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BIOMECHANICS OF PERIODONTAL LIGAMENT
SPECIFIC TO CLINICAL ORTHODONTICS

by

STEPHANIE ROSE TOMS

A DISSERTATION

Submitted to the graduate faculty of The University of Alabama at Birmingham,
in partial fulfillment of the requirements for the degree of
Doctor of Philosophy

BIRMINGHAM, ALABAMA

2002

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ABSTRACT OF DISSERTATION
GRADUATE SCHOOL, UNIVERSITY OF ALABAMA AT BIRMINGHAM

Degree Ph.D. Program Biomedical Engineering

Name of Candidate Stephanie Rose Toms

Committee Chair Alan W. Eberhardt

Title Biomechanics of Periodontal Ligament Specific to Clinical Orthodontics

The goal of this effort was to more fully quantify optimum forces for orthodontic loading by experimental testing of periodontal ligament (PDL) specimens from cadaveric premolars and applying these experimental data to finite element analysis (FEA) to study the stresses and strains in the PDL. This project was a first step in developing specific biomechanical data for correlation with existing and future clinical experiences of the PDL response to orthodontic loading. Laboratory testing of cadaveric specimens was performed, with an overall intent to quantify both the nonlinear and viscoelastic properties of this tissue.

The periodontal ligament was described mathematically by the quasi-linear viscoelasticity (QLV) model. The experimental data demonstrated that the theory accurately predicted peak stresses of the PDL during cyclic extrusive ramp loading. The findings support the use of QLV to characterize PDL stress-strain behavior for the many complex loading scenarios encountered in dentistry.

Material properties of the periodontal ligament were demonstrated to be nonlinear and anisotropic for specimens of tooth/ligament/bone. Low force magnitude stress-strain curves for specimens in both intrusion and extrusion displayed distinct linear and toe regions. Stiffness of the ligament was found to be higher for intrusion than extrusion, suggesting anisotropic material properties. The stress distribution in the periodontal

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ligament was complex and not constant along the root under conditions of intrusive and extrusive loading.

Two finite element (FE) models were made, one with a uniform PDL width and one with the anatomical varying width of a tested premolar. Linear and nonlinear material properties were assigned to the ligament in a parametric analysis. The FE predicted stresses in the PDL that were substantially different when comparing linear and nonlinear material properties of the ligament. The two-dimensional parametric study of a mandibular premolar subjected to tipping and extrusive orthodontic forces indicated that the incorporation of nonlinear material properties of the ligament resulted in substantially different predicted maximum principal and shear stresses. Of clinical interest is that the center of rotation moved away from the long axis of the tooth when nonlinear material properties were assigned to the PDL.

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DEDICATION

To my family and friends for providing

continuous support throughout this arduous endeavor.

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ACKNOWLEDGMENTS

I am grateful to my research advisor, Dr. Alan Eberhardt, for offering direction and assistance throughout the progression of this study. Many thanks are extended to my committee members, Drs. Lionel Sadowsky, Jack Lemons, William Davidson, and Linda Lucas, for the valuable insights and guidance each has offered throughout this effort. The successful outcome would not have been possible without the help of many, including Greg Dakin, David Beason, Patty Lott, Noel Clark, and Preston Beck.

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LIST OF ABBREVIATIONS

CR	Center of rotation
FE	Finite element
FEA	Finite element analysis
GLM	General linear model
PDL	Periodontal ligament
QLV	Quasi-linear viscoelasticity
UAB	University of Alabama at Birmingham

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INTRODUCTION

Introduced as early as 1000 B.C., orthodontics has been an area of specialty concerned with applying forces to teeth to correct malocclusions and achieve balance of the facial proportions.[1,2] Capable of delivering forces and moments to crowns of teeth, orthodontic appliances initiate the migration of the roots to new positions in the alveolus. Clinically, the desire is to safely relocate the teeth as rapidly as possible by applying forces within a window of magnitude considered optimal. Too little force prolongs treatment times unnecessarily, whereas excessive force causes pain and undermining bone resorption. Excessive forces have also been implicated in tooth root resorption.[1]

The periodontal ligament (PDL) transfers forces at the crown to the supporting alveolus. Housed between two hard tissues, cementum and cortical bone, this collagenous ligament protects the tooth and bone from functional masticatory forces. The method of PDL support of teeth is complex but likely combines structural capabilities of the ligament fibers and hydrodynamic damping mechanisms.

Although the PDL adapts to accommodate forces of mastication, it is also the mediator of orthodontic forces. In contrast to the intermittent, high impact nature of mastication (e.g., hundreds of Newtons for < 1 sec), clinically applied orthodontic loading is light and continuous (e.g., 1 N for weeks).[1]

When an optimum force is applied orthodontically, the stresses produced in the PDL alter the homeostatic physiologic environment, and consequential cellular activity

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initiates bone remodeling. Low magnitude forces are believed to partially occlude the vasculature, thereby signaling cells local to the ligament to resorb bone in compressed regions at the socket wall. In contrast, high forces choke the vessels, starving the nearby cells and tissues of oxygen and nutrition. During the undermining resorption caused by excessive force, cells from bone are recruited to excavate the necrosed tissue from beneath the socket wall. Whereas light force produces a steady saunter of the root through bone, heavy force causes abrupt starts and stops of migration synchronous with collapse of necrosed bone and cementum.[1,2] The stressed environment of the PDL is the decisive factor regulating a healthy or potentially pathologic orthodontic tooth migration.

Quantification of the elusive window of optimum orthodontic force has been attempted through clinical experimentation. Measurement errors have haunted clinical characterizations of tooth movement because orthodontic displacements tend to be (1) small (1 mm/month), (2) nonlinear and timedependent, and (3) different among individuals. Hence, recommendations of optimum orthodontic stress based on clinical trials span a wide range (e.g., 0.007 to 0.14 MPa) and are restricted to only the most common and least difficult to measure, namely canine distalization. Other common displacements (i.e., tipping, rotation, intrusion, extrusion) are difficult to isolate and have been excluded from most clinical experimentation.

While quantification of optimal forces for an in vivo remodeling process has not been accomplished, researchers have attempted biomechanical characterization of the periodontal ligament. The general nonlinear and visco-elastic behaviors of this tissue have been known for several decades,[3-5] but a complete mathematical description has not been presented. In addition, the forces used in many experiments simulate mastication

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and are far outside the range deemed appropriate by the clinical community for orthodontic forces. Based on the functional arrangement of periodontal ligament fibers, researchers have speculated that the PDL is anisotropic but have offered limited supportive mechanical data.

Thus, optimum orthodontic force has not been adequately quantified by either clinical or laboratory experimentation. Without guidance from the scientific community, clinicians rely on trial and error when activating orthodontic appliances. This "shoot from the hip" approach is a disadvantage to clinicians who risk causing pain to the patient and initiating pathologic bone resorption.

The ultimate goal of this effort was to more fully quantify optimum forces for orthodontic loading by applying finite element analysis (FEA) to study the stresses and strains in the PDL. This project was a first step in developing specific biomechanical data related to clinical experience and scientific understanding of the PDL response to orthodontic magnitudes of loading. The largest obstacle to date in appropriately modeling effects of orthodontic loading is the lack of a biomechanical description of the human periodontal ligament. Thus, laboratory testing of cadaveric specimens was performed, with an intent to quantify both the nonlinear and viscoelastic properties of this tissue. Since the tissue was hypothesized to be anisotropic, material properties were investigated in directions of both intrusive and extrusive shear loading.

Hypotheses

Hypothesis 1 asks if temporal and elastic behavior of periodontal ligament can be described mathematically by the quasi-linear viscoelasticity model originally proposed by

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Fung.[6] Hypothesis 2 asks if material properties of the periodontal ligament are nonlinear and anisotropic. Hypothesis 3 states that the stress distribution in the periodontal ligament is complex and not constant along the root for intrusive and extrusive loads. Hypothesis 4 states that the finite element predicted stresses in periodontal ligament by orthodontic force are dependent on assigned material properties of the PDL. Linear material properties assigned to the ligament result in higher predicted stresses compared to nonlinear material properties.

Aims

The first aim was to develop an experimental procedure suitable for measuring and quantifying material properties of the periodontal ligament. The second aim was to develop a quasilinear viscoelastic model of the human periodontal ligament. The third aim was to quantify periodontal ligament in vitro nonlinear stiffness in intrusion and extrusion over a range of stresses recommended for orthodontic therapy. The fourth aim was to use the FE method to describe the stress field in the dental structures for intrusive.

The manuscripts submitted for publication investigating the hypotheses were a result of the research performed by the author. The first paper investigates Hypothesis 1 by applying quasi-linear viscoelasticity to cadaveric specimens of mandibular premolars. The second paper investigates Hypotheses 2 and 3 by testing premolars from two skeletally mature populations in intrusion and extrusion. The third paper investigates Hypothesis 4 by performing a parametric FE analysis to determine the effect of using linear and nonlinear material properties for periodontal ligament.

