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Finite Element Analysis of Titanium Alloy-Graphene based mandible plate

Titanium alloy based maxillofacial plates and implants are widely used in fracture treatment and reconstructions. Filler materials Graphene Nanoplatlets(GNPs) were used in Titanium alloy maxillofacial plate and a Finite Element Model (FEM) was designed to reconstruct a fractured human mandible. 50N and 500N bite forces were applied on the mandible and stress distribution using Von mises failure theory across the plate sections was analyzed. A pure plate was critically stressed at a section near the mandible fracture region for a Von mises stress of nearly 27.5GPa while this stress got reduced by nearly 10%-22% with the presence of minor composition of GNPs in the plate. GNPs orientation in parallel (21.1 GPa) to the plate axis were more effective in comparison to other orientations(90^0,45^0 and 135^0) and the location variation of these GNPs along the plate had no significant effect on the stress distribution. The fatigue analyses showed that, under these stresses and forces the plate with GNP was able to endure for nearly 7000 days, while pure Titanium plate could fail by fatigue in approximately 70 days. Hence, presence of minor compositions of GNPs could enhance endurance life of the Titanium plate by reducing stress concentrations at critical sections of the plate.

Keywords: FEA; FEM; GNP; maxillofacial; endurance; stress

Introduction

Exceptional mechanical properties with smaller mass density of graphene (Potenza et al. 2017; Papageorgiou et al. 2017) material has attracted lot of interest among scientists for improving the properties of biomedical implant materials. Biomedical implants (Pacifici et al. 2016; Azevedo and Hippert 2002) made up of different types of metal alloys are being widely used for orthopaedic, dental, maxillofacial and craniofacial reconstruction applications. Size and weight reduction for implants has always been a major concern among surgeons and scientists, for which composite material development has widely been explored over the years. Composite filler material must possess high strength, lower mass and biocompatibility for its suitability as biomedical implant filler. Carbon materials (Mathur et al. 2008; Jindal et al, 2014; Papageorgiou et al. 2017) in the form of Carbon Nanotubes(CNTs) and Graphene possess high mechanical strength and smaller size. Graphene has shown tremendous potential for enhancing mechanical properties of polymer (Mathur et al. 2008; Jindal et al. 2015) and metal (Bakshi et al. 2010) composite materials without altering their mass significantly. Graphene can be used experimentally in multiple forms (Papageorgiou et al. 2017) such as microplates, nanoplates, oxides, nanosheets etc. On a bulk level, Graphene (Potenza et al. 2017; Liu et al. 2012, Azevedo and Hippert 2002) has a thermal conductivity of 3000W/mK, elastic modulus nearly 1TPa, ultimate tensile strength 130GPa, shear modulus of 53 GPa, Poisson's ratio of 0.19 and mass density of nearly 700kg/m^3. These major properties of graphene play an important role for enhancement of mechanical properties of any composite material. All these properties of graphene are dependent upon chirality, layer thickness, orientation, direction of loading, forms etc. hence lot of variations (Sakhaee-Pour 2009; Zheng et al. 2014; Politano and Chiarello 2015;) based on these parameters have also been reported. Graphene and its various forms have shown biocompatibility (Reina et al. 2017) for different applications like drug delivery, tissue engineering, bio sensing and implants. The ability of graphene to improve the mechanical and biological (Gu et al. 2014) properties of implants or scaffold materials, by promoting adhesion, proliferation, and osteogenic differentiation have also been demonstrated in several studies. Graphene coated nitinol (Podila et al. 2013) has been proposed as a viable candidate for stents, however, numerous challenges remain due to exogenous material cytotoxicity, bio- and hemo-compatibility. The metallic nature of these alloys results in poor bio- and hemo-compatibility due to lack of cell adhesion, proliferation, and thrombosis.

Among the bio-medical implants, Titanium alloy(Ti-6Al-4V) (Niinomi 1998; Pacifici et al. 2016) based maxillofacial plates are widely used for jaw fracture treatment and reconstructions. Based on the method of manufacturing of these Titanium alloy plates their elastic moduli and fatigue strength vary between 110-114 GPa and 600-816 MPa respectively. Apart from the basic Ti-6Al-4V, various other alloys like Ti-5Al-2.5Fe, Ti-6Al-7Nb etc. have also been developed to improve other properties like corrosion resistance, fatigue strength etc. Plates of variable thickness and lengths are used, based on the type of fractures. Plates need to be evaluated for strength under various jaw movement conditions for which various FEM techniques are adopted. FEM is also used to design different shapes, combinations and thickness of these plates to evaluate their effects on strength enhancement for withstanding higher mandible stresses. Gutwald et al (2017) evaluated customized mandibular reconstruction plate strengths using mechanical testing and FEM. He reported that maximum stress was significantly reduced by nearly 31% by increasing the bar width from 5.5mm to 6.5mm. Goulart et al (2015) used FEM by applying Von Mises yielding criteria for evaluating the effectiveness of using 2 plates instead of single for recovery of bone fractures and observed that two locking plates promoted a better mechanical resistance for complex mandible fractures. Atilgan et al (2010) used ANSYS software for FEM analysis by applying Von Mises yielding criteria to evaluate mechanical stresses in the plate by simulating masticatory forces in the human jaw. This analysis provided an insight into the location of stress intensifiers and breaking points on the plate, helping to improve the design of the plates.

