Bilinear elastic property of the periodontal ligament for simulation using a finite element mandible model

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This study aimed to introduce a procedure for determining the bilinear elastic moduli (E1 and E2) of the periodontal ligament for a mathematical tooth model to analyse stress in the mandible. The bone and tooth morphology were scanned from a dry skull and an extracted intact tooth, respectively, and reconstructed in a three-dimensional finite element model. The model showed good agreement with previously reported *in vivo* premolar movement when an E1 for the first phase tooth movement of 0.05 MPa and an E2 for the second phase of 8.0 MPa with ε_{12} of 0.075 were adopted. The mandible model analysis indicated that a remarkably high maximum compressive stress in the cervical cortical bone and the tensile stress in areas of masticatory muscle attachment were found. Future stress analyses using a jaw model may follow the process of determination of bilinear moduli to enhance accurate simulation with less calculation time.

Keywords: Finite element analysis, Elastic modulus, Mandibular bone

INTRODUCTION

The effect of masticatory forces on the supporting mandible is not sufficiently understood in terms of stress and strain. To determine the influence of masticatory forces on potential risks of damage in the oral tissues, the stress distributions created in the oral structures under function must be determined¹. The three-dimensional finite element (FE) method has been used to estimate the stress distribution within soft and hard tissues². In such mathematical models, tooth movement is ideally represented as a nonlinear behaviour, because the relationship between applied force and tooth displacement is expressed by a non-linear curve rather than by a straight line. According to a classic paper from the 1950s³, the incisor tooth was largely displaced during a small horizontal force up to 1 N, though the increment of the displacement was very small at a force above 100 N, resulting in the conclusion that this displacement was a 2-phase movement.

Application of the non-linear material properties of the periodontal ligament (PDL) to simulate tooth movement allowed accurate prediction of stress in periodontal tissues⁴⁻⁶. However, because non-linear analysis requires a large number of load steps compared with linear structural analysis, the non-linear solutions in a tooth model usually result in a tremendous computer running time. To overcome the disadvantages of both linear and non-linear analyses, an alternative methodology using 2 moduli for approximation of the non-linear curve was advocated⁷. Measurements of the

load-displacement relationship of teeth in rats⁴ and pigs⁸ were approximated by bilinear models. A decision process of the bilinear moduli should be conducted for each model, usually by the inverse problem approach so that each model accurately simulates the load-displacement relationship of a tooth. However, a method to determine the bilinear elastic moduli is not established.

In this study, a three-dimensional FE model was created to reproduce the load-displacement of the mandibular second premolar. The aim of the study was to introduce a procedure for determining bilinear elastic moduli, and to analyse the principal stress distribution in the supporting mandibular bone under the simulated occlusal bite force generated by the masticatory muscles.

MATERIALS AND METHODS

A finite element model

The model consisted of the mandibular right second premolar, the periodontal ligament (PDL), and the cancellous and cortical bone. The outline morphology of the bone and the tooth were scanned from a dry skull and an extracted intact tooth, respectively (Figs. 1a and b). For this purpose, optical scanner ATOS was used (ATOS Standard 3D; GOM mbH, Braunschweig, Germany). In this specific case, the device was calibrated for the camera and projector lenses focal length of 35 mm and 17 mm, respectively. The accuracy of the device is about 0.1 mm. The tooth had a crown length, from the occlusal cusp to the cement-enamel junction, of 8.1 mm and a root length, from the cement-enamel junction to the root apex, of 13.4 mm. The morphological data were reconstructed in a three-dimensional solid volume in the

