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Numerical simulation of the biomechanical behaviour of multi-rooted teeth

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SUMMARY The elastic properties of the periodontal ligament (PDL) in eight multi-rooted teeth were examined in a combined experimental and numerical study in six minipigs. The initial tooth movement of the mandibular primary molars surrounded by the periodontium was registered three-dimensionally (3D) in an optomechanical measuring system. The dissections were then embedded in resin and cut in transverse sections. Based on these sections, 3D finite element (FE) models were constructed and numerically loaded with the same force systems as used in the experiment.

The material behaviour of the PDL registered in the experiment was non-linear and could be approximated with a bilinear parameter set consisting of two Young's moduli, E_1 and E_2, and one ultimate strain, ε_{12}, separating both elastic regimes. When a deficient congruence existed between the experimental and numerical force/deflection curves the material parameters were varied to obtain a satisfactory congruence. The material behaviour determined for these specimens delivered mean values of E_1 = 0.05 MPa, E_2 = 0.18 MPa and ε_{12} = 6.4 per cent for the elastic behaviour of the multi-rooted minipig teeth. There was no significant difference in the material parameters determined for specimens with two, four or six roots. The results were in close agreement with the material parameters of the PDL, determined in previous investigations of single-rooted human and pig teeth.

Introduction

Orthodontic tooth movements can be induced by different force systems. According to the level and duration of the applied force, different types of tooth movement can be produced. Initial tooth displacement is caused by short-term loading, associated with an intra-alveolar root deflection, producing local stress and strain distributions in the desmodont. Under these preconditions, the deformation of the alveolar bone is reversible and of very low magnitude. If the tooth deflection is maintained for a very long time, the stresses and strains in the periodontal ligament (PDL) will trigger bone remodelling processes that result in a permanent change in tooth position.

The degree of initial tooth displacement is related to the material properties of the different structures, such as the tooth, the bone and, in particular, the PDL. Based upon the high elasticity of the PDL compared with bone and tooth, it is especially the PDL that determines the extent of tooth movement (Nägerl and Kubein-Meesenburg, 1993; Bourauel *et al.*, 1999). The elastic properties of the PDL, published in former studies, show a broad variation. The values for Young's modulus, stated in literature, differ by a factor of 10^5 (Kawarizadeh *et al.*, 2003b). This variation in the results can be attributed to the complex structure of the PDL, and the different modelling assumptions for the mechanical behaviour resulting from this. Further reasons are differing study designs, especially with respect to experimentation.

The aim of this study was to investigate the elastic properties of the PDL by analysing initial tooth displacements of minipig teeth with two, four, five, and six roots. The elastic properties of the PDL, which have already been determined for single-rooted teeth and for rat molar specimens, employing the same method, should be verified on multi-rooted porcine teeth. A combined experimental and numerical method was used for this study. The numerical part of the investigation was performed using the finite element (FE) method, which is a method to subdivide a geometrically complex structure into a finite number of simple geometric elements. These are interconnected in so-called nodes, thus building up the FE mesh. Specific material parameters are assigned to each element of the mesh.

Most FE studies in orthodontics have been performed with respect to the behaviour of single-rooted teeth. Until now, only a few have dealt with the simulation of the behaviour of multi-rooted teeth (Katona *et al.*, 1995; Melsen, 2001; Kawarizadeh, 2002; Cattaneo *et al.*, 2003; Kawarizadeh *et al.*, 2003a, b).

Material and methods

The initial tooth movement was measured on a total of eight multi-rooted primary molars of 3–12-month-old minipigs. This race of pig was chosen as its teeth closely resemble human teeth in terms of their development, size, and physiology (Douglas, 1972). Pigs are particularly suitable as experimental animals for various reasons (Weaver *et al.*, 1962): just like humans they are omnivores with a grinding chewing movement and also go through a phase of primary teeth with a development similar to that of human teeth.

The pigs were used in an animal experimental study at the Department of Experimental Surgery of the University of Bonn, which was ethically approved. After finalization of the animal experiments, the mandibular jaw sections were used for the present research. The teeth were removed from the lower jaw, together with the surrounding alveolar bone, immediately following sacrifice. No root resorption was observed radiographically.