These methods can also assist in designing customized and individualized plates of different geometry and shapes. Chen et al (2010) observed the influence of number of screws on the fatigue life of locking compression plates using SolidWorks software by evaluating principal stresses. Biomechanical analyses provided an estimate on plate and screw combinations to provide rigid and flexible fixations, where flexible fixations enhanced the fatigue life of the plate. Papakyriacou et al (2000) reported the effects of corrosive environment for Titanium alloys (Ti–6Al–7Nb) used for dental implant materials by observing fatigue properties. There was a decrease in endurance limit by nearly 20% when implants were exposed to corrosive environments and a beneficial influence of surface structuring by blasting and shot peening on the fatigue properties was also found. Mahathi et al (2013) used Von Mises theory using ANSYS software to evaluate the stress on a fractured mandible bone for different types of plate designs by applying bite force. An improvised 3D modified plate was designed for minimal stress in the plate, screw and bone. Hence, the reported work by various scientists clearly indicates rising interest on improving the mechanical strength of biomedical implants. FEM techniques have been widely used for characterisation to save on manufacturing costs. Various software, failure theories, plate types, geometries etc. have been the preferred methods to explore these properties and accordingly produced satisfactory results in several cases. Along with the plate designs, FEM can also be used to evaluate the influence of a composite filler material on the mechanical properties of plates. Graphene, despite of being a mechanically strong material, has not been exhaustively explored for maxillofacial plate applications.

For this paper a basic Titanium alloy based thin maxillofacial plate (Mandible fractured model) with a minimal quantity of Graphene Nanoplatlets (GNPs) using SolidWorks software has been modelled and analysed. The influence of GNPs in different orientations and locations in the plate for stress and endurance has been analysed under the application of compressive bite force on the mandible.

Materials and Methods

Finite Element Model

A mandible bone model with a 1 mm fracture was used and a Titanium alloy (Ti-6Al-4V) based 1 mm thick plate was used for its fracture osteosynthesis. As shown in Figure 1, the plate was placed at the suitable location for fracture osteosynthesis and a compressive bite force (Raabe et al, 2009 ; Gutwald et al. 2017) 50N and 500N was applied at the mandible with fixed supports at the opposing end.

The Titanium plate was modelled as shown in Figure 2 with customized screws represented by a cylinder (7 mm length) and a rigidly connected head (2.6mm diameter) to the bone and plate respectively (Chen et al. 2010). Four unicortical screws were used with plate of thickness 1 mm, length 16.5mm, diameter 3 mm and volume 22.02 mm^3. The plate and screws were Ti-6Al-4V alloy based, hence their mechanical properties were considered as- Elastic modulus 105 GPa, Poisson ratio 0.31, yield strength 827 MPa and mass density 4429 kg/m^3.