CAD program (Rhinoceros version 3.0; Robert McNeel and Associates) and in the preprocessor of the FE program (ANSYS 11.0; ANSYS Inc., Canonsburg, PA, USA) in the following way: The data in STL-format created by the ATOS were exported into the Rhinoceros. The reconstruction of the individual parts was carried out and afterwards exported through IGES-format into the Ansys for the final arrangement of the model. The position of the tooth model in the mandible was determined based on the typical radiographic view seen in the Caucasian adults of healthy periodontal condition. A 0.25 mm-thick homogeneous layer of the PDL was attached to the root surface. The bone was modelled as a cancellous core surrounded by the cortical bone with an approximate thickness between 0.2 mm and 2.5 mm, depending on the location. The smallest value was used for the thin cortical bone layer around the tooth socket. The value of 2.5 mm was used for the rest of the model since it is a typical thickness in mandible^{9,10}. The cortical bone of the whole mandible model was meshed by a 4-node triangular shell element (cortical bone in general; free mesh) and an 8-node quadrilateral shell element (lamina dura; mapped mesh). The cancellous bone was meshed by a 10-node tetrahedral solid element (free mesh). Enamel, dentin, and periodontium were meshed by a 20-node hexagonal solid element (mapped mesh). The decision to exclude the pulp chamber and the dentine structure from the model was based on the preliminary test in addition to the previous study⁵, in which the effects of these factors were found to be negligible upon the comparative evaluations of the stress distributions in the periodontal structures and the supporting bone. The model consisted of 151,578 elements. The element edge length on the surface boundaries for the tooth was 0.25–0.50 mm and was 2 mm for the bone.

To determine the bilinear moduli of the PDL, a segmented bone model was constructed by retrieving a block from the right premolar vicinity of the mandible model (Fig. 1c). The maximum bucco-lingual width, mesial-distal length, and vertical height of the segment model were 18 mm, 20 mm, and 25 mm, respectively. The model was meshed by structurally solid elements defined by 20 nodes having 3 degrees of freedom in tetrahedral bodies consisting of 61,266 elements. The mesh size and arrangement were determined by preliminary convergence tests for consistency of the maximum principal stress in the cortical bone¹¹.

Material Properties

The tooth and the bone structures were assumed as homogeneous, isotropic, and linear elastic materials. The modulus of elasticity (E) and Poisson's ratio (μ) of each tissue were referred from previous studies^{7,12–16} and are shown in Table 1. Nine combination groups of different bilinear elastic moduli of the PDL for each phase ($E1$ and $E2$) were assumed for comparison (M1–M9, Table 2). Values of $E1$ and $E2$ which were to be investigated were proposed on the basis of earlier papers^{7,8,12,13}. In these papers $E1$ and $E2$ ranged from 0.05 MPa to 0.15 MPa and from 0.18 MPa to 5.24 MPa,

Fig. 1 Three-dimensional finite element models. a: The mandibular bone reconstructed from a dry skull. The segmented area is shown in red. b: Meshed second premolar tooth model without (left) and with (right) the periodontal ligament. c: Meshed segment model with the cortical (red) and cancellous bone (purple) structures.

Table 1 The modulus of elasticity (E) and Poisson's ratio (μ) of the tooth structures and the bone. Data were referred from previous studies^{7,10–14}.

	E (MPa)	μ
Cortical bone	16,000	0.3
Cancellous bone	690	0.3
Dentin	19,000	0.3
Enamel	84,000	0.3

Table 2 Nine combination groups of different elastic moduli of the PDL for the first and second phases ($E1$ and $E2$) with strain ranges below and over $\epsilon_{12}=0.075$, respectively.

	$E1$ (MPa)	$E2$ (MPa)
M1	0.05	0.1
M2	0.05	0.5
M3	0.05	0.9
M4	0.10	0.1
M5	0.10	0.5
M6	0.10	0.9
M7	0.05	2.5
M8	0.05	5.0
M9	0.05	10.0