Figure 1 reflects the experimental approach described below in a summary form. The jaw segments that had been removed were placed in envelopes soaked with 0.9 per cent NaCl. The lower portion of each bone segment was placed in a metal carrier and embedded in resin (Technovit 4004®, Kulzer, Germany). Occlusally a screw pin was attached to the crown, which served to attach an aluminium cube with three laser diodes arranged orthogonally to one another, and thus corresponding to a Cartesian co-ordinate system. The measurements were carried out in an optoelectronic measurement set-up, the mobility measurement system (Hinterkausen *et al.*, 1998), which comprised a mechanical section for the application of the force/torque systems and an optoelectronic component for the non-invasive measurement of tooth displacement. The individual components of the experimental set-up are outlined in Figure 2a. The preparation embedded in resin was provided with a hollow of 1 mm buccally, 2 mm beneath the incisal edge on the centre of the crown and in the experimental set-up positioned at a 90 degree angle to the power arm of the level of the force/torque sensor (Figure 2b).

Forces of up to a maximum value of 6 N were applied gradually through the hollow on the tooth via the force/torque sensor. The tooth displacement led to a corresponding displacement of the laser diodes attached to the crown, which were recorded three-dimensionally (3D) by optoelectronic planar sensors (position sensitive detectors) and transmitted to a control computer. A waiting period of 40 seconds had to be kept between each load step and the subsequent measurement of the force/displacement behaviour in order to minimize the influence of hydrodynamic flow processes in the PDL. Force/displacement diagrams could be produced based on the values measured. Following measurement, which took 1.5–2 hours,

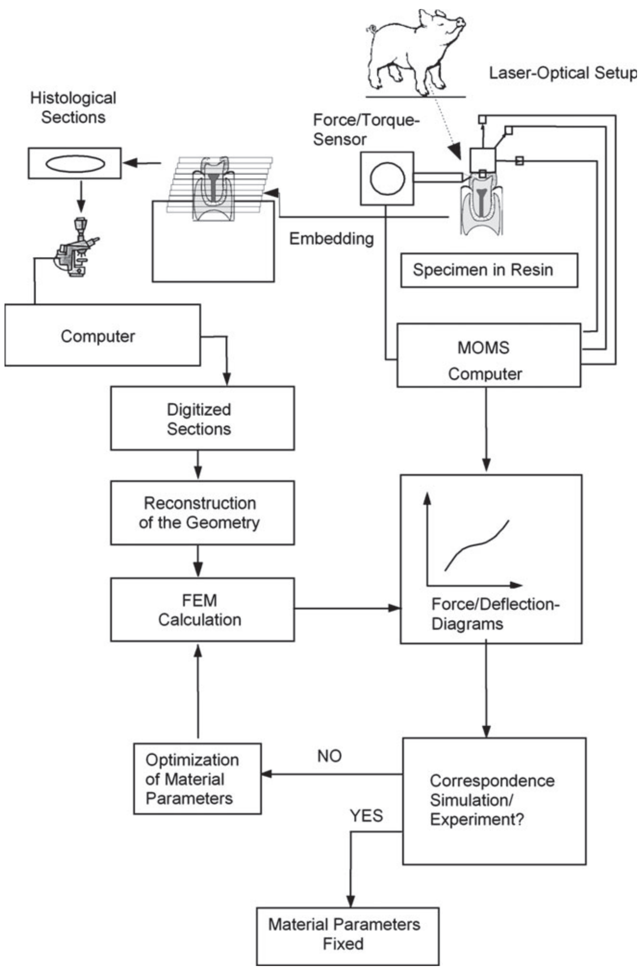

Figure 1 Schematic diagram of the basic principles of the study.