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QUASI-LINEAR VISCOELASTIC BEHAVIOR OF THE HUMAN PERIODONTAL LIGAMENT

by

S. R. TOMS, G. J. DAKIN, J. E. LEMONS, AND A. W. EBERHARDT

In press, *Journal of Biomechanics*

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Abstract

Previous studies have not produced a comprehensive mathematical description of the nonlinear viscoelastic stress-strain behavior of the periodontal ligament (PDL). In the present study, the quasi-linear viscoelasticity (QLV) model was applied to mechanical tests of the human PDL. Transverse sections of cadaveric premolars were subjected to relaxation tests and loading to failure perpendicular to the plane of section. Distinct and repeatable toe and linear regions of stress-strain behavior were observed. The amount of strain associated with the toe region differed as a function of anatomical location along the tooth root. Stress relaxation behavior was comparable for different anatomical locations. Model-predicted peak tissue stresses for cyclic loading were within $6.2 \pm 5.0\%$ of experimental values, demonstrating that the QLV approach provided an improved, accurate quantification of PDL mechanical response. Success of the QLV approach supports its usefulness in future efforts of experimental characterization of PDL mechanical behavior.

Introduction

The human periodontal ligament (PDL) stabilizes the tooth in bone and provides nutritive, proprioceptive, and reparative functions.[1] It is composed of collagenous fibers and a gelatinous ground substance, including cells and neurovascular tissue. Biomechanically, the ligament demonstrates nonlinear viscoelasticity;[2-5] however, detailed quantification of this complex behavior has not previously been performed.

Patient outcomes associated with dental treatments are strongly influenced by the mechanical support of the PDL. Functional masticatory forces (e.g., hundreds of New-

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tons for < 1 sec) are relevant in prosthodontics and periodontics, whereas low, continuous forces (e.g., 1 N for weeks)[6] are typically applied in orthodontic treatments. Quantification of mechanical behavior of the PDL, specific to these different ranges of loading, has not been reported. Finite element analyses (FEAs) that have simulated clinical experiments of dental implants,[7] operative dentistry,[8] prosthodontics,[9] and orthodontics[10] may be limited by their use of relatively simple (linear elastic) material properties of the PDL.

In the present study, the quasi-linear viscoelasticity (QLV) theory[11] was used to quantify the nonlinear, time-dependent PDL stress-strain behavior. We hypothesized that the mathematical approach would accurately predict stresses in the tissue when subjected to cyclic loading. The purpose was to establish the technique as an improvement over previous works, one that allows for accurate, simultaneous description of nonlinear and time-dependent behavior. Addition of QLV properties may also improve the biofidelity of future computer models of masticatory and orthodontic loading.

Methods

Tooth specimens were harvested from two fresh frozen human heads obtained through the University of Alabama at Birmingham (UAB) Willed Body Program. All procedures were approved by the UAB Institutional Review Board (E990513003). The donors were 78- and 79-year-old White males whose causes of death were cardiac arrest and emphysema, respectively. After thawing, each mandible was isolated, and external soft tissue was removed. Radiographs were taken of all teeth to identify long axis orientation. One premolar was identified from each cadaver for this study. Although each

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premolar had suffered some bone loss, no periodontal pocketing (indicative of active disease) was present in either specimen.

Using a method similar to that of Mandel et al[12], both harvested mandibles were sectioned anterior to the canine and distal to the second premolar to isolate the tooth of interest and adjacent mandibular bone. The block specimens of mandible were radiographed to determine cutting planes. The crown side of the tooth/bone block was mounted in dental acrylic to facilitate fixation. Twelve transverse sections, approximately 0.85 mm thick, were made using a water-irrigated Isomet circular saw (Buehler, Lake Bluff, Illinois). Five specimens were obtained from the 78-year-old donor (A1-A5), and seven specimens were obtained from the 79-year-old donor (B1-B7). To further isolate the chosen premolars, the thin sections were cut interdentally (Fig 1). The specimens were frozen at minus 20°C in a saline environment until testing.

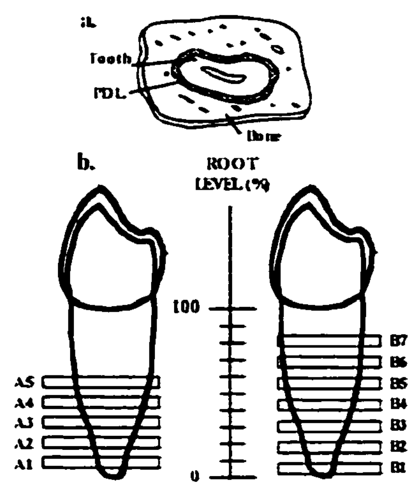

Fig 1. Harvested cadaveric specimen of a mandibular premolar. a) Isometric view, b) region of harvest of the 12 specimens. Drawings are not to scale.

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Digital photographs were taken of the specimens using a Micro-Vu optical metrological system (Micro-Vu Corporation, Windsor, CA) from both apical and coronal views. Prior to testing, ligament width and tooth perimeter were obtained by measuring the digital photographic images with Sigma Scan 4.0 (Jandel Corporation, Chicago, IL) software (Table 1). The ligament width (W_L) was defined as the average of 16 measurements, that is, eight measurements from each view evenly spaced around the tooth perimeter. Tooth perimeter (P) was taken as the average of the apical and coronal perimeter measurements, and specimen thickness (T) was defined as the average of four evenly spaced caliper measurements of the tooth thickness (Fig 2).

Fixtures were fabricated to clamp the bony part of the specimen and allow for extrusive testing on specimens immersed in saline solution. Custom washers were machined (Fig. 2) to closely approximate the contour of the PDL and support as much bone as possible. The specimens were centered under an indenter, which was attached to the actuator of a materials testing machine (MTS 858 Mini Bionix, MTS Corporation, Eden Prairie, MN) through a 100 N load cell.

Following previous studies[12-14] stress area (A_S) for extrusive loading was defined as $A_S = TP$. Stress was calculated as force/A_S, and extrusive shear strain was the angular deformation of the ligament $\gamma = \tan^{-1}(\Delta l / W_L)$, where Δl was actuator displacement (Fig 2b and 2c). Finally, shear modulus was determined by the slope of the linear region of the stress-strain curve beyond the toe region.

Each of the 12 specimens was preconditioned to strains listed in Table 1 (at least five cycles of linear ramp loading and unloading at 0.2 mm/min) to convert the ligaments to an in vitro test state, as previously established.[12] The specimens were stored over-

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Table 1. Soft and hard tissue dimensions and strain conditions for the eight specimens.

Specimen	A1	A2	A3	A4	A5
Measurements					
Lig.width ± SD (mm), W_L	0.20 ± 0.06	0.21 ± 0.05	0.17 ± 0.04	0.14 ± 0.03	0.15 ± 0.04
Perimeter ± SD (mm), P	9.15 ± 1.69	12.32 ± 1.23	14.80 ± 0.57	16.12 ± 0.43	17.05 ± 0.47
Thickness ± SD (mm), T	0.82 ± 0.02	0.87 ± 0.02	0.84 ± 0.01	0.87 ± 0.01	0.89 ± 0.02
Stress area (mm^2), A_S	7.49	10.73	12.40	14.08	15.12
Preconditioning					
Max ramp shear strain (rad)	0.559	0.546	0.640	0.733	0.699
Min ramp shear strain (rad)	0.268	0.261	0.316	0.380	0.354
Stress Relaxation Test					
Shear strain (rad)	0.559	0.546	0.640	0.733	0.699

Specimen	B1	B2	B7
Measurements			
Lig.width ± SD (mm), W_L	0.21 ± 0.04	0.22 ± 0.08	0.21 ± 0.08
Perimeter ± SD (mm), P	6.47 ± 1.78	9.01 ± 1.01	16.05 ± 0.77
Thickness ± SD (mm), T	0.85 ± 0.01	1.11 ± 0.04	0.89 ± 0.01
Stress area (mm^2), A_S	5.50	9.98	14.32
Preconditioning			
Max ramp shear strain (rad)	0.464	0.464	0.575
Min ramp shear strain (rad)	0.169	0.180	0.300
Stress Relaxation Test			
Shear strain (rad)	0.464	0.464	0.575