respectively. The proposed values were intended to cover evenly already known values and also to investigate values which were not taken into account so far. The values of E1 and E2 were used in strain ranges below and over $\varepsilon_{12}=0.075^{(7)}$, respectively^{17,18}. For the finite element method, a bilinear material was modeled using “multilinear elastic model option” which was included in the Ansys material library. The bilinear properties were input into the program as the stress-strain relationship of the PDL represented by two moduli, or two lines in the X-Y coordinate. In detail, the program requires for the multilinear material curve “n” pairs of values (for the constant temperature): stress 1 – strain 1, stress 2–strain 2, up to stress n–strain n. As for the bilinear material ($n=2$), these stress and strain values were calculated from the characteristics E1, E2 and ε_{12} . Therefore, the nonlinear relationship between the stress and strain for the PDL was simply composed of the two linear parts. For all the bilinear properties tested, the displacements at the top of the buccal cusp by using the segment model with these bilinear properties were plotted as a function of the output vertical forces (Fig. 2a) and were analysed by comparing with previously reported experimental data¹⁹. As the boundary condition, zero displacement was prescribed for the nodes of the lower surface of the cortical bone in all directions. The bilinear material was modeled by using a pre-defined ‘multilinear model’ which is part of Ansys material library. E1 and E2 were investigated by running consecutive solutions governed by macros written in Ansys Parametric Design Language (APDL).

Loading and boundary conditions

The bilinear property obtained by the segment model was used in the calculations of the mandible model (Fig. 2b). The masticatory forces were assumed at the areas of the masticatory muscle attachments on the bone surface for *M. masseter* (F_{MR} and F_{ML} on the right and left sides, respectively, Fig. 2b), *M. temporalis*, (F_{TR} and F_{TL}) and *M. pterygoideus medialis* (F_{PR} and F_{PL}). The upper surfaces of the right and left condyles were fixed in all directions. A preliminary analysis was carried out to obtain optimal force magnitudes so that the resultant occlusal force in the second premolar constraint was 190 N¹⁸, which was applied in the vertical direction to the tooth. The preliminary analysis was based on the model of the same shape and material properties. The only difference was that all active muscles were modelled using finite ‘link’ element (with the tension-only option). The stiffness of the active-muscle elements is supposed to be much higher than the other materials, e.g. Young’s modulus of more than 100,000 MPa. ‘Free’ ends of the muscles were constrained in all directions. Nodes on the bilateral condyles were fixed in all direction as well. The inner force resultants in the muscles were determined on the basis of the principles of equilibrium: 54 N for the left *M. masseter*, 116 N for the right *M. masseter*, 4 N for the left *M. temporalis*, 85 N for the right *M. temporalis*, 78 N for the left *M. pterygoideus medialis*, and 115 N for the right *M. pterygoideus medialis*. Obtained values were

Fig. 2 Loading and boundary conditions. a: Buccolingual cross section view of the segment model. The vertical loading (F) and the resultant displacement (Δ) are indicated with the location of fixation (triangles). b: The mandible model. Red arrows indicate the location and direction of the load generated by each muscle (see text for detail).

similar in order of magnitude to those reported previously²¹. Note that the right side of the mandible is the biting side and the left side is the balancing side. In the ‘main’ analysis, the determined masticatory forces were applied and the boundary condition was modified: The occlusal force of 190 N used in the preliminary analysis was removed and instead the zero displacement was prescribed for nodes on the occlusal surface of the tooth in the vertical direction. The principal stress distribution in the model was calculated under the loading condition.

Additional calculations were performed to evaluate the maximum principal strain of the mandibular bone, with decreased masticatory forces, which were determined by multiplying the original forces by scale factors of 0.1, 0.05, 0.01 and 0.005. For control, the maximum principal strain at the same node was obtained using a linear elastic modulus of 8.0 MPa. These were conducted to evaluate the influence of the bilinear property on the nonlinear characteristics of the maximum principal strain in the mandible model. All calculations were conducted on a hardware platform with Intel® Core™ i7 CPU 950/3.07GHz RAM 12.0 GB and the operation system Windows 7. The approximate calculation time for the segmented and the mandible models were 10 min and 20 min, respectively.