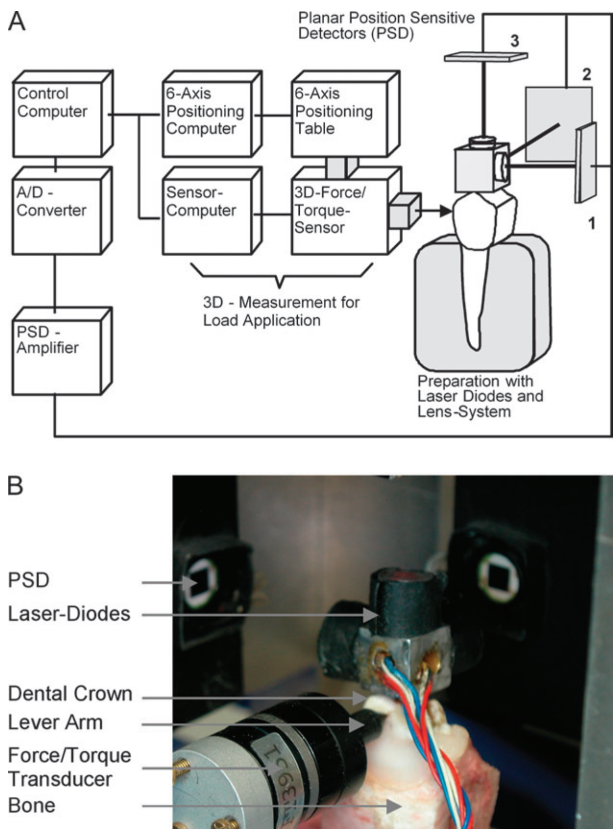

Figure 2 (A) Schematic diagram of the components of the experimental set-up. (B) The set-up of an integrated specimen adjusted such that the laser diodes point to the surfaces of the planar sensors.

the tooth with surrounding tissue including two brass bits arranged parallel to one another was completely occlusally and lingually embedded in resin. The preparation was then cut into parallel sections that had an average thickness of 1.25 mm with a precision inner diameter saw (Microtom 1600, Leitz, Wetzlar, Germany). A good level of contrast between the tooth hard substance, the PDL and the bone could be produced by sprinkling each section with toluidine blue solution (Toluidine blue O, Chroma companies, 0.1 per cent distilled in water). The sections were enlarged under a microscope and digitally recorded with a scanner camera.

The Computer-aided Generator for Orthodontic Geometries (CAGOG) program (Haase, 1996) made it possible to geometrically reconstruct the respective preparation. The individual sections were assigned to one another based on the brass bits and the anatomy of the tooth, screw pin, PDL and bones during each cut was reconstructed by means of FE meshes (Figure 3). The FE program COSMOS/M 2.8 (Structural Research and Analysis Corp., Los Angeles, California, USA) semi-automatically generated a 3D FE model (Figure 4) on the basis of the individual meshes. This FE model was now numerically loaded with the same force as the corresponding tooth during the experiment. The Young's moduli used for bone and tooth structures were taken from early experiments by Spears *et al.* (1993) (Table 1). Initially, standard parameters were used for the elasticity property of the PDL and these were then varied by means of a comparison of the measured and calculated tooth displacement until such time as the calculated tooth displacement was as close as possible to the measured displacement. In general, a good correlation of experimental and numerical results was reached after five to 10 runs of calculations with different material parameters of the PDL. Convergence in the individual non-linear calculations was highly dependent on mesh density, force level and overall geometry of the model. Thus, the automatic stepping option of the COSMOS solver was used. Typical convergence cycles were between three and 25 iterations for each individual time step.

In an earlier study, a sensitivity analysis was performed with all relevant parameters, such as mesh density, element type, number of elements, Young's modulus and Poisson's ratio of the PDL, to determine the influence of the respective value on the calculated tooth deflection (Vollmer *et al.*, 2000). These investigations showed that with the assumption of homogeneous and isotropic material behaviour for all relevant structures, the simulation of orthodontic force application presupposes a Poisson's ratio of 0.3. Higher values would reduce tooth deflections significantly and could only reproduce the experimental tooth deflection in time-dependent calculations, simulating hydrodynamic phenomena, which was not intended in this study.