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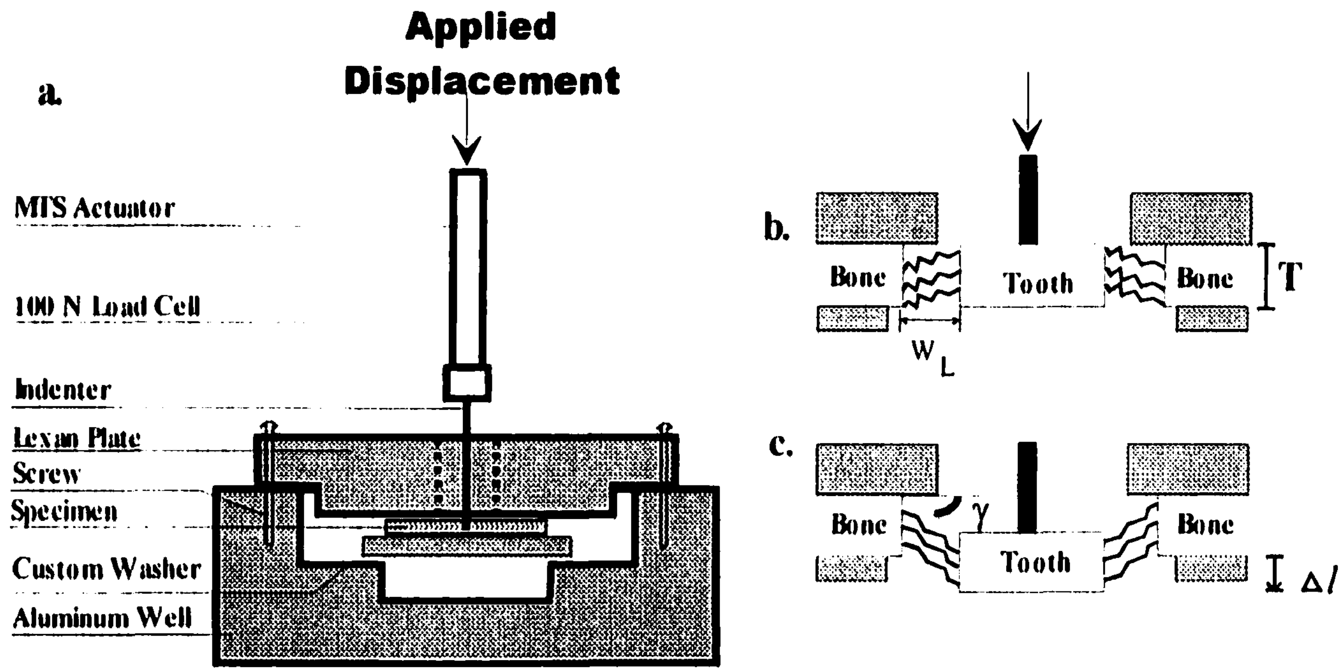

Fig 2. Specimen fixture in the MTS. a) Downward motion of the MTS actuator moves the indenter through an opening in the lexan clamping plate, applying a load to the center of the tooth, b) magnified view of specimen clamped between the lexan and washer for loading in extrusion before, and c) after load application. Drawings are not to scale.

night in an unloaded refrigerated saline environment to rehydrate the collagen fibers.[13,15]

The following day, specimens were preconditioned a second time, at which point repeatable load-displacement behavior was observed. Stress relaxation tests were performed where step-displacements (Table 1) were achieved at the maximum MTS ramp speed (approximately 3.9 mm/sec) and held for 50 min. After overnight recovery, the tissues were preconditioned, cyclically loaded at the previous strain levels for eight cycles, and then extrusively loaded to failure at 0.2 mm/min.[12] Upon completion of the testing, each specimen was examined by light microscopy under various magnifications to ensure that the ligament failed and the tooth did not fracture.

According to the QLV theory,[11] stress in a tissue subjected to a step strain is

$$\sigma[\lambda(\tau);\tau] = G(\tau) * \sigma^{e}(\lambda), \qquad (1)$$

where G(t) is the reduced relaxation function, and $\sigma^{e}(\lambda)$ is the nonlinear elastic stress for an applied strain λ. In the present study, a decaying exponential equation 2 was chosen to describe the temporal behavior

$$G(t) = ae^{-bt} + ce^{-dt} + ge^{-ht}, \qquad (2)$$

where coefficients a, c, and g and exponents b, d, and h were found by least-squares curvefit. Stress-strain behavior (pre-yield) was characterized by applying a rising exponential,

$$\sigma^{e}(\lambda) = A(e^{B\lambda} - 1) \qquad A>0 \text{ and } B>0 \qquad (3)$$

to the load to failure test data, including data points up to the strain amplitude used in cyclic loading. Data from the cyclic loading were used to test the predictive capacity of the experimentally derived QLV constants.[16]

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Results

Of the 12 specimens tested, 3 were excluded because of tooth fracture, and 1 was excluded due to ligament failure during preconditioning. The calculated elastic response parameters *A* and *B* were substantially different for each specimen (Table 2). Variability in toe size and linear slope were apparent among the eight specimens (Fig 3).

Table 2. Shear stiffness and curve-fit parameters for stress-strain equation

Parameters for Specimen A			
	Shear	$\sigma^e(\gamma)=A(e^{B\gamma}-1)$	
Spec.	Modulus	A	B
A1	5.96	8.92E-03	8.79
A2	4.17	1.30E-03	11.30
A3	3.02	3.22E-05	14.30
A4	3.12	1.39E-03	8.11
A5	1.85	1.17E-05	13.57
avg.	3.62	2.33E-03	11.21
SD	1.54	3.74E-03	2.77

Parameters for Specimen B			
	Shear	$\sigma^e(\gamma)=A(e^{B\gamma}-1)$	
Spec.	Modulus	A	B
B1	2.28	2.50E-02	6.34
B2	3.13	1.73E-03	11.19
B7	6.08	1.56E-02	7.72
avg.	3.83	1.41E-02	8.41
SD	1.99	1.17E-02	2.50

The relaxation response did not reach an asymptote (Table 3) within the 50 min test period. Constraints were imposed such that $0.154 < b < 0.156$, $0.002 < d < 0.008$, and $0 < h < 0.00015$, which resulted in accurate curvefits ($r^2 > 0.9$) and suggested that G(t) was similar for all specimens. Noteworthy was the very low decay rate of the slow component h (mean = 3.521E-05) reflecting the long-term behavior of the relaxation response, which although small in magnitude was still greater than zero.

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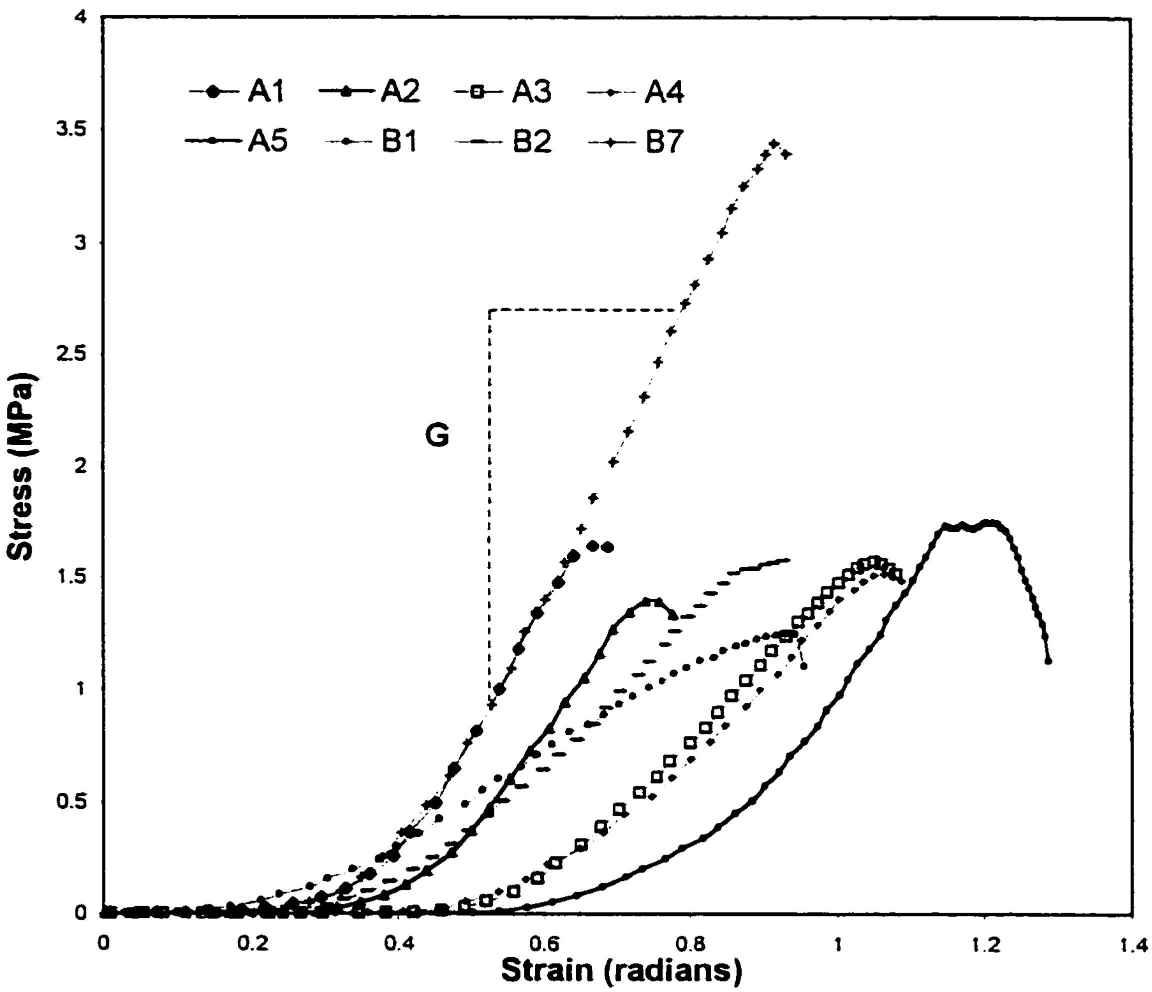

Fig 3. Stress-strain response of PDL under ramp loading to failure. Toe size and modulus were different for the eight specimens. The shear modulus was determined for the curves as shown.