RESULTS

The vertical displacement of the tooth cusp of the segmented model as a function of the load up to 2 N is shown with experimental data from a previous report¹⁹ in Fig. 3. A higher modulus of 0.1 MPa for E1 was entered into M4, M5, and M6 that was not suited for a rapid increment of the initial tooth movement. Figure 4 shows

Fig. 3 The load-displacement relationship of the segment model for the small load range. The reported experimental data were shown by the dotted curve¹⁹⁾.

Fig. 4 The load-displacement relationship of the segment model for a load up to 200 N. The dotted horizontal line represents the reported vertical intrusion of 0.12 mm²²⁾.

the load-displacement relationship of the rest of the models (M1 to M2, and M7 to M9) under high load up to 200 N. The dotted horizontal line represents a presumed vertical intrusion of 0.12 mm for a typical healthy mandibular premolar tooth under the maximum clenching effort²²⁾. The M1 to M3 showed considerably higher displacement compared with the reference intrusion due to their lower E2 values, thus not considered for further selecting process. Plots of the vertical displacement as a function of E2 are shown in Fig. 5. The approximated relationship can be expressed by the curve $y=0.4994x^{-0.742}$, with a coefficient of correlation (R^2) of 0.9912, where x is E2 and y is vertical displacement. Accordingly, the reported displacement of 0.12 was obtained by an x value of approximately 8 MPa. The result showed that the movement of the segment model agreed with previously reported *in vivo* premolar movement when an E1 for the first phase tooth movement of 0.05 MPa and an E2 for the second phase of 8.0 MPa were adopted.

Distributions of the maximum first principal stress (tensile stress) in the cortical bone are shown in Fig. 6a. Concentration of the tensile stress up to 10.3 MPa was found in some regions of the masticatory muscle attachment and on the alveolar cancellous bone. Increased tensile stress was apparent in the oblique line of the mandible, mainly on the right side. A considerable increase in tensile stress was also found in the region near the bottom of the tooth socket. Figure 6b shows the distributions of the minimum third principal stress (maximum compressive stress) in the mandible. Remarkably high values were found in the neighbourhood of cervical areas, close to the contact with a model tooth and in the area towards the angle of the mandible. An increased pressure load was also apparent on the back side, close to the ramus of the mandible. Concentration of compressive stress was found in the cancellous bone

Fig. 5 Plotted vertical displacement under the load of 200 N as a function of the E2 (E1=0.05). The approximated relation was represented by the dotted curve $y=0.4994x^{-0.742}$ with a coefficient of correlation (R^2) of 0.9912. The horizontal line indicates the reported vertical displacement of 0.12 mm²²⁾.

near the apex of the tooth. A series of cross sections in mesiodistal planes are presented for the maximum compressive stress distributions of the cancellous bone (Fig. 7).

The maximum principal strain of the alveolar cancellous bone was shown at a site near the tooth socket. The maximum principal strain as a function of the load up to 20 N (Fig. 8) was graphed for both the bilinear and the linear properties. For the bilinear model, the maximum principal strain increased non-linearly with the increase of the load, while the strain-load relationship was linear proportional for the linear model.

a First Principal (tensile) stress **b Third Principal (compressive) stress**

Fig. 6 Principal stress contour graphics of the mandible model. The first principal tensile stress (a) and the third principal compressive stress (b) distributions are shown by the whole mandible (left) and of the cross-sectioned distal half at the premolar (right).

Fig. 7 The third principal (compressive) stress distributions of the cancellous bone on a series of cross sections by mesial-distal planes in the second premolar vicinity.

Fig. 8 The relationship of the load and the maximum principal strain of the cancellous bone near the root apex. Solid line indicates the calculated data by the bilinear property ($E_1=0.05$ MPa, $E_2=8$ MPa), while dotted line represents the result of the linear analysis ($E=8$ MPa).

As a result, the magnitude of the maximum strain of the mandible model incorporating the linear property was not consistent with that incorporating the bilinear model.