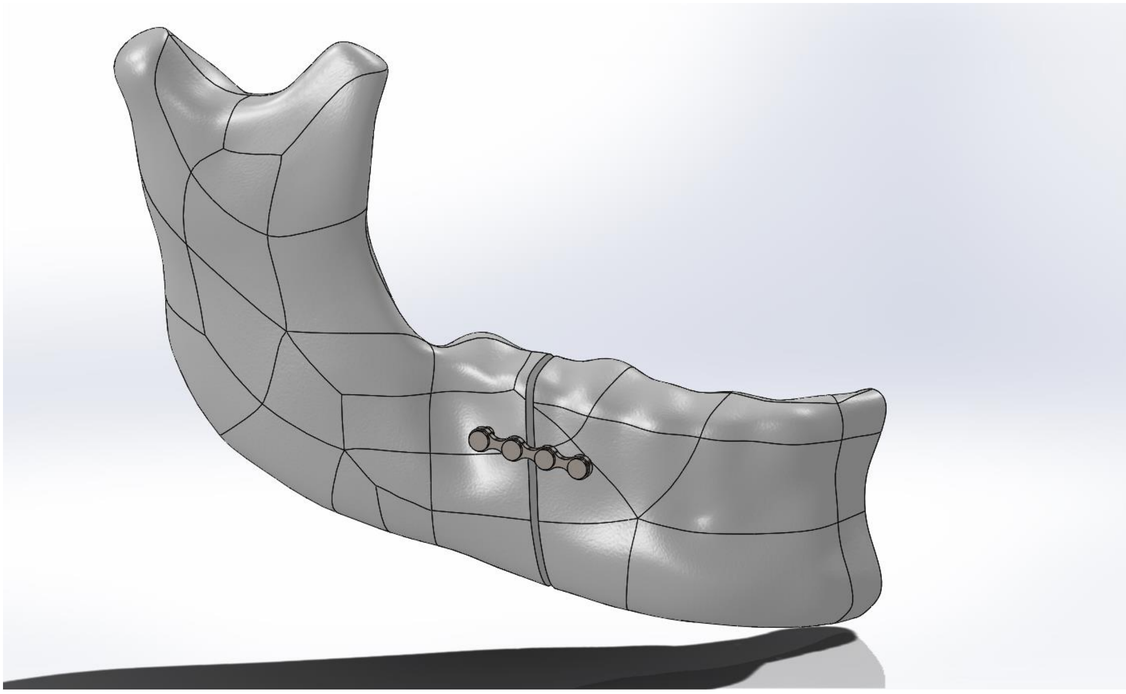
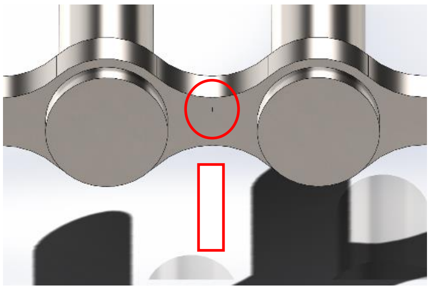


Figure 1. Fractured mandible with a Titanium plate

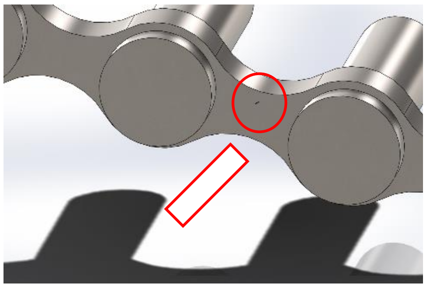
Figure 2. Maxillofacial plate with screws

Based on this model, other plate models (Figure 3(a-d)) were designed with GNP embedded on the surface and centre plate near the exact fracture location, as this was the expected breaking (Gutwald et al., 2017) or most vulnerable section of the plate during mandible movement. To evaluate the effect of angular orientation of GNPs, four different orientations were modelled for analysis. GNP (Papageorgiou et al., 2017) dimensions were taken as a thin multilayer cuboid sheet of 10^5 x 10^4 x 10^2 nm with an equivalent bulk density of 700kg/m^3, Young's modulus 1TPa and Poisson's ratio 0.2. Mandible bone elastic modulus was taken as 18GPa, Poisson's ratio 0.394 and mass density 1.8gm/cm^3. Based on the densities and volumes, the given mass of the plate was 97.4mg and GNPs weight nearly 7×10^{-5}µgm. The bulk density for GNP can vary up to

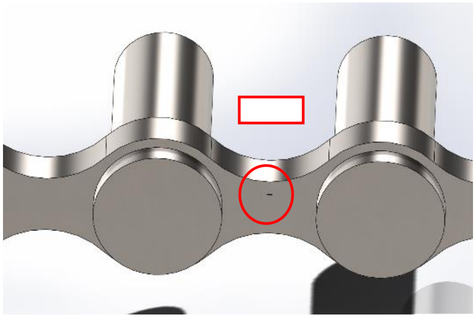
$2000 kg/m^3$ which would result in its weighing mass up to nearly $21x10^{-5}$µgm, which would still remain insignificant to the overall weight of the titanium plate.