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Table 3. Reduced relaxation function of eight PDL specimens determined by curve-fitting.

	$G(t) = ae^{-bt} + ce^{-dt} + ge^{-ht}$					
Specimen	a	b	c	d	g	h
A1	0.0856	0.1540	0.0800	0.0020	0.8244	1.2597E-05
A2	0.0846	0.1540	0.1480	0.0028	0.7623	3.0033E-05
A3	0.1633	0.1540	0.1174	0.0042	0.7363	7.0327E-05
A4	0.0772	0.1540	0.1373	0.0020	0.7641	3.3649E-05
A5	0.0785	0.1560	0.1069	0.0072	0.7673	8.6459E-05
B1	0.0946	0.1540	0.1048	0.0049	0.7839	1.2619E-05
B2	0.0925	0.1560	0.1003	0.0022	0.7813	1.5383E-05
B7	0.0410	0.1560	0.0800	0.0050	0.8616	2.0576E-05
average	0.0897	0.1548	0.1093	0.0038	0.7852	3.5205E-05
SD	0.0341	0.0010	0.0244	0.0019	0.0398	2.8076E-05

No constraints were placed on the multipliers. Constraints on coefficients in exponents: $0.154 < b < 0.156$, $0.002 < d < 0.008$, $0 < h < 0.00015$.

The average error between the QLV predicted peak values for the cyclic loadings and those calculated as force/A_S was $-6.2 \pm 5.0\%$, with a maximum error of -11% (example Fig 4).

Discussion

The present work demonstrated that QLV theory accurately predicted peak stresses of PDL during cyclic ramp loading, using independently derived equations of stress relaxation and nonlinear stress-strain. These findings support the use of QLV to characterize PDL stress-strain behavior for the many complex loading scenarios encountered in dentistry.

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High variability was observed in toe size and modulus among the specimens (Fig 3). These differences may relate to collagen fiber orientation as a function of anatomical

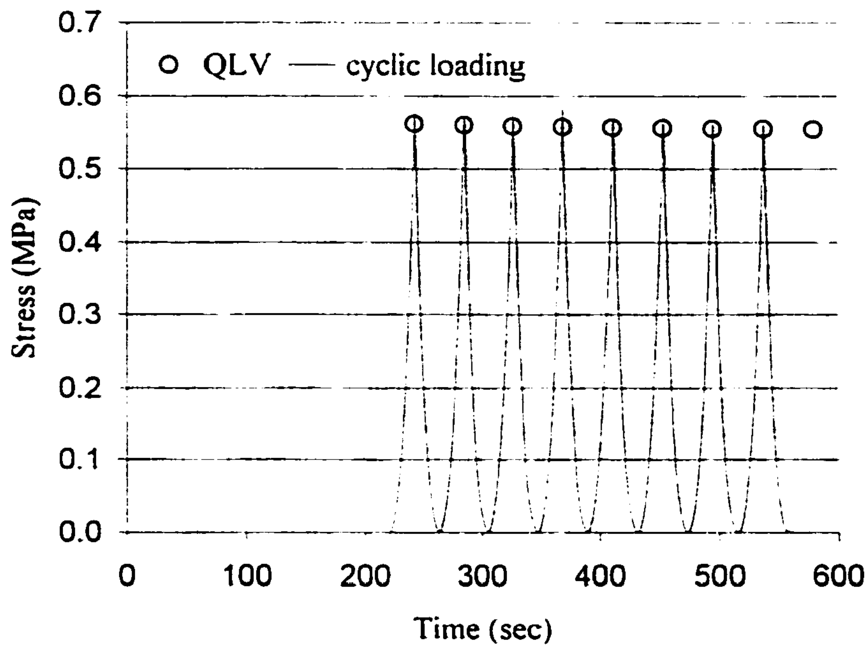

Fig 4. Example plot of cyclic ramp loading of PDL (Specimen A2). Open circles indicate QLV calculated peak stresses. Close agreement was found between the QLV prediction and experimental values.

location along the root. Berkovitz[17] reported that collagen fibers are more obliquely oriented along the midroot than at the apex or cervical margin, and others have observed a correlation between anatomic location and biomechanical behavior.[12] The tests indicated distinct toe and linear regions, suggesting that for dental structures subjected to masticatory forces at least a bilinear expression of elastic modulus is warranted. Accurate quantification of the toe region is necessary for studies of orthodontic (low force) biomechan-

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ics. QLV offers a means of separately addressing orthodontic and masticatory tissue response.

The temporal behavior of the ligament appeared similar for our sample of mandibular premolars. We selected an average G(t) (Table 3) for our calculations. Others have demonstrated viscoelastic behavior in human and primate PDL but have not offered quantification.[18-22] In vivo tests using monkeys indicated that G(t) could vary among teeth by comparing maxillary and mandibular central incisors.[2] The stress relaxation test in this investigation was run for 50 min; however, shorter times may be adequate for studies where the influences of masticatory (large, short duration) forces are the subject.

A more truly elastic response for characterizing the coefficients of the rising exponential elastic stress-strain function would have been achieved by utilizing a faster deformation rate and is an acknowledged limitation of our approach. The current results may not be representative of the general population since we only tested older, healthy, White males. Future efforts should therefore include variables of age and periodontal disease status. In addition, as the size of the toe region decreases and the linear modulus increases with age,[23] testing on a younger population is recommended. This study used mandibular premolars, but PDL behavior may vary among teeth (premolar, canine, incisor) and arch (maxillary, mandibular). Furthermore, the oblique fiber orientations[1] may result in different stress-strain behavior for intrusion, rotation, and tipping forces. The present demonstration that the QLV technique is valid for the PDL suggests an improved approach to study differences in mechanical behavior associated with age, disease state, anatomy, and loading.

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NONLINEAR STRESS-STRAIN BEHAVIOR OF PERIODONTAL LIGAMENT UNDER ORTHODONTIC LOADING

by

STEPHANIE R. TOMS, JACK E. LEMONS,
ALFRED A. BARTOLUCCI, AND ALAN W. EBERHARDT

In press, *American Journal of Orthodontics and Dentofacial Orthopedics*

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Abstract

Previous studies of periodontal ligament (PDL) have applied high forces to the dental units to examine stress-strain behavior of this soft tissue. In the present study, cadaveric specimens of mandibular premolars from two young adult and two elderly adult donors were tested to determine biomechanical behavior of the PDL over an orthodontic force range. Transverse specimens were prepared from nine premolars and subjected to loading in intrusion and extrusion. Stress-strain curves for both loading directions had distinct toe and linear regions, demonstrating nonlinear behavior of the periodontal ligament. The average linear shear modulus was higher for intrusion than extrusion. Toe extrusive modulus was higher for the young group, and extrusive toe size was larger for the elderly group. In extrusion the average modulus was higher for cervical margin and apex regions than midroot regions. The size of the toe region was smaller for intrusion than extrusion. The results indicate age-dependent, location dependent, and load direction dependent nonlinear properties of the human PDL and suggest that analytical computer simulations of orthodontic tooth movements may benefit from incorporating nonlinear material properties of the PDL.

Introduction

The periodontal ligament (PDL) has been described as the principal tissue that regulates orthodontic tooth movement.[1] Orthodontic forces, by altering blood flow and the localized electrochemical environment, upset the homeostatic environment of the PDL space, initiating a biochemical and cellular cascade that resurfaces the bony contour of the alveolus. Whereas light forces applied to a tooth result in partial obstruction of

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PDL vasculature and frontal resorption of bone, heavy forces choke the vessels and necrose surrounding tissue by starving them of oxygen and nutrition. Unlike the physiologic bone remodelling induced by light force, heavy forces cause hyalinization of the PDL and undermining bone resorption and have been implicated in root resorption.[1-4]

The precise definition of light orthodontic force has been the subject of numerous clinical investigations. Experiments to date have focused on canine distalization, which is a procedure aimed to move one tooth per quadrant while leaving the other teeth fixed. The procedure is necessitated clinically in patients with Class II dental malocclusions where the treatment plan includes first premolar extractions and retraction of the anterior segments. Quantification of translatory movement during canine distalization has been complicated by the limited accuracy of measurements of extremely small displacements (less than 1 mm) over extended periods (days, weeks, and months) as well as undesired rotations and tipping of teeth under study. Recommendations of optimum stress in the PDL for canine distalization range from 0.00687 to 0.039 MPa (Table 1). Clinical experiments investigating optimum force for other tooth movements (tipping, rotation, intrusion, extrusion) have not been reported. Movements of this kind are difficult to isolate, as forces are delivered to many teeth by engagement of an archwire in brackets, and teeth tend to move relative to one another.