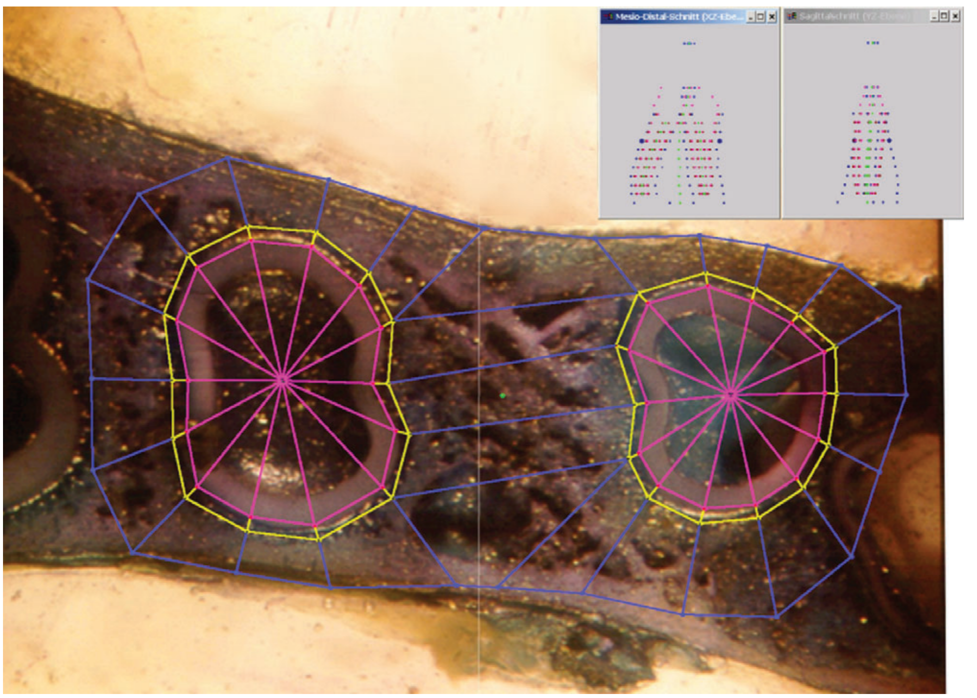

Figure 3 Histological section through the root region of a two-rooted primary pig molar. The different structures are identified by polygons, representing a planar finite element mesh (green: centre of the tooth/roots; red: outer surface of enamel/cementum; yellow: margin of alveolus; blue: outer surface of alveolar bone). The figures in the small boxes represent a preview of the mesio-distal and sagittal cuts.

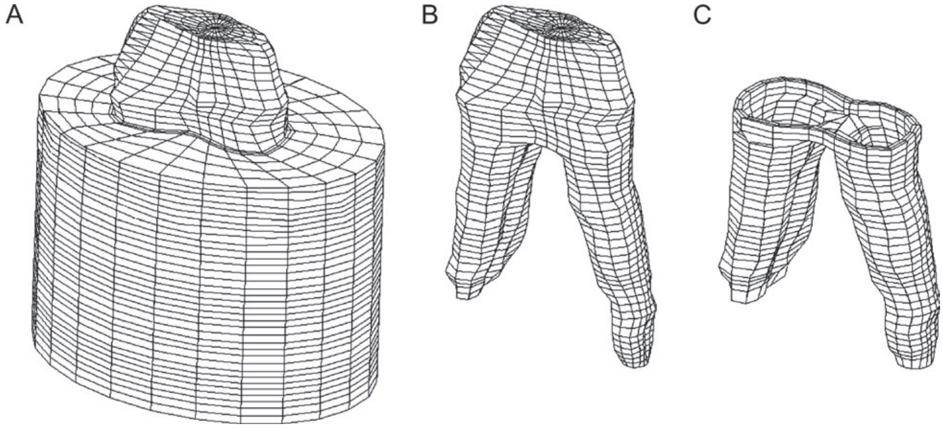

Figure 4 Three-dimensional finite element mesh of a three-rooted lower porcine molar. (A) Tooth with bone and ligament, (B) tooth and (C) periodontal ligament.

Table 1 Material parameters of tooth, bone and periodontal ligament used in this study. Values for tooth and bone are taken from Spears *et al.* (1993).

