Title	In Silico Analysis of the Biomechanical Stability of Commercially Pure Ti and Ti-15Mo Plates for the Treatment of Mandibular Angle Fracture
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Note	

Original paper

***In silico* analysis of the biomechanical stability of commercially pure Ti and Ti-15Mo plates for the treatment of mandibular angle fracture**

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Abstract

Purpose: To investigate the influence of different materials and fixation methods on maximum principal stress and displacement in reconstruction plates using *in silico* three-dimensional finite element analysis (3D-FEA).

Methods: CAD models of the mandible and teeth were constructed. CHAMPY and AO/ASIF plates and fixation screws were designed with CAD software. 3D-FEA was performed by image-based CAE software. Maximum and minimum values of biomechanical stability, maximum principal stress and displacement distribution were compared in CHAMPY and AO/ASIF plates made from commercially pure titanium grade 2 (cp-Ti) and titanium-molybdenum (14.47%wt) alloy (Ti-15Mo).

Results: For plates fixed on a fractured left angle of mandible model, the maximum/minimum values of MPS in the cp-Ti-constructed CHAMPY plate, upper AO/ASIF plate, and lower AO/ASIF plate were 19.5/20.3%, 15.2/25.3%, and 21.4/4.6% lower, respectively, than for plates made from Ti-15Mo. In the same model, the maximum/minimum values of displacements in cp-Ti-constructed CHAMPY plate, upper AO/ASIF plate, and lower AO/ASIF plate were 1.6/3.8%, 3.1/2.7%, and 5.4/10.4% higher, respectively, than for plates made from Ti-15Mo.

Conclusion. This *in silico* 3D-FEA demonstrates that Ti-15Mo plates have greater load-bearing capability.

Keywords: Mandibular fracture; Finite element analysis; Ti-15Mo alloy; Osteosynthesis, fracture.

INTRODUCTION

Mandibular angle fractures most commonly occur in 20- to 40-year-old males, generally as the result of personal assault, falls, or motorized vehicle accidents [1, 2]. Treatment of these fractures is challenging due to the difficulty of treating a sensitive load-bearing region that is susceptible to infection. In recent years, validation studies have been conducted to develop optimized reconstruction plates with appropriate mechanical properties and therefore reduce the healing period of the fracture [3]. Precise evaluation of the mechanical stresses that develop in a fractured mandible is essential to this optimization process.

There are two main avenues to reducing stress shielding and damage to the blood supply in fractured bone [4-7]. The first is to modify the bone-plate material. The second is to reduce the contact between the bone and the plates. Few studies have investigated the combined effects of these two parameters on stress shielding in the fractured bone [6].

Various types of internal fixation devices are used to promote the stabilization of bone structure [5, 8]. Reconstruction plates should be biocompatible and have appropriate mechanical properties for the support of fractured bone [5-7, 9, 10]. Conventional reconstruction plates are fabricated from metals such as cobalt-chromium, stainless steel, and titanium alloys. These plates have acceptable bio-compatibility, provide excellent reduction of bone fragments and have the required strength to stabilize and support the fracture. Titanium alloys are also the preferred material for the manufacture of miniplates and screws because of its stiffness, strength, and biocompatibility, which help these devices to maintain the relative position of bone segments. Ti-15Mo—a titanium-molybdenum system alloy containing 14.47%wt molybdenum—is known to exhibit high corrosion resistance, high electrochemical stability, and excellent biocompatibility [11] closer to commercially pure titanium grade 2 (cp-Ti) [12]. In terms of elastic modulus, Ti-15Mo closely approximates to that of human bone (~30 GPa) [13], unlike cp-Ti.

The primary goal of a bone plate should be to provide the maximum stability in the bone fracture region with the minimum amount of implanted material. Achieving this goal will reduce patient complications and overall patient discomfort. Greater biomechanical understanding allows the designer to take a more structured perspective on the design and composition of bone plates [4]. Three-dimensional finite element analysis (3D-FEA)—a computational technique, originally developed by engineers to model the mechanical behavior of structures such as buildings, aircraft, and engine parts—can determine the displacements, stresses and strains over an irregular solid body given the complex material behavior and loading conditions imposed on that body. 3D-FEA has been used previously to evaluate the treatment of facial fractures [9, 14-16] and its use in evaluating plating techniques has been shown to be promising [9].

The aim of this study was to use *in silico* 3D-FEA to investigate the maximum principal stress and displacement in two types of reconstructive fixation plate (CHAMPY and AO/ASIF) made from two types of material (cp-Ti and Ti-15Mo).

MATERIALS AND METHODS

CAD models simulating angle fractures

CAD models of the mandible and teeth for *in silico* 3D-FEA were constructed from a three-dimensional whole-body model for an adult human male [17]. Plates (CHAMPY and AO/ASIF types) and fixation screws were designed with CAD software (Solidworks2011; Dassault Systèmes Solidworks Corp, MA, USA) (**Fig. 1**). Each 1.0-mm-thick plate included four screw holes of 2.0 mm in diameter. The CHAMPY plate was fixed to the isolated left angle of mandible model by four $\phi 2.0 \times 6.0$ mm screws made of alpha-beta titanium alloy (Ti-6Al-4V; ASTM F136-12a). The AO/ASIF system consists of upper and lower plates fixed to the isolated left angle of mandible model by four $\phi 2.0 \times 6.0$ mm Ti-6Al-4V screws (upper plate) and four other screws of $\phi 2.0 \times 12.0$ mm (lower plate).

Three-dimensional finite element analysis

3D-FEA was performed by image-based CAE software (VOXELCON2015; Quint Corp., Tokyo, Japan). Material properties used for 3D-FEA are shown in Table 1. The voxel numbers of each CAD model are shown in Table 2. Both mandibular rami were fixed and a 3.0-mm force displacement corresponding to maximum failed load of *in vitro* experiment [18] was applied through the vertical axis of the mandibular central incisors (**Fig. 2**). For the evaluation of biomechanical stability, we measured the maximum principal stress (MPS) used as a failure criterion of titanium alloy [19, 20] and displacement distribution in models reconstructed with CHAMPY and AO/ASIF plates made from either cp-Ti (ASTM F67-06) or Ti-15Mo (ASTM F2066-08). Maximum and minimum values were acquired of each of these parameters.