Computer simulations of orthodontic scenarios have been instrumental in identifying the centers of rotation of teeth[5] and quantifying stress profiles in PDL.[6-7] Accuracy of computer models is dependent on the assigned mechanical properties of the bone, tooth, and PDL. More specifically, modulus of elasticity and Poisson's ratio are required

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as mathematical inputs for finite element simulations. Tooth[8] and bone[9] moduli are well documented; however, comprehensive values for the PDL have not been reported.[10]

The purpose of the present study was to quantify PDL mechanical behavior related to the clinical experience of orthodontic loading. Cadaveric specimens of human mandibular premolars were tested in intrusion and extrusion, and the nonlinear stress-strain behavior was quantified. Comparisons were made between elderly and young adult samples, and the influence of load direction and location around the tooth on stress-strain behavior were examined. The descriptions presented may be ultimately used to improve the biofidelity of computer simulations of orthodontic tooth movements.

Table 1. Optimum stress levels for canine retraction.

Report	Year	Published Value	Conversion (MPa)
Lee[19]	1965	150-260 g/cm2	0.01470-0.02550
Hixon et al[20]	1969	3-4 g/mm2	0.02009-0.03900
Bench[21]	1978	100-200 g/cm2	0.01000-0.02000
Quinn & Yoshikawa[22]	1985	70-140 g/cm2	0.00687-0.01370
Lee[23]	1996	197g/cm2	0.02
Iwasaki et al[24]	2000	4 kPa, 13 kPa	0.004, 0.013

"Conversion" values are the published values in units of MPa, consistent with the present study.

Methods

Tooth specimens were harvested from four fresh frozen human cadavers obtained through the University of Alabama at Birmingham (UAB) Willed Body Program. All procedures were approved by the UAB Institutional Review Board (E990513003). The

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"young" donors were 24- and 27-year-old White males, and the "elderly" donors were 78- and 79-year-old white males. Causes of death were gunshot wound, asphyxia, cardiac arrest, and emphysema, respectively.

After thawing, each mandible was isolated, and external soft tissue was removed. In a method similar to others,[11] each harvested mandible was sectioned anterior to the first premolar and distal to the second premolar to isolate these teeth and adjacent mandibular bone. The block specimens were radiographed to determine cutting planes. The crown side of the teeth/bone blocks were mounted in dental acrylic to facilitate fixation. Transverse sections, approximately 0.85 mm thick, were made using a water irrigated Isomet circular saw (Buehler, Lake Bluff, IL). To further isolate the chosen premolars, the thin sections were cut interdentally (Fig 1a). A total of 56 specimens was harvested, 44 from the young group and 12 from the elderly group. The specimens were categorized by location (apex, midroot, cervical margin) as shown in Fig 1b. Digital photographs were taken of the specimens using a Micro-Vu optical metrological system (Micro-Vu Corporation, Windsor,CA) from both the apical and coronal views. The specimens were frozen at -20°C in a saline environment until testing. Seven premolars were tested from the young group, whereas only one premolar was tested from each elderly donor due to incomplete dentitions. Although each tooth from the latter group had suffered some bone loss, no periodontal pocketing was present in either specimen. Bone loss was not radiographically evident in any tested teeth from the young donors.

Prior to testing, ligament width and tooth perimeter were obtained by measuring the digital photographic images with Sigma Scan 4.0 software (Jandel Corporation, Chicago, IL). The ligament width (W_L) was defined as the average of 16 measurements,

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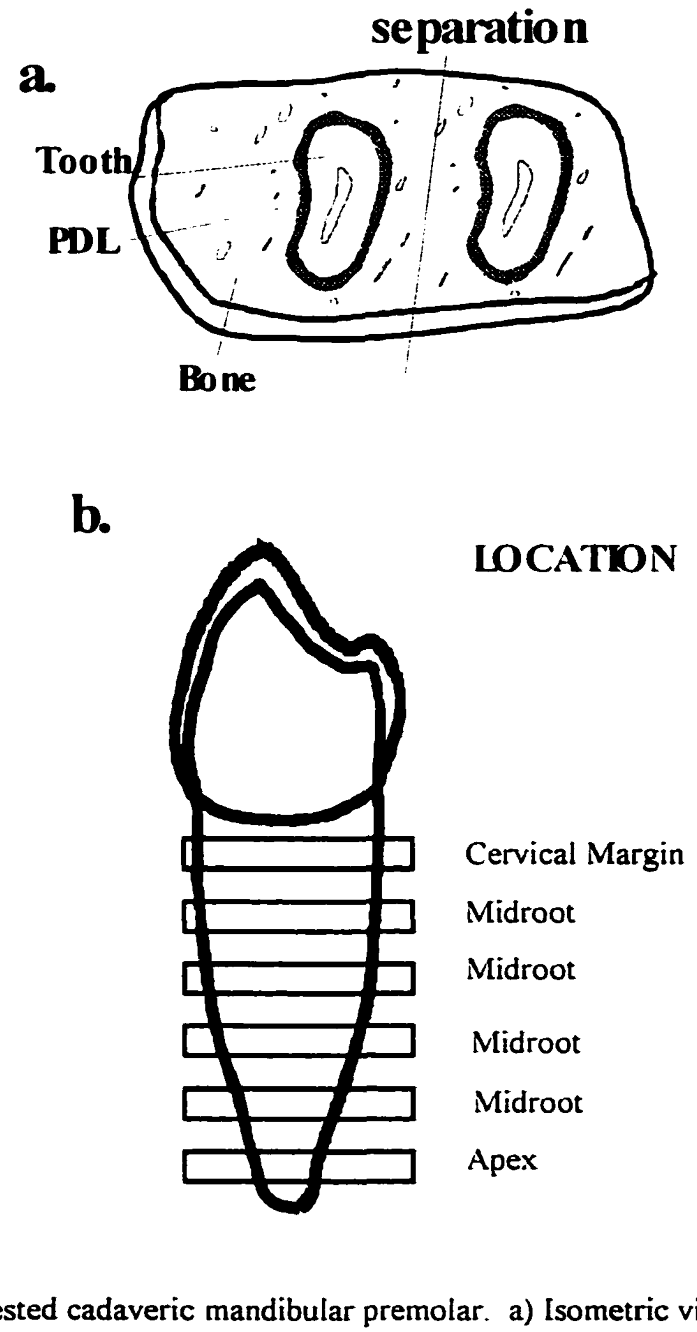

Fig 1. Harvested cadaveric mandibular premolar. a) Isometric view of specimen indicating site of interdental separation, b) specimens were categorized by region of harvest. Drawings are not to scale.

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that is, eight evenly spaced measurements from each of the apical and coronal views. Tooth perimeter (P) was the mean of the apical and coronal perimeter measurements, and specimen thickness (T) was defined as the average of four evenly spaced caliper measurements of the tooth thickness (Fig 2).

Following methods presented in previous studies,[11-12] stress area (A_S) for extrusive loading was defined as $A_S = TP$. Stress was calculated as the applied force/A_S, and elongation, Δl, was the actuator displacement. Extrusive shear strain was the angular deformation of the ligament, $\gamma = \tan^{-1}(\Delta l / W_L)$ (Fig 2b and 2c), and linear stiffness was determined as the slope of the linear region of the stress-strain curve. Toe stiffness was calculated as slope of the toe region beginning at the origin (Fig 3). Linear regressions were used to determine the slope of the two regions of the stress-strain curves.

Fixtures were fabricated to clamp the bony part of each specimen firmly and allow for extrusive and intrusive loading of the specimens immersed in saline solution (Fig 2). Custom washers were machined to closely approximate the contour of each PDL section and support as much bone as possible. The specimens were centered under an indentor which was attached to the actuator of a materials testing machine (MTS 858 Mini Bionix, MTS Corporation, Eden Prairie, MN). During extrusive testing, the specimen was clamped apical side up, whereas the coronal side was up during intrusive loading.