Material	Young's modulus (MPa)	Poisson's ratio μ
Tooth	20 000	0.30
Bone	2000	0.30
Periodontal ligament	Bilinear	0.30

FE models can be produced with a maximum of two roots with the CAGOG software. Accordingly, in the four-rooted teeth, the two mesial roots had to be joined together, as well as the two distal roots, for the modelling of the pig teeth used in the present investigation. In teeth with five roots, the mesial roots were joined with the centrally located root and the two distal roots were combined. In six-rooted teeth, three roots were combined. The differentiation of the tooth into enamel and dentine or a subdivision of the bone into trabecular and cortical substance would only have had a 0.1 per cent influence on the tooth displacement calculated (Haase, 1996). For this reason, the tooth and the bone were modelled isotropically, which led to a simplification of the calculations.

Results

Material parameters

As demonstrated in previous experiments (Siebers, 1999; Poppe *et al.*, 2002), the non-linear force/displacement behaviour could be described in a bilinear manner (Figure 5) by means of two straight lines, i.e. by using two different Young's moduli. The gradient of the first straight line corresponds to the first Young's modulus and the gradient of the second straight line to the second. The first calculation was carried out with standard parameters. During previous tests on human teeth, the calculated results achieved a

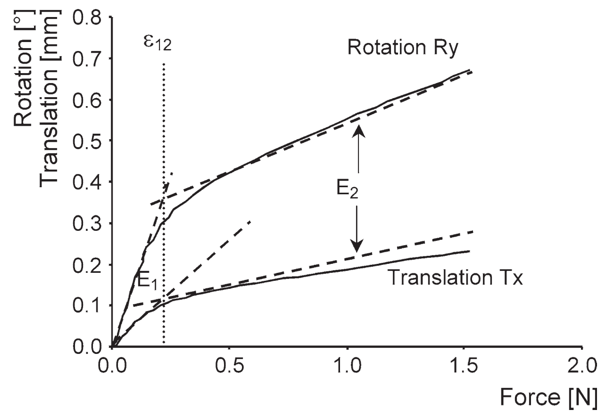

Figure 5 Approximation of the calculated curve to the measured force/deflection behaviour assuming a bilinear material behaviour of the periodontal ligament. The ultimate strain, ε_{12}, is the limit of the region with a low Young's modulus E_1 and the transition to a higher stiffness with modulus E_2.

good level of similarity with the measured result (Vollmer, 1998): $E_1 = 0.05$; $E_2 = 0.22$; $\varepsilon_{12} = 7.5$ per cent; $\mu = 0.3$. The ultimate strain, ε_{12}, characterizes the point of intersection of the first and second straight lines. The calculated and measured translation and rotation movement in the main displacement direction were set against one another. The Young's moduli of the PDL and the ultimate strain were varied until the calculated force/displacement curve tallied as accurately as possible with the measured displacement. The last set of parameters used, by means of which a good level of consistency of the measured and the calculated force/displacement curve was achieved, was deemed as being the final result (Figure 6). The averages of E_1, E_2 and the ultimate strain, ε_{12}, were calculated from the material parameters determined for all the preparations (Table 2).

The extent of the element displacement under force was displayed in colour on the FE model following the completion of the calculations. Elements that were greatly

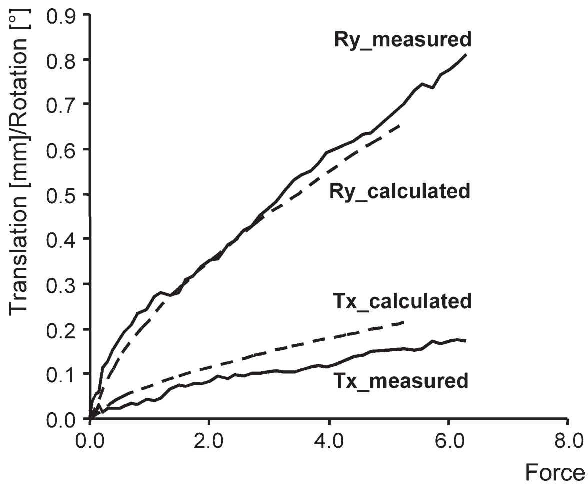

Figure 6 Calculated force/deflection curve after variation of the material parameters to reach an optimum approximation to the measured translation (Tx) and rotation (Ry).