RESULTS

Maximum principal stress

Table 3 summarizes maximum and minimum values of MPS in plates made from cp-Ti and Ti-15Mo. It can be seen that the maximum/minimum values of MPS in the CHAMPY plate, upper AO/ASIF plate, and lower AO/ASIF plate were 19.5/20.3%, 15.2/25.4%, and 21.4/4.56% higher, respectively, in plates made from cp-Ti than in those made from Ti-15Mo. For both the cp-Ti and Ti-15Mo CHAMPY plates, the maximum and minimum values of MPS were observed in the upper-middle and lower-middle areas of the plates, respectively (**Fig. 3**). For AO/ASIF plates (irrespective of material), the maximum MPS values were observed in the upper-middle section of the upper plate, while the minimum MPS values were found inside the first screw hole on the bottom plate (**Fig. 4**).

Displacement

Table 4 shows maximum/minimum values of displacements occurring in plates made from cp-Ti and Ti-15Mo. The maximum/minimum values of displacements in the CHAMPY plate, upper AO/ASIF plate, and lower AO/ASIF plate were 1.6/3.8%, 3.1/2.7%, and 5.4/10.4% higher in Ti-15Mo plates than in cp-Ti plates. Irrespective of material, maximum values of displacement in CHAMPY plates were observed at the mesial end of the plate, whereas minimum values were at the distal end (**Fig. 5**). In the AO/ASIF model, maximum values of displacement were found at the proximal end of the upper plate, while minimum values were obtained from the distal sections of the lower plate, regardless of material (**Fig. 6**).

DISCUSSION

A previous *in vitro* single load failure test of a synthetic mandible model concluded that AO/ASIF plates made of a titanium-molybdenum system alloy containing 14.47 wt% of molybdenum (Ti-15Mo) were more resistant to load and displacement than CHAMPY plates [18]. However, the mechanism by which this improved resistance was conferred could not be determined. The present *in silico* study demonstrated the distribution of stress and displacement in reconstruction plates and investigated the biomechanical stability of CHAMPY and AO/ASIF plates fabricated from commercially pure titanium grade 2 (cp-Ti) and Ti-15Mo.

Von Mises stress is known as a superior failure criterion for ductile materials such as metals during *in silico* analysis. However, because of the scalar nature of its values, Von Mises stress cannot determine whether observed stresses are compressive or tensile. Maximum principal stress (MPS)—a vector value—is a useful parameter for identifying the location(s) of those compressive and tensile stresses. Displacement observed in the reconstruction plates is helpful to understand a relative displacement of fractured bones. In this study, MPS and displacement were calculated by three-dimensional finite element analysis to evaluate the biomechanical stability of the types of plates used in treatment of mandibular angle fracture.

Ti-15Mo plates have been shown to exhibit lower MPS and higher tensile strength than plates made from cp-Ti [21, 22], strongly suggesting that Ti-15Mo provides greater resistance than cp-Ti for a same amount of load/displacement. Furthermore, we observed that the maximum and minimum values of MPS were focused respectively in the upper-middle and lower-middle of the CHAMPY plate, characteristic of a flexural mode of stress. Conversely, the concentration of maximum and minimum forces in the AO/ASIF plates suggested that they might inhibit flexural stress.

The addition of molybdenum to titanium is believed to reduce the Young's modulus of the resultant alloy [23-25] and give it similar material properties to human mandibular bone [26]. In the case of the CHAMPY plate and the upper AO/ASIF plate, the maximum and minimum values of displacements were observed in peripheral areas of the plates, whereas the minimum displacement in the lower AO/ASIF plate was shifted towards the middle of the plate. This altered center of rotation in the lower AO/ASIF plate could reduce the relative displacement of the fractured bones it re-apposes. There is further scope to improve this stability by optimizing the position and orientation of the plates. However, the use of two plates rather than one represents an increased risk of complications [4]. Ti-15Mo has properties that make it superior to Ti-6Al-4V as the material from which the screws are fabricated, notably that it has similar material properties to human mandibular bone [18] and appears to inhibit the strain concentration that is known to induce bone resorption [27].

Within the limitations of *in silico* 3D-FEA (namely the linear properties used for the mandible and teeth), our results suggest that Ti-15Mo is a suitable material for bone reconstruction plates. Further *in silico* study considering anisotropic and non-homogeneous properties of the mandible [28, 29] may be helpful in further optimizing fracture fixation methods for patients.

CONCLUSIONS

This *in silico* three-dimensional finite element analysis demonstrated that plates made from Ti-15Mo possess greater load-bearing capacity than those made from cp-Ti. From these findings, it can be predicted that the superior performance of CHAMPY plates made from Ti-15Mo may enable a shorter treatment period with greater longevity in clinical service.

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ACCEPTED MANUSCRIPT

FIGURE LEGENDS

Figure 1. CAD models used for *in silico* finite element analysis with (a) CHAMPY plate and (b) AO/ASIF plates. Yellow and red areas correspond to the mandible, white areas to the teeth, while the light gray and dark gray denote the plate and screws, respectively.

Figure 2. Voxel models and boundary conditions used for *in silico* finite element analysis with (a) CHAMPY plate and (b) AO/ASIF plates. Yellow denotes the loaded areas and direction of force (arrow), whereas red indicates fixed areas.

Figure 3. Maximum principal stress distribution obtained in CHAMPY plates fabricated from (a) cp-Ti and (b) Ti-15Mo. Red and blue arrows indicate the position of the maximum and minimum values, respectively, of the maximum principal stresses in these CHAMPY plates.

Figure 4. Maximum principal stress distribution obtained in AO/ASIF plates fabricated from (a) cp-Ti and (b) Ti-15Mo. Red and blue arrows indicate the position of the maximum and minimum values, respectively, of the maximum principal stresses in these

AO/ASIF plates.