Consistent with traditional testing of other soft tissues, each specimen was cyclically loaded in extrusion (at least three cycles of ramp loading and unloading at 0.2 mm/min), whereby "structural improvement" of the PDL was attained and the ligament was converted to an in vitro testing state.[13] Rather large strains were necessary to reorient

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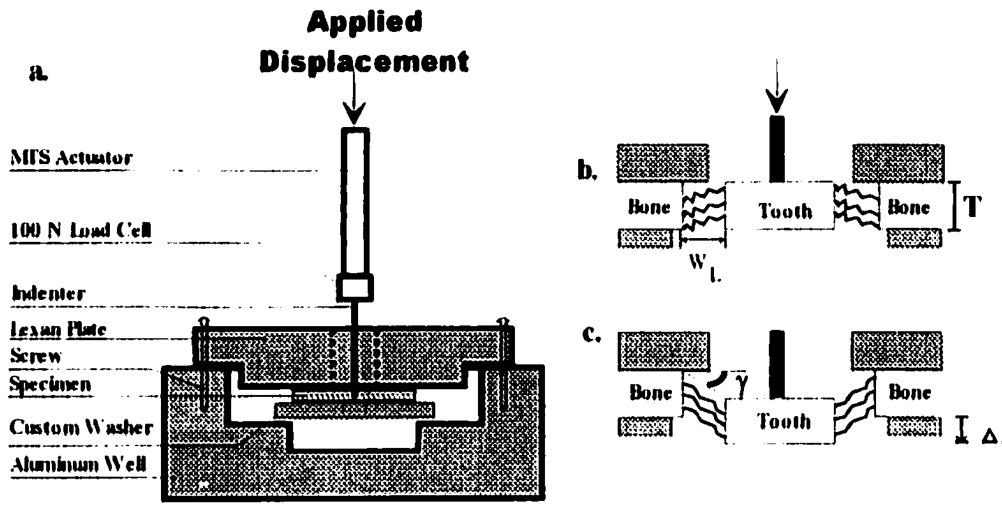

Fig 2. Specimen fixture in MTS. a) Downward motion of the MTS actuator moves the indenter through an opening in the lexan plate, applying a load to the center of the tooth; b) magnified view of specimen clamped between the lexan and washer for loading in extrusion before; and c) after load application. Drawings are not to scale.

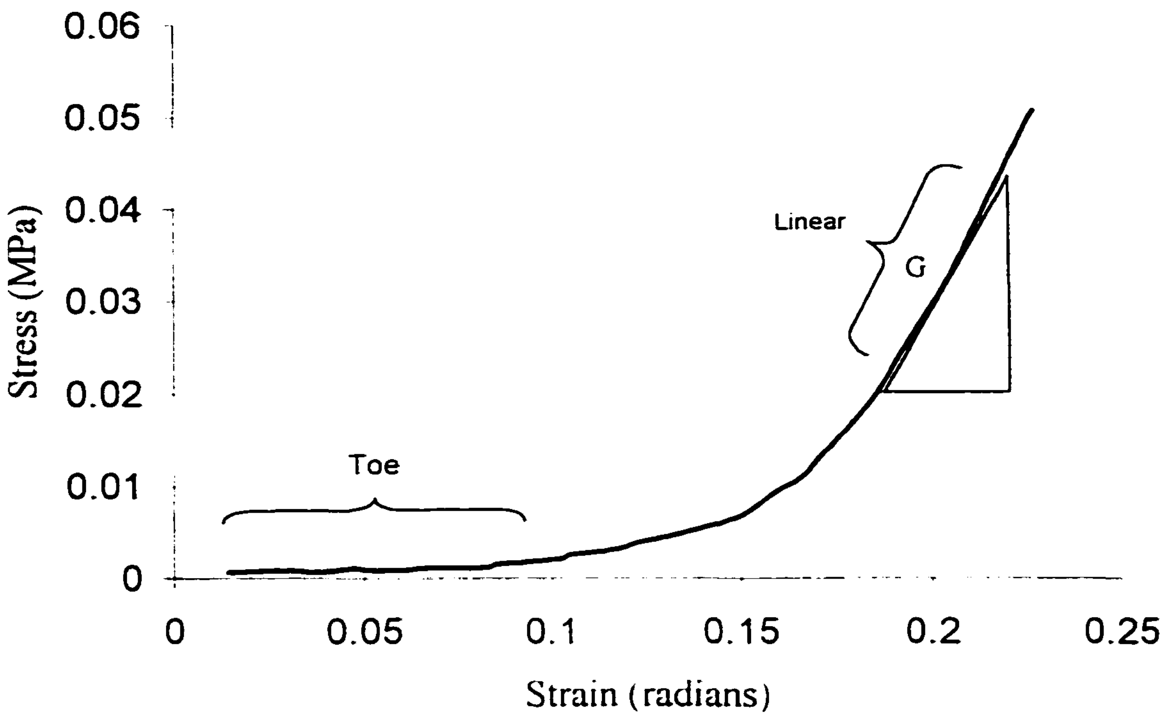

Fig 3. Nonlinear elastic behavior of PDL under low stress. Toe modulus was calculated as slope of the toe region beginning at the origin. Linear modulus was calculated as the slope of the linear region. Moduli were calculated for intrusion and extrusion.

the fibers in the direction of load.[14] Preliminary testing revealed that the periodontal ligament exhibited irreversible stress-strain responses after a sequence of cyclic stretching and relaxation similar to previous findings.[13] Overnight recovery in an unloaded refrigerated saline environment resulted in repeatable stress-strain behavior, as observed previously.[12, 15]

After overnight recovery, the tissue was cyclically loaded for three cycles to the strain required to produce 0.05 MPa ligament stress. Load-displacement data for each specimen were taken from at least the third cycle of loading. The specimens were

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refrigerated for 2 h, then removed from the test fixture, and turned over for testing in intrusion.

To determine the strain necessary to stress the ligament to an orthodontic level, midroot specimens were strained to 0.2 radians. If stress was below 0.05 MPa, the ligament was strained beyond the initial 0.2 radians in increments of 0.05 radians until at least 0.05 MPa was reached, after which the ligament was strained two additional cycles at the maximum strain. Apex and cervical margin specimens were initially strained to 0.14 radians because these specimens broke most often in preliminary testing. Data for intrusive loading were taken from the third cycle of loading at the strain required to reach 0.05 MPa stress. Some ligaments failed during this iterative process. Specimens from the elderly population were not tested in intrusion.

Data were analyzed to determine differences in calculated shear moduli based on donor age, load direction, and anatomic location. The General Linear Model (GLM) was used to compare stiffness in extrusion for the young and elderly specimens ($\alpha = 0.1$). Intrusive modulus versus extrusive modulus for all specimens was compared using paired *t* tests, whereas unpaired *t* tests were used to compare intrusive moduli based on location and extrusive moduli based on location. The extent of the toe region was analyzed using unpaired *t* tests to compare differences based on load direction and age. Differences among groups analyzed with *t* tests were deemed significant at $\alpha = 0.1$.

Results

Of the 56 specimens tested, data from 22 young specimens and 8 elderly specimens were included in the analyses presented. Data from the remaining specimens were

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excluded due to ligament failure during testing. The coefficients of determination, r^2, illustrate goodness of fit of the linear regressions to the experimental data.

Distinct linear and toe regions were observed for all specimens in both loading directions (Figs 4, 5, and 6). After examination of the curves, toe regions were defined as the region from the origin to 0.005 MPa stress, and linear regions were defined from 0.015 to 0.05 MPa. Average linear and toe moduli for extrusion and intrusion and average size of toe were tabulated (Table 2).

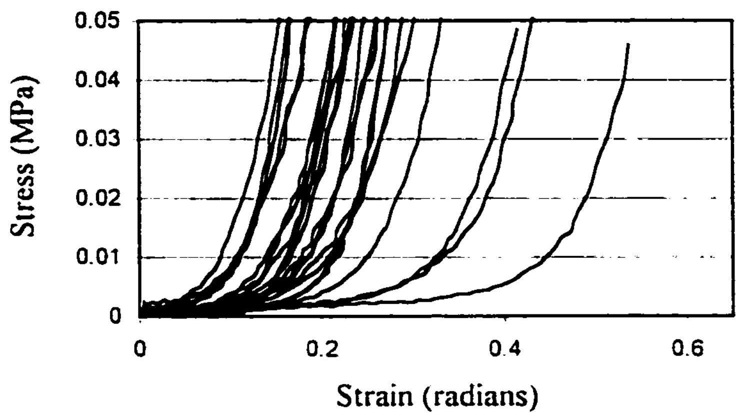

Fig 4. Extrusive shear behavior for the young premolars. The toe on each curve extends to 0.005 MPa and the linear region extends from 0.015 to 0.05 MPa.

The average linear modulus in intrusion (1.043 ± 0.349 MPa/rad) was significantly higher than that for extrusion (0.688 ± 0.136 MPa/rad). No significant difference was found for toe modulus for intrusion (.037 ± 0.050 MPa/rad) and extrusion (0.019 ± 0.03 MPa/rad) due to wide scatter (Table 3).