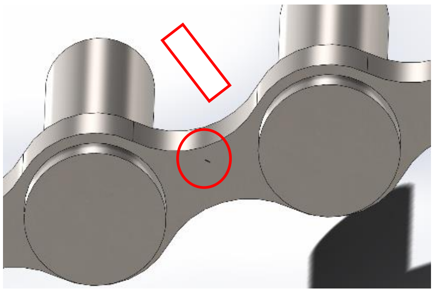
(a) GNP aligned perpendicular to the plate axis



(b) GNP aligned 45^{0} to the plate axis



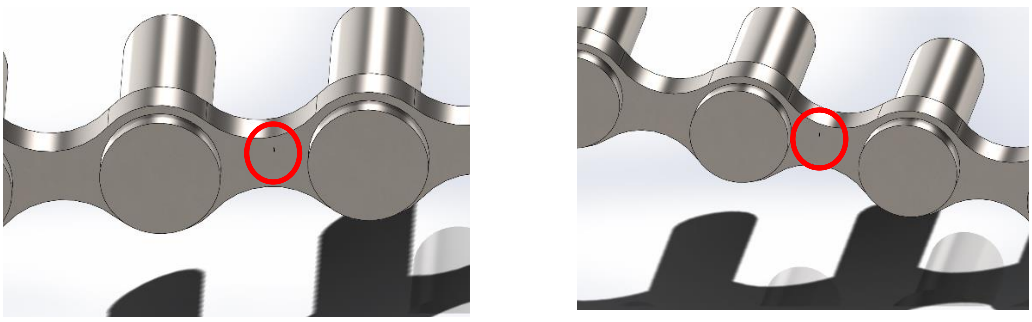
(c) GNP aligned parallel to the plate axis



(d) GNP aligned 135^{0} to the plate axis

Figure 3. Different angular orientations of GNP with plate.

In addition to the angular orientation variations, models with distributed GNPs at other locations were also designed as shown in Figure 4(a, b) where the placement of GNPs was offset from both the left and right side of the centre.



(a) GNP displaced 0.23mm towards right side

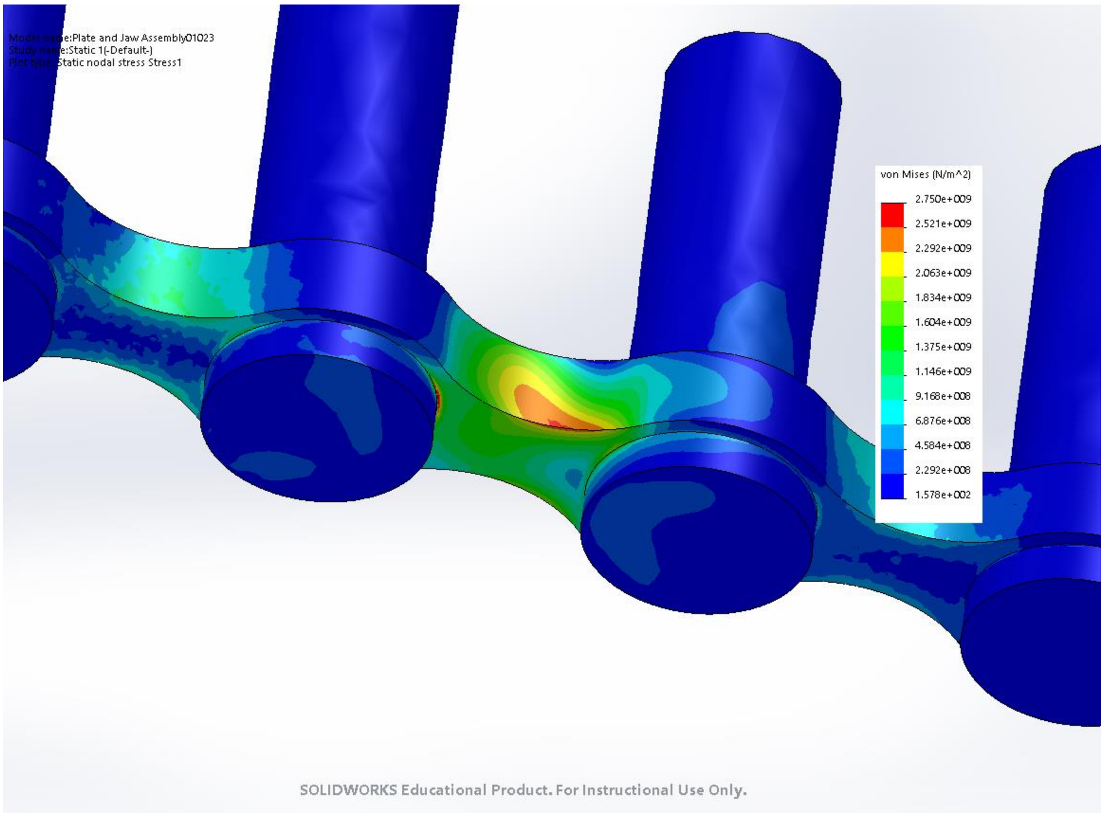
(b) GNP displaced 0.23mm towards left side

Figure 4. Offset locations of GNPs on the plate.