Table 2 Mean and standard deviation of Young's moduli of the periodontal ligament, determined in the present study.

Material parameter	Mean	Standard deviation
E_1 (MPa)	0.05	0.02
E_2 (MPa)	0.18	0.12
ε_{12} (%)	6.4	1.2

displaced were shown in red, while those that were minimally displaced were shown in dark blue (Figure 7).

Dependency of the results upon the number of roots

The grouping of several roots to form a total of two roots during the preparation of the FE models necessarily led to geometric inaccuracies. One aspect to consider was the extent this geometric simplification influenced the simulated tooth movement and thus also affected the determination of the material parameters. The average values of the parameters used for both tooth groups were individually determined to compare the material parameters obtained for the two-, four- and six-rooted primary molars (Table 3). The E_1 values of elasticity and the ultimate strains only revealed very slight differences; the E_2 values were the same. On the basis of these results, a geometric simplification of four-rooted teeth does not lead to significant deviations from the standard set of parameters during the determination of the material parameters.

Discussion

The material behaviour of the PDL has been investigated in several studies. A large amount of fluctuation is conspicuous when comparing the data with respect to elastic properties. This is due, on the one hand, to the use of differing experimental

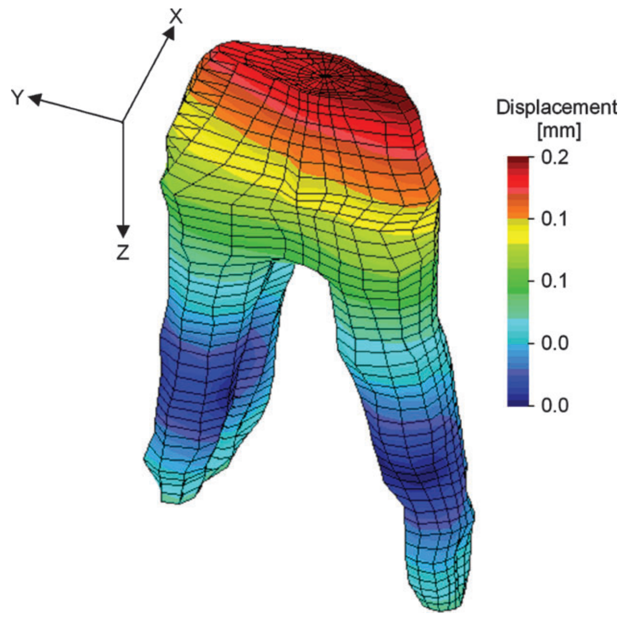

Figure 7 Finite element model of a multi-rooted pig primary molar, displaying a colour-coded representation of the calculated tooth deflection.

Table 3 Mean and standard deviation of Young's moduli of pig premolars with two and four to six roots.

	Two-rooted premolars ($n = 4$)	Four- to six-rooted premolars ($n = 4$)
E_1 (MPa)	0.05 (0.01)	0.04 (0.01)
E_2 (MPa)	0.18 (0.14)	0.18 (0.11)
ε_{12} (%)	6.4 (1.6)	6.3 (0.58)

methods and, on the other, to the complex structure of the PDL, which in some cases was greatly simplified or even not considered at all (Baeten, 1975; Dermaut *et al.*, 1986; Nägerl *et al.*, 1991). The elastic behaviour of the PDL has been described as being linear in the majority of studies. However, the description of elastic behaviour with just one Young's modulus is too imprecise, as the tooth displacement at the beginning of the force application is much greater due to the decurling of the wavy structure of the collagenous fibres, whereby only an extension of the fibre system is present until it is torn. In addition, fluid displacements within the PDL must be considered (Wills *et al.*, 1972).

The non-linear mechanical behaviour of the PDL has been proven in several investigations (Mühlemann and Zander, 1954; Christiansen and Burstone, 1969; Wills *et al.*, 1972; Daly *et al.*, 1974; Picton and Wills, 1978; Tanne *et al.*, 1995; Siebers, 1999; Yoshida *et al.*, 2001; Toms *et al.*, 2002). In this study, the computational approximation of the mechanical behaviour of the PDL was carried out with a set of parameters that consisted of two differing Young's moduli and an ultimate strain. This approach has been used previously (Vollmer, 1998; Siebers, 1999; Kawarizadeh, 2002) and allows a good level of computational approximation with the non-linear force/displacement behaviour of the tooth investigated.

