predict how the increases in the surface area would reduce the stresses in the screw. Nevertheless, the development of a more complex computational model is a part of our future work. Future studies should analyze the impact of changing material properties on the model. It is expected that materials with higher stiffness will decrease the chances of stripping; however, the combined influence of design and altered material properties will need to be evaluated.

In summary, this study has yielded the first qualitative results of stresses and stress concentration in an Mg-based IFS drive, in response to the torque required during surgery. This is an area that has been limited in its study. Results suggest that when a new material is introduced, new designs must also be considered. As a result, the Mg-based IFS was made fully driven with a quadrangle drive design. A renewed interest in using Mg-based biomaterials for orthopaedic applications is built on the ability of Mg-based alloys to degrade [12]. This degradation eliminates the need for removal surgeries. This work highlights the importance of screw drive design in creating an effective ACL IFS.

### Discussion

**Table 2** Maximum von Mises stress (MPa) of the different designs.

| Screw drive | 3.1 mm depth | 3.1 mm depth | 13.1 mm depth | 13.1 mm depth | Hexagonal | 224 | 196 | 53 | 48 |
|------------|--------------|--------------|---------------|---------------|-----------|-----|-----|----|----|
|            | 2.9 mm width | 2.9 mm width | 2.3 mm width  | 2.3 mm width  | Quadrangle| 298 | 209 | 60 | 47 |
|            |              |              | 212           | 72            | Torx      | 246 | 212 | 72 | 49 |
|            |              |              | 197           | 95            | Trigonal  | 428 | 197 | 95 | 52 |
|            |              |              | 245           | 81            | Trilobe   | 320 | 245 | 81 | 57 |
|            |              |              | 280           | 141           | Turbine   | 466 | 280 | 141| 66 |

![Figure 7](image_url) The relationship between surface area and maximum von Mises stress from the parametric analysis including 24 simulations (6 drive designs, 4 combinations of drive depth and drive width each).
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