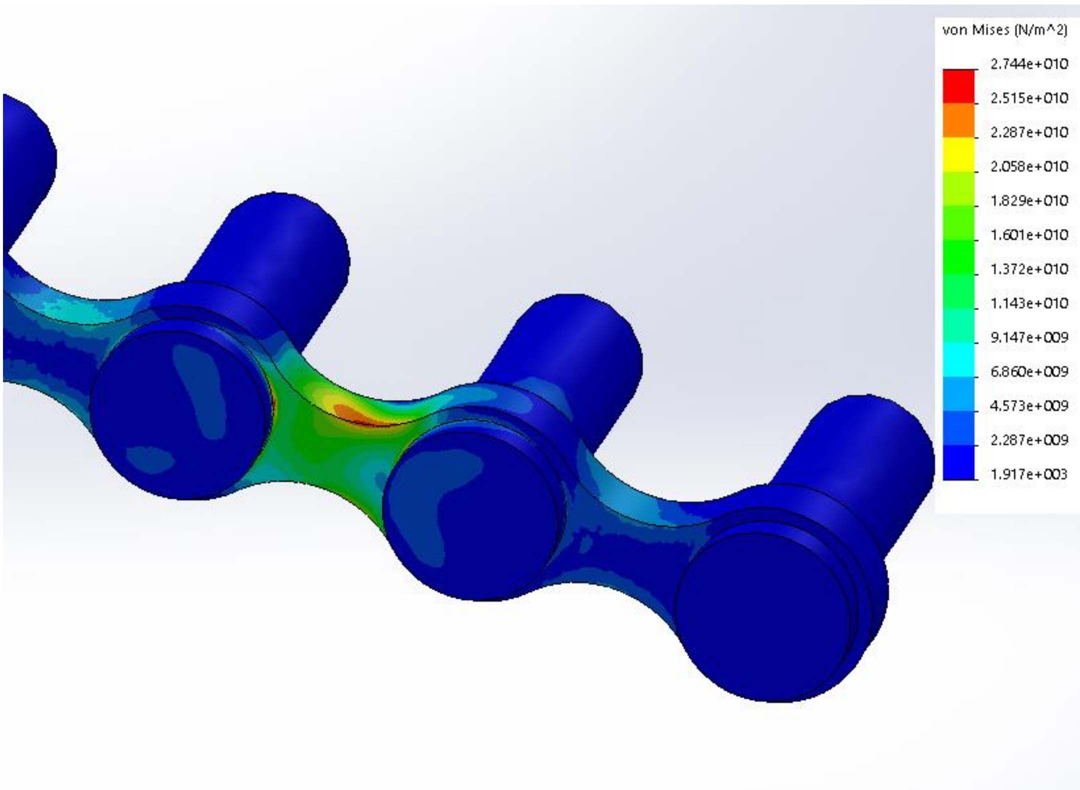
Fixed compressive forces were applied on all these models for 50N and 500N to evaluate the critical stress point on the plates.