Figure 5. Displacement distribution obtained in CHAMPY plates fabricated from (a) cp-Ti and (b) Ti-15Mo. Red and blue arrows indicate the position of the maximum and minimum values of displacements, respectively.

Figure 6. Displacement distribution obtained in AO/ASIF plates fabricated from (a) cp-Ti and (b) Ti-15Mo. Red and blue arrows indicate the position of the maximum and minimum values of displacements, respectively.

TABLES

Table 1. Material properties used for *in silico* finite element analysis. Young's modulus and Poisson's ratio represent elasticity of materials.

	Mandible and teeth	Plate (cp-Ti)	Plate (Ti-15Mo)	Screw (Ti-6Al-4V)
Young's modulus (MPa)	624.24	107000	75000	110000
Poisson's ratio	0.2817	0.34	0.34	0.34

Table 2. Number of voxels for components of finite element models. Voxel resolution was standardized to 0.1 mm.

	Mandible	Teeth	Upper plate	Bottom plate	Screw (ϕ2.0 × 6.0 mm)	Screw (ϕ2.0 × 12mm)
CHAMPY	35955373	7966020	83665	-	39990	-
AO/ASIF	35909282	7966020	83665	83271	39990	89214

Table 3. Maximum/minimum values of maximum principal stress (MPa) in plates made from cp-Ti and Ti-15Mo.

	cp-Ti	Ti-15Mo
CHAMPY	1226.0/-149.7	986.8/-119.3
AO/ASIF		
Upper plate	1037.9/-83.8	879.8/-62.6
Lower plate	623.1/-182.0	489.6/-173.7

Table 4. Maximum/minimum values of displacements (mm) in plates made from cp-Ti and Ti-15Mo.

	cp-Ti	Ti-15Mo
CHAMPY	0.852/0.0684	0.866/0.0710
AO/ASIF		
Upper plate	0.513/0.150	0.529/0.154
Lower plate	0.314/0.0308	0.331/0.0340

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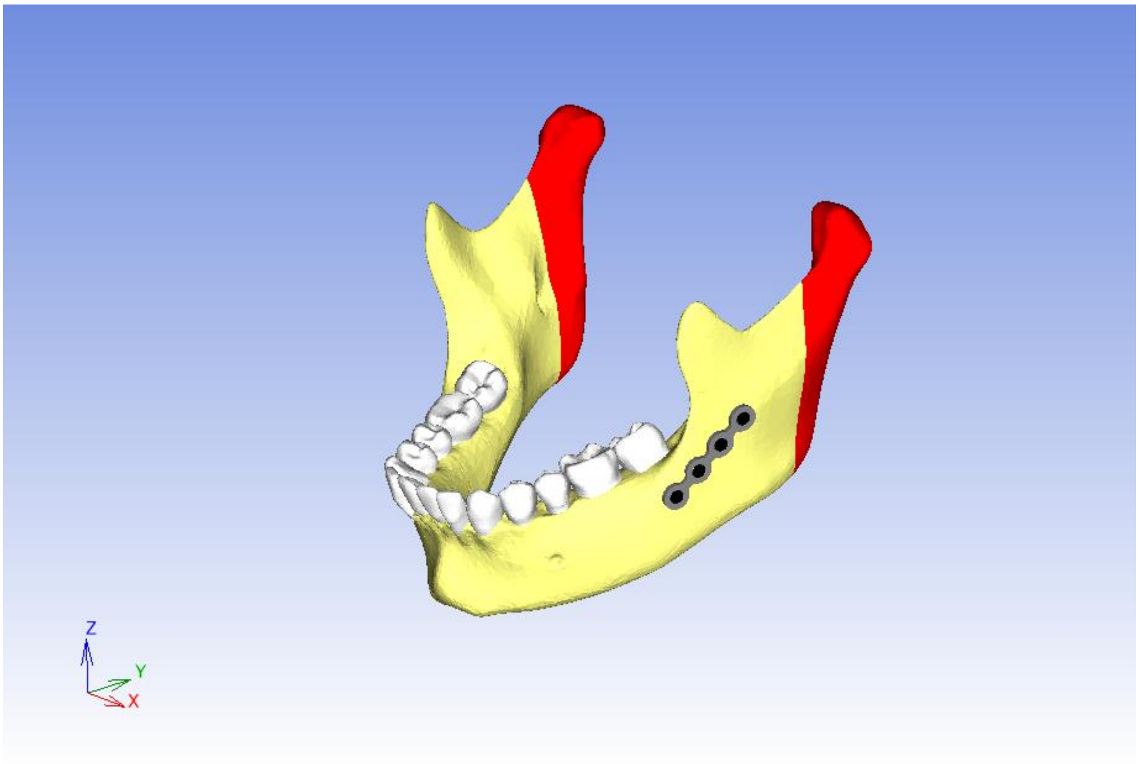
Figures