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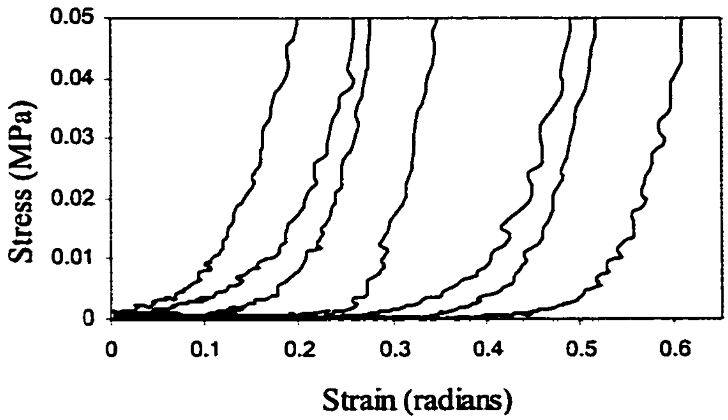

Fig 5. Extrusive shear behavior for the elderly premolars.

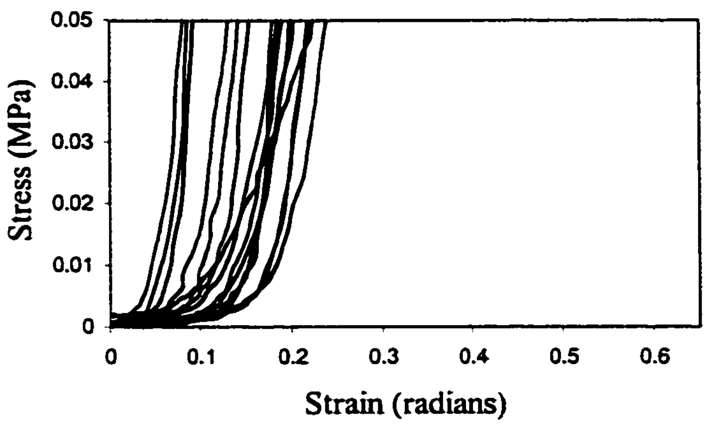

Fig 6. Intrusive shear behavior for the young premolars.

The average linear modulus for the elderly group (0.631 ± 0.091 MPa/rad) was not significantly different from that of the young group (0.688 ± 0.136 MPa/rad). The mean toe modulus for the elderly group (0.0191 ± 0.018 MPa/rad), however, was significantly different from the young group (0.0419 ± 0.030 MPa/rad).

No significant differences in intrusion moduli (linear and toe) comparing midroot specimens to the non-midroot (cervical margin and apex) specimens were observed. No

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Table 2. Average PDL moduli for linear and toe regions in intrusion and extrusion (MPa/rad) and size of toe region (rad) for all anatomical regions (a,b), and separated by region (c,d), where MR = midroot and non-MR = apical and cervical.

Extrusion

	Linear Mod. ± SD	Toe Mod. ± SD	Toe Size ± SD
Young	0.688 ± 0.136	0.0419 ± 0.030	.1628 ± .0778
Elderly	0.631 ± 0.091	0.0191 ± 0.018	.2693 ± .1531

Intrusion

	Linear Mod. ± SD	Toe Mod. ± SD	Toe Size ± SD
Young	1.043 ± 0.349	0.037 ± 0.050	.106 ± .0778

Extrusion

	Linear Mod. ± SD	Toe Mod. ± SD	Toe Size ± SD
Young MR	0.6363 ± 0.110	0.0430 ± 0.0318	.1739 ± .0819
Young non-MR	0.825 ± .097	.0383 ± .0236	.1318 ± .0565
Elderly	0.6597 ± 0.098	0.0100 ± 0.0072	.0963 ± .0482
Elderly non-MR	.6016 ± .087	.0283 ± .0211	.2262 ± .2012

Intrusion

	Linear Mod. ± SD	Toe Mod. ± SD	Toe Size ± SD
Young MR	1.0054 ± 0.2548	0.0483 ± 0.0398	.1161 ± .0411
Young non-MR	1.1457 ± .5754	.0549 ± .0311	.0783 ± .0224

significant difference was found for the toe modulus in extrusion. However, the linear modulus in extrusion was significantly different for the midroot and non-midroot locations (Table 3).

The extent of the toe region was smaller for intrusion (0.1060 ± 0.0778 rad) than extrusion (0.1628 ± 0.0778 rad). In addition, the size of the toe was significantly larger

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Table 3. Results of statistical analyses of PDL biomechanical data.

Analysis	*p*
Linear, young, Int. vs. Ext.	0.001
Linear, Ext., Young vs. Eld.	NS
Toe, Young, Int. vs. Ext	NS
Toe, Ext., Young vs. Eld.	0.053
Linear, Young, Int., MR vs. non-MR	NS
Linear, Young, Ext, MR vs. non-MR	0.002
Toe, Young, Ext., MR vs non-MR	NS
Toe, Eld., Ext., MR vs non-MR	NS
Toe Size, Young, Int. vs Ext.	0.024
Toe Size, Ext., Young vs. Eld.	0.017
Toe Size, Ext., MR vs non-MR	NS
Toe Size, Int., Young, MR vs. non-MR	NS

MR = Midroot

for the elderly population (0.2693 ± 0.1531 rad) than for the young population in extrusion (0.1628 ± 0.0778) (Table 3).

No significant difference in toe size was found based on anatomic location for either intrusive or extrusive loading (Table 3).

Discussion

The current study offers unique information about the nonlinear elasticity of the PDL in the range of orthodontic forces for intrusive and extrusive loading of young and elderly samples. Although limited in sample size, the data acquired in the cadaveric testing reveal complex elastic behavior of PDL from which four generalizations can be made.

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The linear modulus was higher in intrusion than extrusion, indicating that less force was required to achieve an orthodontic level of stress in intrusion than extrusion. The authors conjecture that the ligament orientation and tapering anatomy of the root were factors in this phenomenon. The findings are in agreement with the clinical recommendation of using lighter forces for intrusion than extrusion.[1]

Extrusive stress-strain behavior of the ligament was dependent on anatomic location, and moduli were higher at the cervical margin and apex than along the midroot regions. The same behavior may be the case for intrusive loading, but the data were insufficient since many of the ligaments failed during testing. Others have reported that anatomical location influenced stress-strain behavior when applying forces in the masticatory range.[11] The clinical implication of this finding may be understood by considering that the tooth is suspended in bone by ligamentous attachments. Our results indicate that the attachments in the midroot region have lower stiffness than those at the cervical margin and apex. Some have postulated that a force placed at the center of resistance of a tooth will cause translation of the tooth, which is a reasonable assumption for uniform linear behavior of the PDL.[16-17] Data presented here assert that PDL mechanical behavior is not uniform along the tooth root (Table 2), that is toe and linear moduli in the midroot regions are different from those at the cervical margin and apex areas. Thus, a force at the center of resistance may cause the tooth to tip and rotate. The magnitude and extent of these untoward movements may be better understood with finite element models that incorporate nonlinear moduli of the PDL.

The size of the toe region of the stress-strain curve was dependent on load direction and donor age. The very low stiffness of the toe region associated with soft tissues

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has been attributed to uncrimping of collagen fibrils, whereas the linear region corresponds to straightening of the fibers as they assume more load.[18] Here, the toe region was smaller in intrusion than extrusion. The oblique fiber orientations of midroot specimens, favoring the direction of intrusive loading, may account for the difference. The present extrusive data indicate that the toe region was larger for the elderly group than for the young group. To our knowledge this represents the first data describing PDL material properties of two skeletally mature samples.

The extrusive data indicated that linear shear modulus is not significantly different for the elderly specimens as compared to the young specimens. Others have associated increase in material properties with age for maturing animals.[18]

The data presented here strongly suggest that in finite element analyses of dental structures, a nonlinear representation of PDL material properties is appropriate, and a linear, homogeneous assumption for this soft tissue may be overly simplistic. Some experimental error may have occurred as a result of the extremely low forces associated with the orthodontic loads. In addition, the mechanical behavior is dependent on load direction, and should be included in computer simulations to increase the accuracy of the complex behavior of the human PDL.

Conclusions

In this study, cadaveric specimens of mandibular premolars from two young adult and two elderly adult donors were tested to determine stress-strain behavior of the periodontal ligament over an orthodontic force range. The following conclusions were found.

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1. Stress-strain curves for both intrusion and extrusion had distinct toe and linear regions, demonstrating nonlinear mechanical behavior of the PDL .

2. The average linear shear modulus was higher for intrusion than extrusion, suggesting anistropic material properties of the PDL.

3. The average linear shear modulus in extrusion was higher for cervical margin and apex regions than for midroot regions in the sample. The average size of the toe region was smaller for intrusion than extrusion.

The data presented here, descriptive of specimens from only four donors, suggest that computer simulations of orthodontic tooth movements may benefit from incorporating nonlinear material properties of the PDL. Additional testing is required before a definitive mathematical description of the stress-strain behavior can be made.