Finite Element Analysis

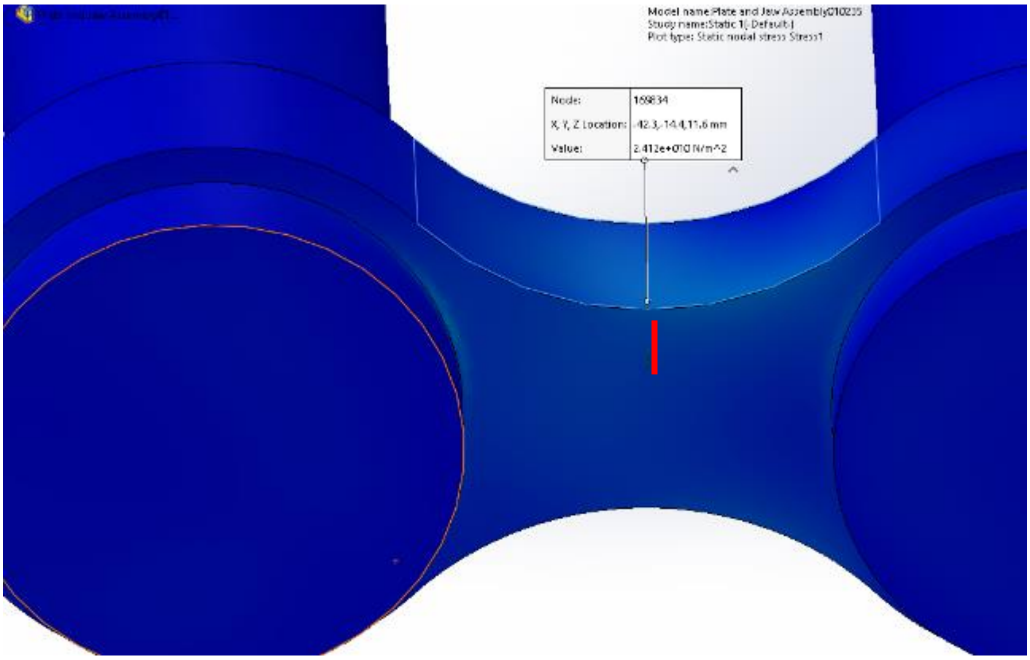
A pure Titanium Alloy plate model was fine meshed (number of mesh elements for the plate was 8924, screws was 1598 and mandible 52526) and a static simulation study for compression was conducted on the mandible with specified (50N and 500N) bite forces. Figures 5(a-b) indicate the maximum stress elements near the middle section and upper surface of the plate at the actual fracture location. The stresses placed on the plate, obtained through Von Mises theory are shown in Table1. To compare the effects of various orientations of GNPs the same study under finer mesh (specifically for GNP) was repeated as shown in Figures 5(c-d). These figures demonstrate, that the stresses were significantly reduced in the same sections of the plate which were identified as vulnerable to failure. Presence of GNPs on the surface itself, reduced the stresses in those plate sections which were earlier most vulnerable for failure. Table 1, gives a comparison of stresses experienced by the plate at the same section for different orientations of GNPs. In addition, stress distribution was also obtained by offsetting(0.23mm, 0.46mm, .69mm and 0.92mm) GNP to various locations along the same section as shown in Figures 5(d-e).



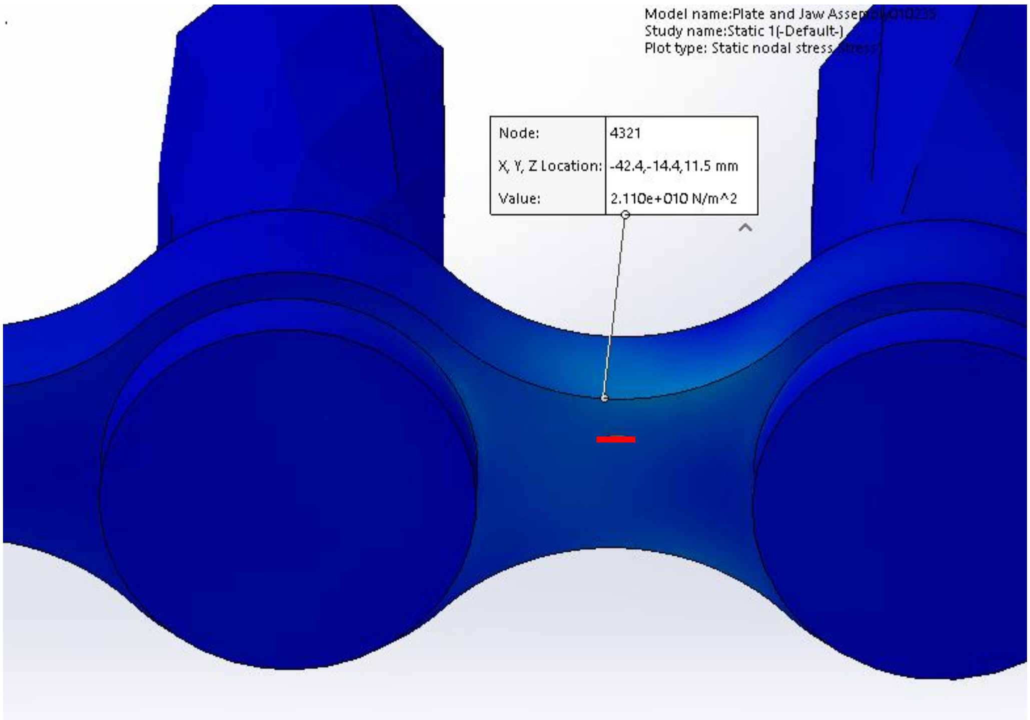
(a) Stressed Titanium plate under 50N bite force