Fig. 1a



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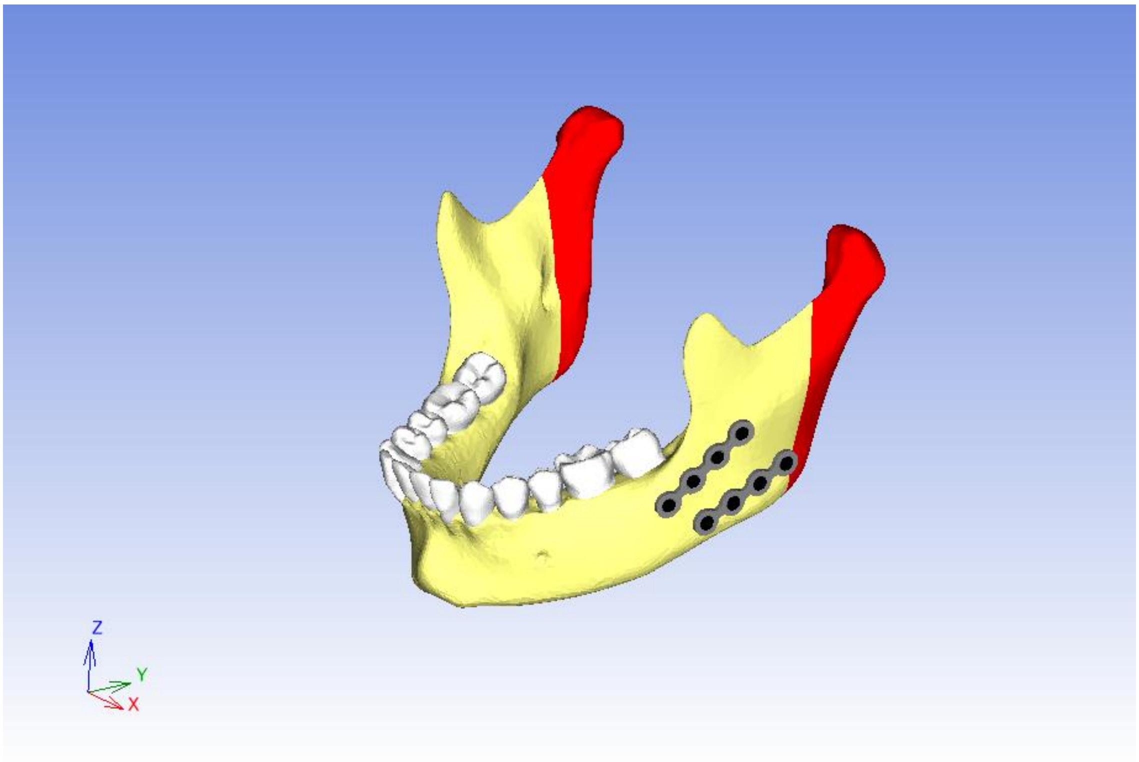

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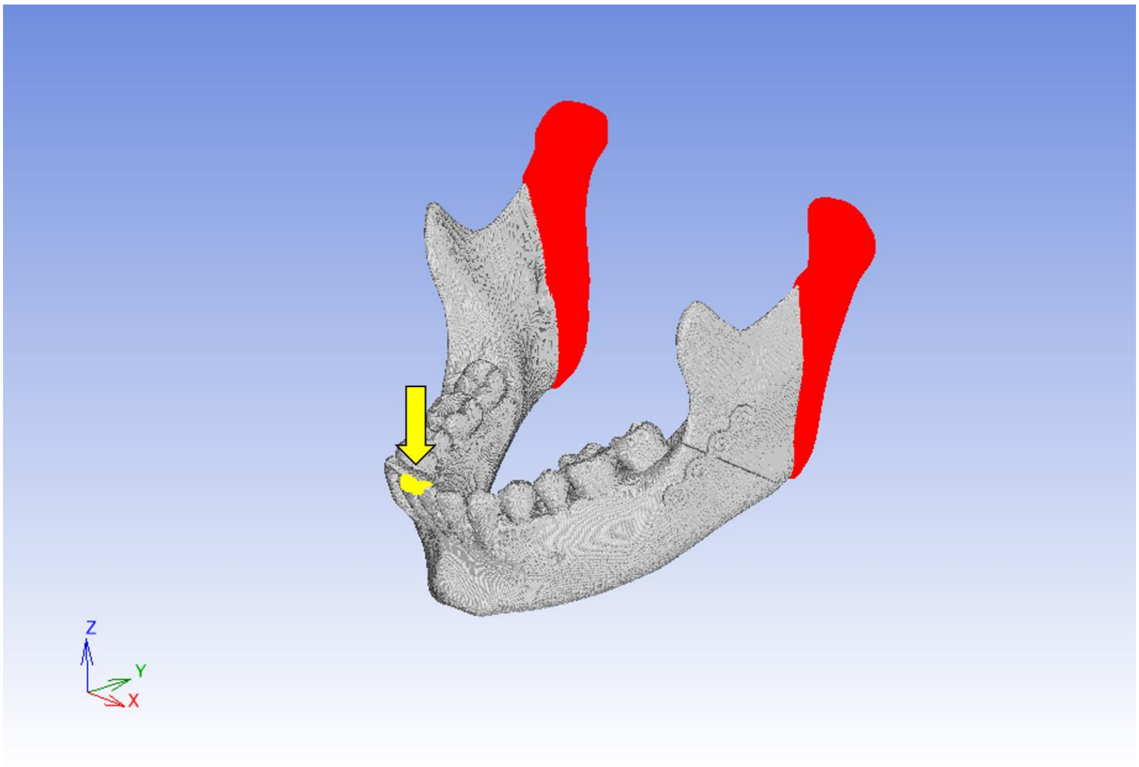

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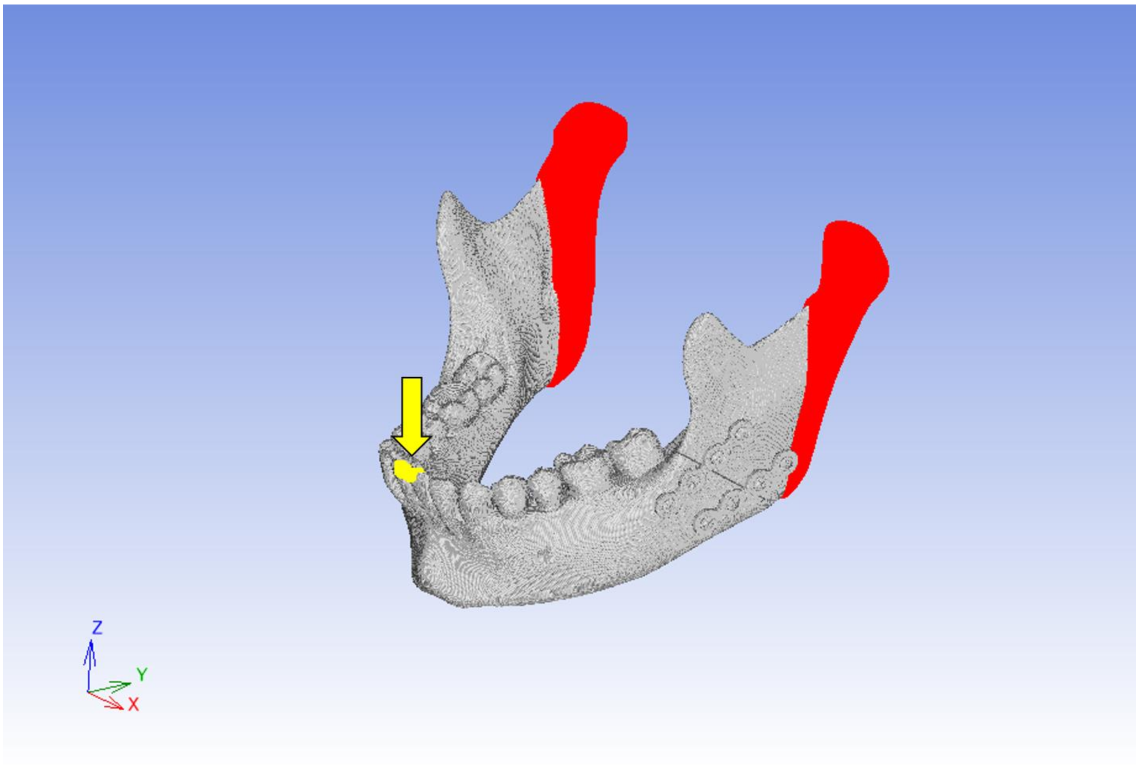