DISCUSSION

Tooth movement as a load-displacement relationship is typically represented by a 2-phase movement. The first phase corresponds to an elastic range of periodontal ligaments, and the second phase corresponds to deformation of alveolar bone with a stretch of the PDLs on the tensile side³. Therefore, the agreement of simulation-based tooth movement with *in vivo* data should be assessed in both the first and second phases of tooth movement. The initial process was conducted for a load less than 2 N. Most available experimental data of the stress-strain relationships of the human PDL were obtained in the range of relatively small tooth movements, presumably because of the limitations of high load applications on human subjects. The nonlinear exponential behaviour of tooth displacement in human subjects has therefore been indicated by cases of relatively low loads, and typically, moduli from 0.12 MPa to 0.96 MPa were obtained under loads between 0 N and 2.0 N²³.

The congruency between numerical force/deflection curves by various bilinear parameters and experimental curves were assessed and obtained from the rat mandibular first molars⁴ and from multi-rooted minipig teeth⁸, and an E_2 of 0.60 MPa and 0.18 MPa⁸, respectively, were derived from these studies. These considerably low values in comparison with those obtained in the current study ($E_2=8.0$ MPa) were

attributed to the fact that the applied loads in these studies were very low, from 0.15 N to 6 N. Models with lower E_2 are likely to create an unrealistically large tooth displacement under a simulated large bite force such as 200 N (see M1–M3 in Figs. 4 and 5). However, in studies using bovine molar teeth²⁴ and teeth from human cadavers²³, the modulus was calculated on the basis of stress-strain plots with more than 0.4% strain that should be created by a large bite force. The former study²³ reported that the elastic modulus of PDL ranged between 4 MPa and 8 MPa, which is in agreement with the result obtained in this study.

To assume the linear elasticity as a constant material property of the periodontal ligament may lead to an erroneous solution in the finite element method. This was clearly shown by the result that the maximum strain of the mandible was not precisely obtained in the linear property model throughout the large load range (Figs. 8). If an intermediate constant is used as the elastic modulus of PDL, the tooth displacement would be too small under a relatively low bite force, and too high under a high load. The use of the linear static model is suitable only for expression of deformation of a tooth under a specific range of applied load. To express this nonlinear behavior of PDL, an elastic property in the form of a stress-strain curve may be input into an FEM program. The load applied to a model is subdivided into a series of multiple load increments. In each step, the program performs a linear solution and checks for convergence. If the convergence criteria are not satisfied, the load vector is reevaluated, and a new solution is obtained. This iterative procedure continues until the problem converges. Thus, the nonlinear solutions on a three-dimensional tooth model often result in an unstable solution or calculation error on the computer.

A bilinear elastic property used in a model that was capable of predicting accurate movements often fails to predict accuracy in models with different morphology and dimensions. The use of bilinear moduli as a definitive property for a future mathematical model with a different morphology is therefore questionable. The methodology to determine the bilinear moduli of the PDL in this study was simple and reasonably applicable for models with similar objectives; therefore, we propose that future studies should follow this procedure to determine the property of each new model.

The stress analyses based on simulation in a jaw is a promising tool for risk assessment of damage and degradation of the bone and soft tissues. It is useful for the preclinical phase evaluation of implant placement and orthodontic treatment²⁵. Such a structural analysis allows determination of deformations, strains, and stresses that are caused by applied force, pressure, and thermal change. This method helps tremendously to indicate the distribution of stresses in biomaterials and human tissue that cannot be measured *in vivo*. On the basis of the stress contour graphics of sectioned tooth, it is clear that the maximum tensile stress is located close to the tooth apex, where stress value is affected by intrusion of the tooth and also by the limited thickness of

cortical bone. The maximum stress of the model of this study did not exceed 3 MPa, and this finding is consistent with the reported contact pressures or principal stresses in human joint areas such as the hip, knee, or elbow, which are usually similar to the maximum stress in the cancellous bone surrounding a tooth^{26,27}. Further studies are needed to enhance the methodological development of bone resorption and necrosis prediction by evaluating the maximum tensile/compression stresses calculated in mechanical simulation using the jaw models.

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