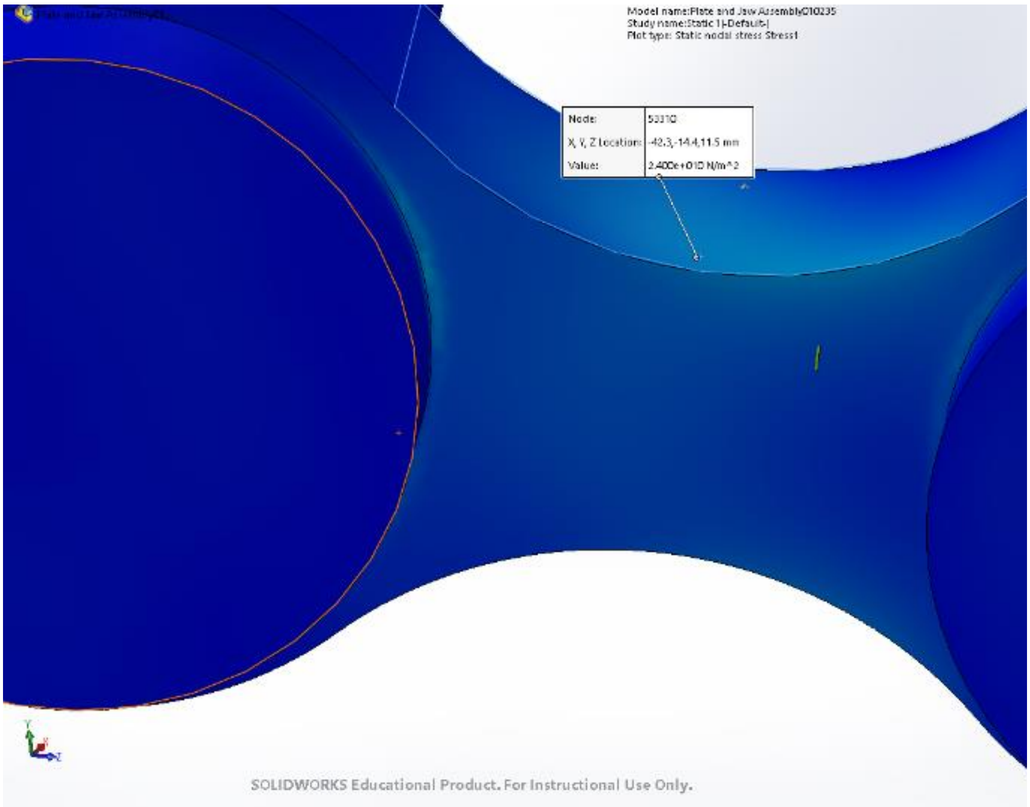
(b) Stressed Titanium plate under 500N bite force



(c) Stressed Titanium plate with GNP embedded perpendicular to the axis under 500N bite force



(d) Stressed Titanium plate with GNP embedded parallel to the axis under 500N bite force



(e) Stressed Titanium plate with GNP embedded perpendicular to the axis and offset under 500N bite force

Figure 5. Stresses across the plate for various GNP combinations

Results

Finite Element Analysis (FEA) results of the various models shown in Table 1 indicate that parallel orientation of GNP to the plate centre line was highly effective in reducing the stress on the plate.

Table 1- Von Mises stresses for pure Titanium alloy plate and embedded GNPs at different angular orientations of GNPs under 50N and 500N bite forces

S.No	Plate material	Angular orientation of GNP with Plate Axis(^{0})	Von Mises stress(GPa) at failure section of plate(50N)	% reduction in stress	Von Mises stress(GPa) at failure section of plate(500N)	% reduction in stress
1	Pure Titanium alloy	-	2.74	-	27.5	-
2	Titanium-GNP	90	2.45	10.91	24.1	12.04
3	Titanium-GNP	45	2.37	13.82	23.4	14.60
4	Titanium-GNP	0	2.13	22.55	21.1	22.99
5	Titanium-GNP	135	2.33	15.27	23.1	15.69

In addition to a change in orientation of GNP, the location of GNP was changed along the same axis by offsetting distance by sets of 0.23mm from the centre along both sides. This process was repeated for all the geometries and it was observed that stress values at the breaking point of the plate were not affected by the GNP position along the plane. This emphasised the phenomenon that the presence of minor compositions of GNP was sufficient to impart higher strength to the plate and nearby location changes have no significant effect on the overall plate strength.

Based on the Von mises stresses obtained, endurance limits and life of the plate were obtained referring to the relation (Chen et al. 2010) below:

$$S_e = S_a\left(1 - \frac{S_m}{S_y}\right)$$

Equivalent stress amplitude/Endurance limit stress(S_e) of the plate was calculated based on elastic modulus(S_y) of the plate material only. Mean stress (S_m) and stress amplitude(S_a) were obtained based on the stress experienced by the plate at the critical stress($S_{max} = 2S_m = 2S_a$) section rather than maximum stress experienced by the plate. For a bite force for 50N, endurance life(cycles) and number of days were calculated using S-N diagram (Papakyriacou et al, 2000) for a survival rate of 50% probability and 1400 chewing cycles per day (Raabe et al, 2009). Since the comparison was between a Titanium plate and minor GNP composition in the plate, only the elastic modulus of the Titanium alloy was considered. Table 2 shows enhanced endurance life of the plate composed of GNP.