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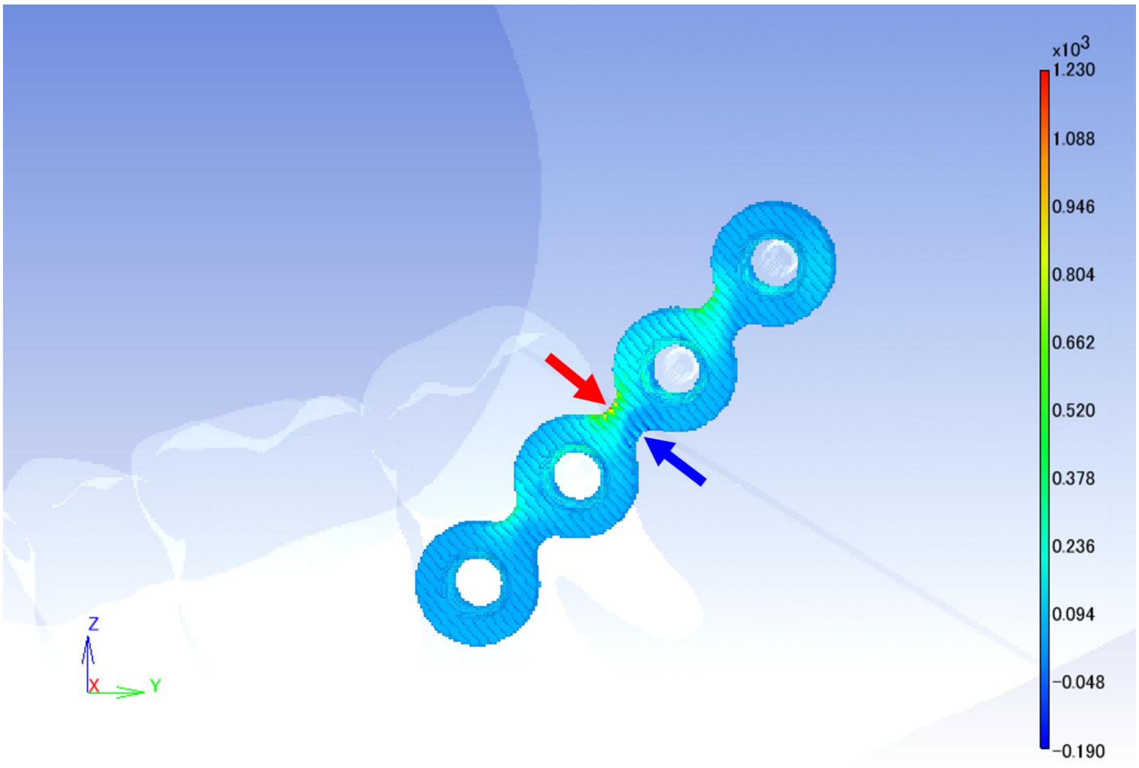
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Z
X
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Fig. 3b