A further study, which took into account the non-linear behaviour of the PDL and described it based on several Young's moduli, has been carried out (Toms and Eberhardt, 2003). They investigated the influence of geometry and material properties of the PDL on tooth movement. A two-dimensional (2D) FE model was generated based on sections of a lower human premolar, in which the PDL was represented once in its natural form and subsequently with an even level of thickness so that two differing models were produced. An extrusion and a tilting movement were simulated on both models. First, linear material properties and, second, non-linear material behaviour of the PDL were assumed. Subsequently, stresses were determined arising during movement of the tooth's root in the periodontium. The stress values produced by the linear FE models differed considerably from those of the non-linear models. The stress values produced with non-linear material behaviour of the PDL were 2.4 times higher than the values calculated with the linear model. In the case of the non-linear model, the maximum stress levels were in the apical section, whereas in the linear model they were at the level of the central root. The non-linear mechanical behaviour of the PDL was not carried out in a bilinear manner during the FE calculations but was instead based on several Young's moduli and ultimate strains. The force/displacement behaviour of the FE model was compared with the experimentally measured force/displacement behaviour in order to verify the non-linear mechanical properties. In contrast to the experimental approach in the present study, the force was not applied to the tooth as a whole, but to the tooth hard substance of the sections. However, this approach must be viewed critically as the original structure of the PDL was damaged by severance of the fibres, which can lead to changes in mechanical behaviour. In addition, the validation of the material properties of the PDL was carried out by means of a comparison of the experimentally measured force/displacement values with the force/displacement values calculated on the basis of the 2D FE models. Set against this, the verification of the material parameters was achieved by comparing the measured data with 3D FE models.

Yoshida *et al.* (2001) carried out a study in which the elastic properties of the PDL were directly derived from measurements of tooth displacements on human cadavers. An upper central incisor was physically moved with a force of up to 2 N and the resulting tooth movement was measured with a magnet system while the force applied was increased. Young's modulus of the PDL was calculated from the force/displacement ratio for various different force areas (Table 4). These values indicated the non-linear elastic behaviour of the PDL. Young's moduli of the first and second force areas only marginally differed from the parameters determined in the present study ($E_1 = 0.05$ and $E_2 = 0.18$). In the following force areas, the values determined by Yoshida *et al.* (2001) correspond more closely to the E_2 module of rat molars ($E_2 = 0.60$) (Kawarizadeh, 2002). Andersen *et al.* (1991) investigated the force/displacement behaviour of human lower premolar specimens while subjected to very light forces. The measurements were carried out invasively by means of strain gauges. A corresponding FE model was generated based on sections and the elastic behaviour of the PDL was determined by comparison of the simulated and calculated tooth movements. A nearly linear mechanical behaviour was determined and a Young's modulus of $E = 0.07$ MPa was ascertained. This value is close to the E_1 modulus found in the present study and, thus, confirms the linear course of the force/displacement movement determined in the lower force region. In their calculations, Andersen *et al.* (1991) assumed a Poisson's ratio of $\mu = 0.49$, which practically equates to incompressibility of the PDL. However, due to the fact that only the first phase of the initial tooth movement was considered, where only very slight deformations of the PDL arise, this assumption was hardly significant with respect to the results.

Table 4 Young's modulus determined for different force levels up to a force of 2 N (Yoshida *et al.*, 2001).

Level of force (N)	0.0 – 0.5	0.5 – 1.0	1.0 – 1.5	1.5 – 2.0
Young's modulus (MPa)	0.12	0.25	0.44	0.69 – 0.96

Conclusions

The elastic properties of the PDL in this numerical and experimental study based on multi-rooted pig primary molars are within the range of the bilinear set of parameters already determined on single-rooted human and pig teeth. They are suitable for 3D numerical simulation of orthodontic tooth movement and thus may contribute towards an improved estimation of secondary tooth movements generated by orthodontic force systems.

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