Table 2- Endurance cycles and life for the plates with and without GNP for a force of 50N

S.No	Plate material	S_e(GPa)	S_m(GPa)	S_y(GPa)	Endurance Life(~Cycles)	Endurance Life(~Days)
1	Pure Ti alloy	0.696	1.38	105	10^5	70
2	Titanium-GNP	0.534	1.07	105	10^7	7000

Discussion

The fabrication process of a graphene and titanium alloy composite material can be a complex and costly process, or alternative melt processing or modern additive manufacturing processes can be explored. With reports on successful biocompatible applications of Graphene on biosensors, drug delivery, tissue engineering etc., it can be used as a suitable filler material for improving mechanical properties of biomedical plates also. Random dispersion of any filler is most effective in enhancing mechanical strength (Jindal et al. 2013; Jindal et al. 2016) especially when its related to nano-composites. Hence, controlling the orientations (Wang et al. 2008) and locations has always been a prime focus in order to save on material cost. During manufacturing, it requires additional methods to control the orientation of fillers and fibres and their effectiveness can only be explored post manufacturing, therefore, finite element studies can provide encouraging data for scientists for making decisions related to manufacturing. Models indicated that if GNPs locations were altered without changing their mass and volume, they produced insignificant changes in stress distributions. Reinforcement of a polymer with random nanoplatelets is expected to have a Young's modulus of around 8/15 of that for a nanocomposite with aligned nanoplatelets deformed parallel (Liu and Brinson 2008) to the axis of alignment, thereby indicating superior effectiveness in mechanical strength of aligned (Li et al. 2016) nanoplatlets. In the analysis of this study, the effectiveness of parallel aligned GNP was also observed to be the highest. The maxillofacial plate with parallel aligned GNP, was accordingly expected to undergo minimal mechanical stress at the breaking point in comparison to all other orientations. The GNP direction which was parallel to the plate axis, was normal to the compressive loading direction which may have acted as a fixed beam support between the two mandibles separated by fracture whereas all other orientations provided a partial support. The fatigue analyses showed that, under these stresses and forces the plate with GNP was able to endure for nearly 7000 days, while pure Titanium plate could fail by fatigue fracture in approximately 70 days.

It is suggested that a successful 3D model of Titanium alloy-graphene maxillofacial plate has been designed for treating a mandible fracture with insignificant mass factor of GNPs in the titanium alloy. Forces of the magnitude of 50N and 500N, equivalent to bite forces were applied on the mandible with the plate attached. The breaking point section in the pure plate was observed near the fracture location and GNPs were placed nearby that location at various angular positions. Presence of GNPs, reduced the stress concentration between 10 to 22% at the breaking section of the plate depending upon the angular orientations with respect to the plate axis. Parallel direction of GNPs showed encouraging results by reducing the stresses by 22% while normal direction GNPs showed only 10% reduction. The suggested reasons for these reduced stresses are mainly the exceptional mechanical properties of Graphene and its derivatives with lower mass densities, which enables them to be embedded in composites without changing the overall mass. Parallel direction of GNPs showed improved results, which could be due to the existing geometrical arrangement of the applied forces and fracture location. It is suggested that, GNPs in parallel direction acted as fixed beam support between the mandibles and thereby reducing the stress distribution in the plate and absorbing major part of the stress along their own layers. Since, GNPs exhibit higher Young's modulus and tensile strength in comparison to Titanium alloy, therefore, lower stresses are transferred to the plate increasing its resistance to failure.

Further, wider studies could be undertaken based on this geometrical arrangement by varying the depth, size and weight of GNPs. Since, it has been observed that mechanical properties of the plate remain unaffected by the location of GNPs, it can assist manufacturing of plate materials whereas add on methods to manipulate filler locations are complex. In addition, since the mass alteration due to GNPs remained insignificant while stresses on the plate varied significantly, more designs and simulations could be conducted with an additional reduction of the size and weight of the plates. Presence of GNPs at the front surface of the plate can facilitate fabrication of the composite plate material, so extensive dispersed embedment of fillers across multiple layers may not be required for strength improvements. Surface interactions and functionalization during plate fabrication with GNPs can produce similar plates with improved mechanical properties. Ultimately the reduced weight and thickness of such plates would benefit both patients and surgeons during surgery and recovery.

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