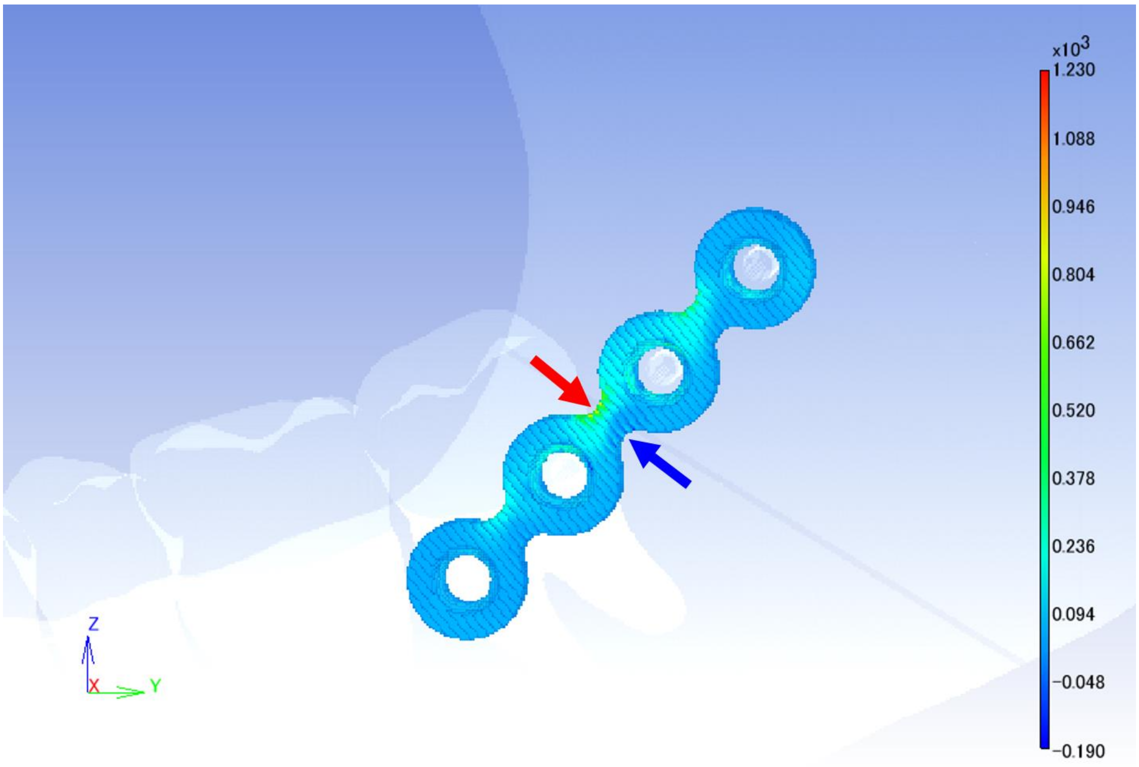
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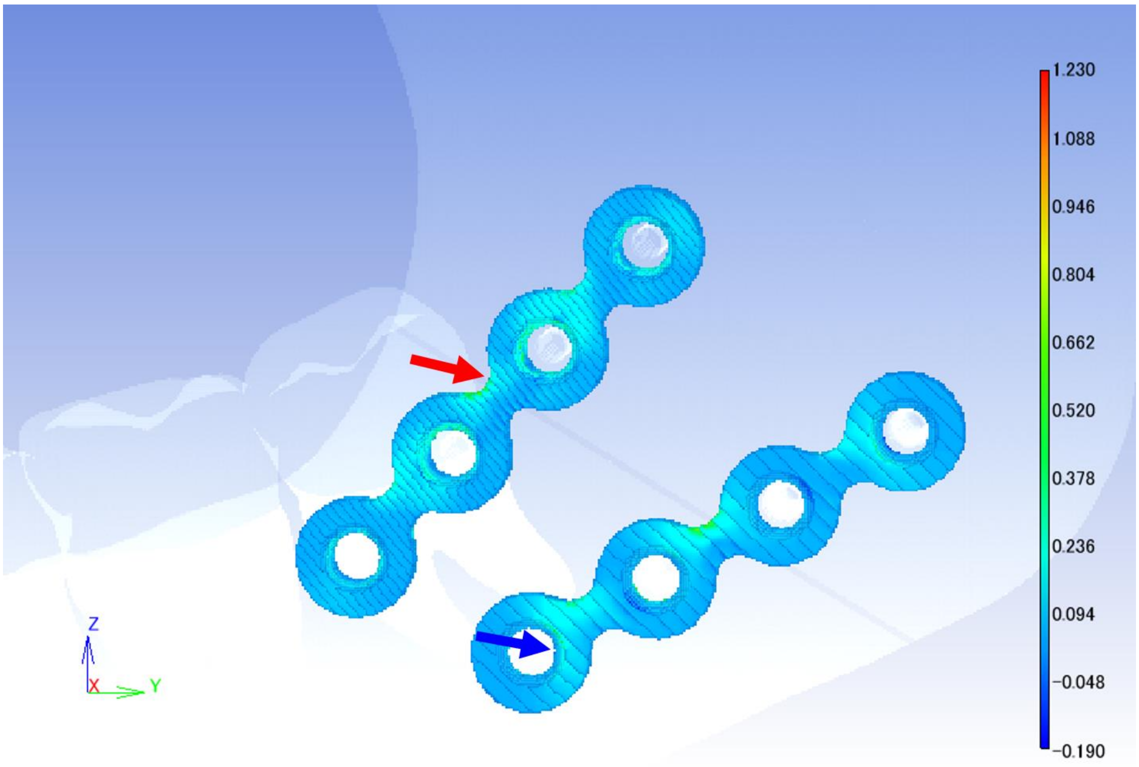
Fig. 4a



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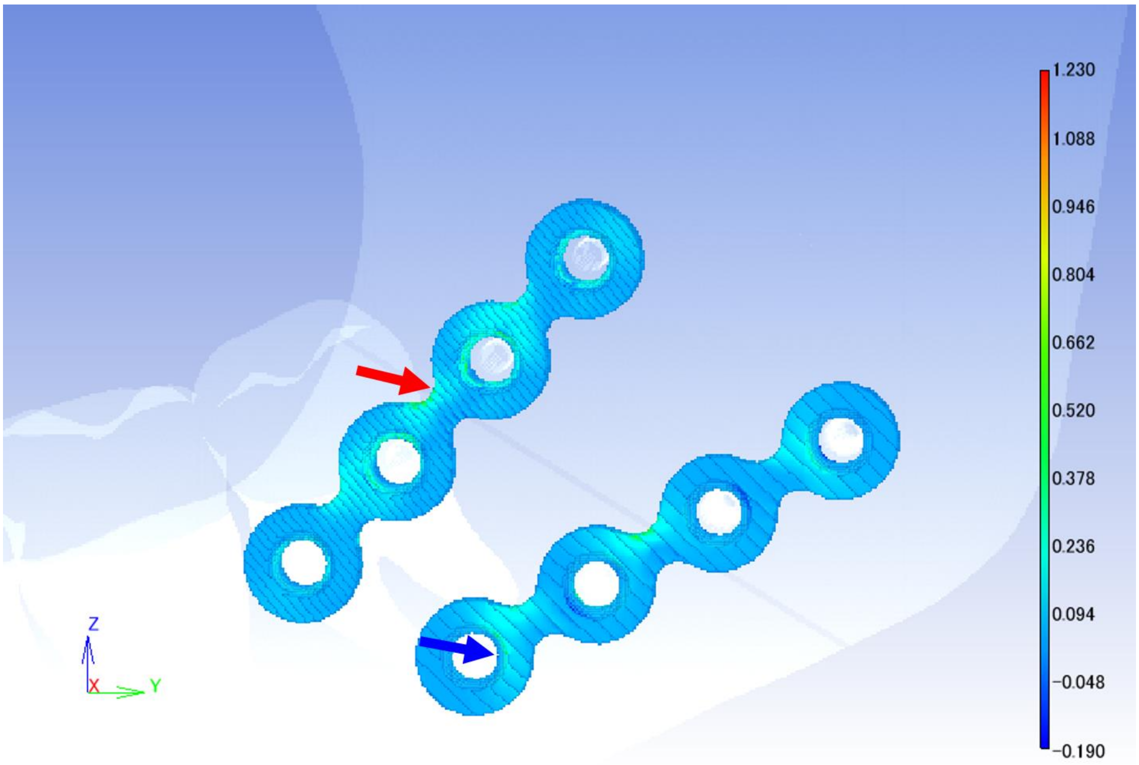

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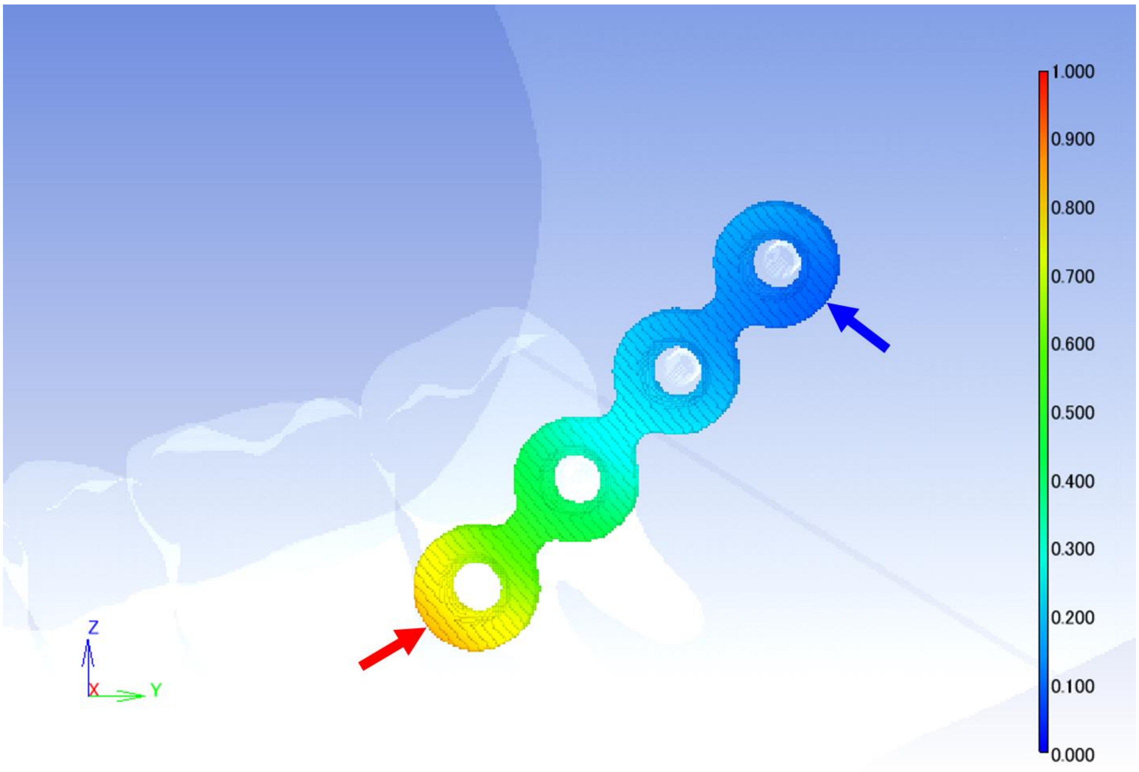

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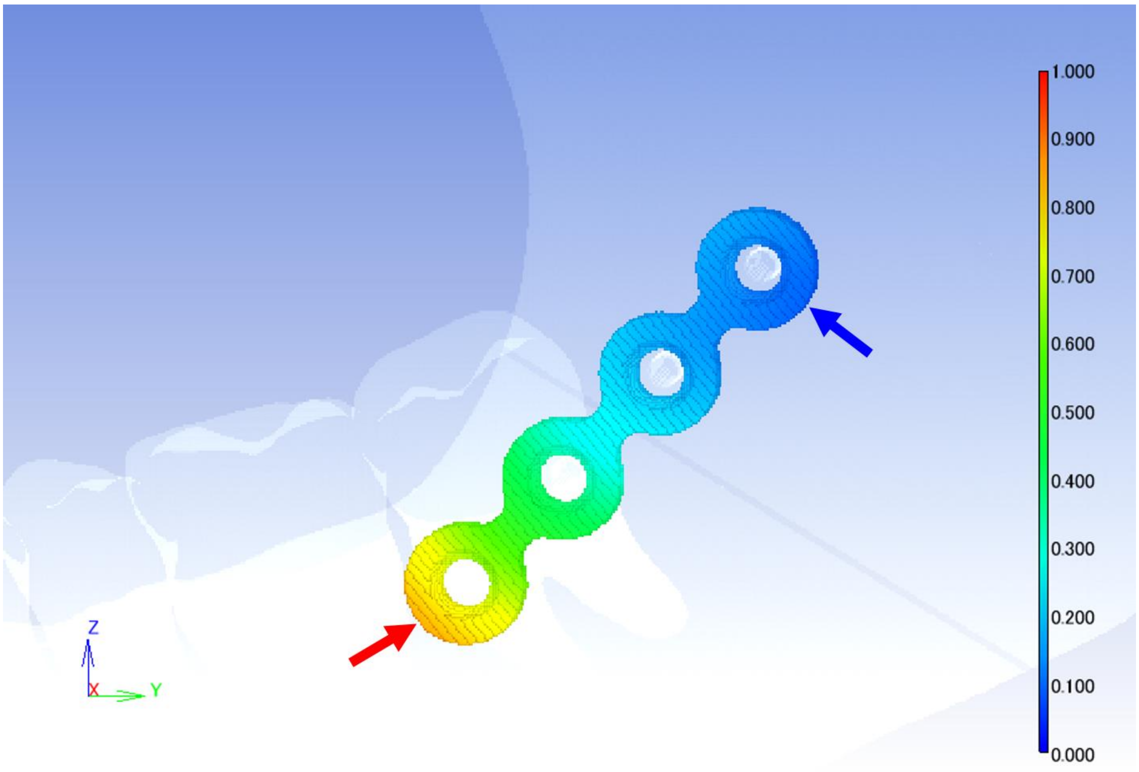

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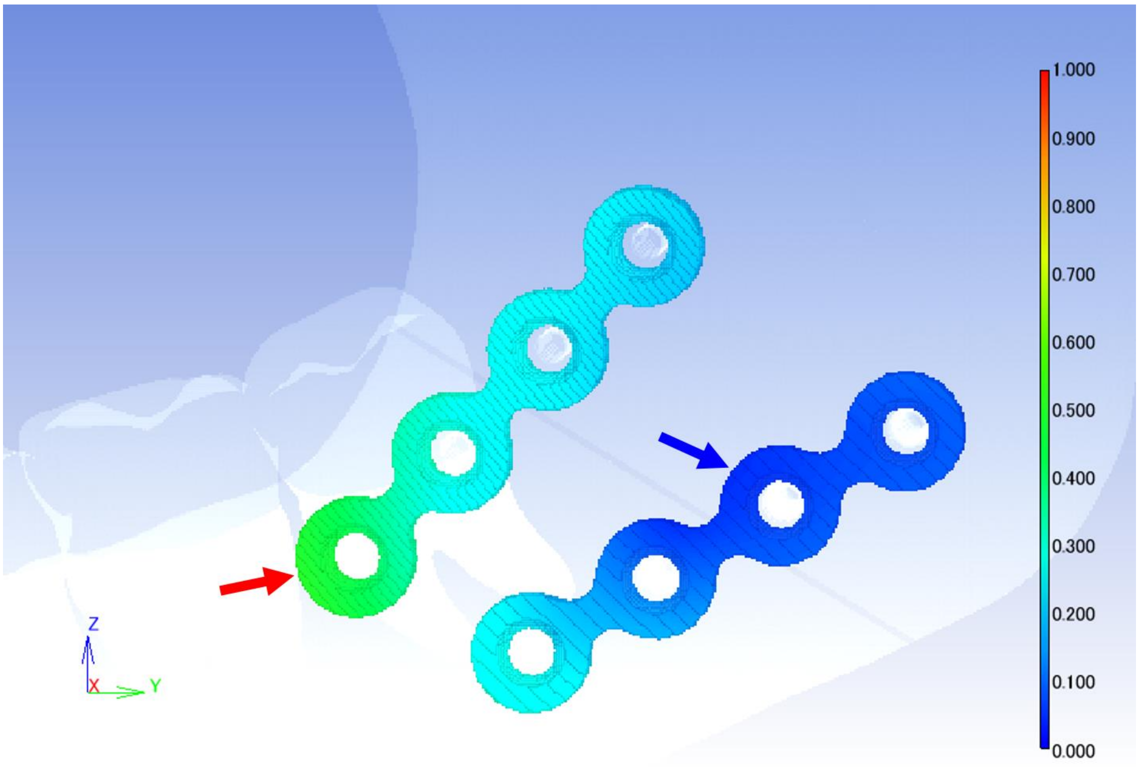

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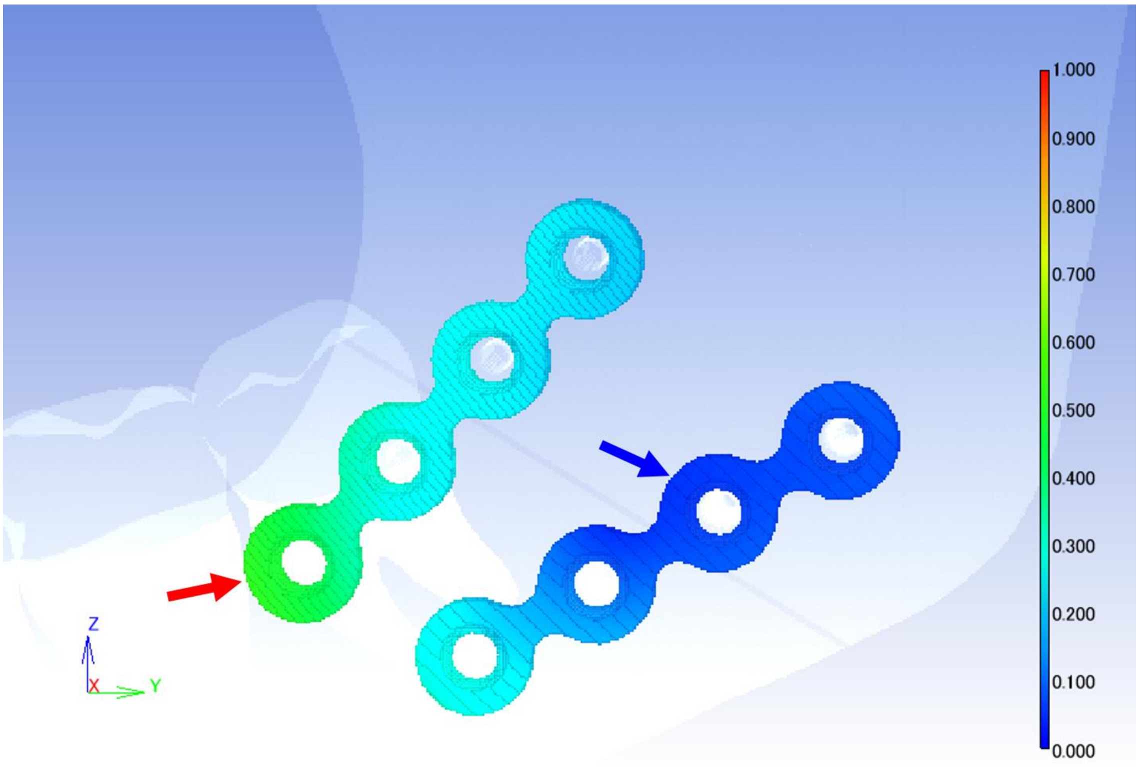

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