Acknowledgments

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A NONLINEAR FINITE ELEMENT ANALYSIS OF THE PERIODONTAL LIGAMENT UNDER ORTHODONTIC TOOTH LOADING

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Abstract

Previous finite element (FE) models of dental structures subjected to orthodontic loading have predominantly assumed linear material properties for the periodontal ligament (PDL). The purpose of the present study was to determine the importance of using nonlinear material properties and nonuniform geometric data in computer predictions of stresses in PDL and tooth movements. Two-dimensional plane-strain FE models of a mandibular premolar were constructed based on anatomical data of transverse sections of tooth/PDL/bone from a 24-year-old cadaveric male. One model had a PDL of uniform width, and the other had a nonuniform width based on geometry of the cadaveric specimen. Each of these was prescribed linear elastic or nonlinear material properties, as obtained in previous experiments. Comparisons were made of the maximum principal stresses and shear stresses in PDL for extrusive and tipping forces. When using linear material properties for PDL, both FE models predicted similar stresses in PDL for extrusive loading, suggesting that incorporation of a biofidelic hourglass shape of the PDL is unnecessary. Incorporation of nonlinear material properties for the PDL, however, resulted in dramatic departure from the stresses predicted by the linear models at the apex and cervical margin, suggesting that the linear model underestimated peak stresses.

Introduction

Application of light and continuous forces to the crown of a tooth is recommended in orthodontics.[1,2] Under low force magnitudes, the periodontal ligament (PDL) vasculature is partially occluded, and cellular activity within the ligament rescaffolds the alveolus. In contrast, heavy forces are more likely to cause ischemia and cell death

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within the ligament, mandating cells in bone to phagocytose necrosed tissue. Whereas light forces cause a physiologic and steady tooth movement, heavy loads induce abrupt starts and stops of migration synchronous with collapse of necrosed bone and cementum.[3] Thus, the stressed condition of the PDL sets the stage for a potentially pathologic tooth movement. Due to geometrical and material complexities, however, few studies have been able to predict an optimal range of forces for orthodontics. Clinicians therefore tend to rely on experience when adjusting appliances.

Finite element analyses (FEAs) offer a means of determining stresses in tooth/ligament/bone structures for a broad range of orthodontic loading scenarios. Centers of rotation of teeth have been analytically determined,[4,5] and stress profiles of the PDL have been quantified for clinical simulations.[6] Each of these computer models assumed homogeneous, isotropic, linear elastic PDL properties and uniform PDL thickness. Accuracy of the models is dependent on assigned constitutive properties. Whereas the hard tissue material properties have been well documented,[7,8] a comprehensive mathematical description for the PDL has not been oncluded in the models and is a source of error in computer simulations of orthodontic tooth movement.[9-11] Recently, we quantified complex stress-strain behavior of PDL of cadaveric mandibular premolars for low force. The data suggested that linear elastic and isotropic assumptions for this soft tissue may be overly simplistic.[12]

The purpose of the present study was to incorporate our experimental data of PDL geometry and nonlinear stress-strain characteristics as input to a finite element model to compare stresses and deformations with models of uniform PDL thickness and containing linear material properties. We hypothesized that incorporation of a sophisticated de-

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scription of PDL mechanical behavior would substantially affect the stresses generated by a tooth subjected to orthodontic forces.

Methods

Two-dimensional plane-strain FE models of a mandibular premolar were constructed using commercial software (COSMOS/M, Version 2.5, Structural Research and Analysis Corporation, Los Angeles, CA). The tooth geometry was based on anatomical data from a previously tested cadaveric specimen of a 24-year-old male. The models (Fig 1) were an assembly of transverse sections of tooth/PDL/bone of the specimen from which stress-strain behavior was determined experimentally.[12] One model had a PDL of uniform width of 250 μm, and the other had a nonuniform PDL width based on the geometry of the cadaveric specimen. The models had 1674 8-node quadrilateral elements and 5205 nodes and were composed of dentin, PDL, and bone. The models had a high density of elements in the PDL (four elements across the thickness), where large displacement gradients were anticipated. A 1 Newton equivalent line load (extrusive or tipping) was delivered in 0.1 N increments to the occluso-gingival midpoint of the crown, and the bone was fixed at the base of the mandible.

Material properties for tooth, bone, and linear PDL (Table 1) were taken from previous FE studies.[13] Nonlinear extrusive material properties for PDL were based on our extrusive stress-strain data of five transverse sections of tooth/PDL/bone.[12] Verification of the nonlinear material properties in the FE model was made by comparing experimental load-displacement behavior of the transverse section to the computer simulation of the experiment (Fig 2)

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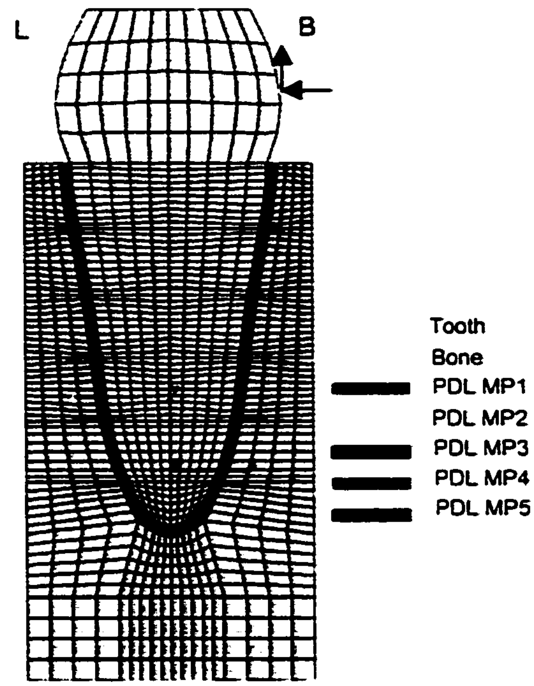

Fig 1. Two-dimensional FE model of a mandibular premolar subjected to extrusive or tipping orthodontic loading at the occluso-gingival midpoint on the buccal (B) aspect of the crown. The PDL thickness in this parametric analysis was either 0.25 mm uniform thickness or non-uniform (not shown). Material properties (MP) of PDL were dependent on anatomic location.

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Table 1. Material properties for the structural elements used in the current study

Material	Young's Modulus (MPa)	Poisson's Ratio
Tooth	19600	0.3
Bone	13700	0.3
PDL (linear elastic)	0.667	0.45
PDL (nonlinear elastic)	experimental data	0.45

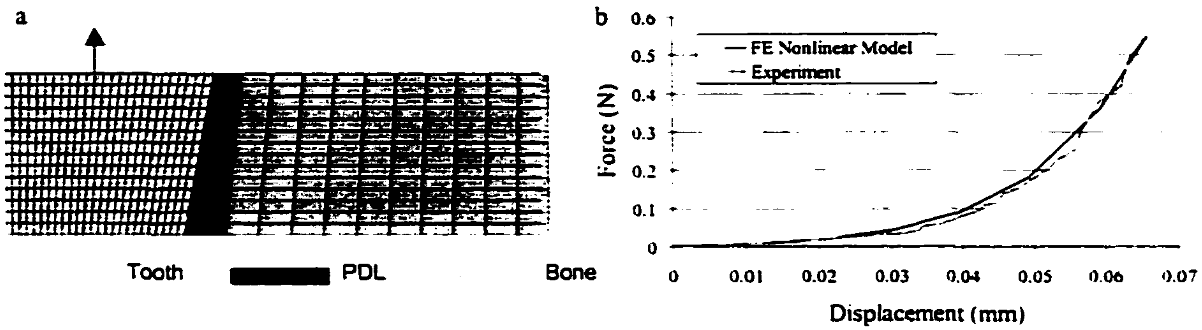

Fig 2. Example model and prediction of an experimental specimen. a) Axisymmetric FE model of a transverse section of experimental tooth/PDL/bone subjected to extrusive orthodontic loading, using nonlinear material properties of the PDL determined experimentally. b) Load and displacement values predicted by the FE model were in agreement with experimental data.

Parametric analysis of the model was performed to determine the effects of PDL thickness variations around the bucco-lingual plane of the PDL, linear versus nonlinear elastic behavior of PDL, and load direction (extrusive or tipping) on PDL stresses and tooth displacements (Table 2). Comparisons were made of the maximum principal stresses and shear stresses in the PDL as predicted by the models. In addition, instantaneous centers of rotation of the mandibular premolar were calculated for each 0.1 N increment of loading as previously described.[4]

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Table 2. Finite element models included in the parametric analysis of stresses in periodontal ligament of a mandibular premolar

Study	Load	Description
Linear/uniform	Extrusive	Linear elastic PDL, uniform PDL thickness (0.25 mm)
Linear/nonuniform	Extrusive	Linear elastic PDL, nonuniform PDL thickness
Nonlinear/extrusion	Extrusive	Nonlinear elastic PDL, nonuniform PDL thickness
Nonlinear/tipping	Tip	Nonlinear elastic PDL, nonuniform PDL thickness

Results

Maximum principal stresses and shear stresses for the uniform and nonuniform linear models were nearly equal for all regions along the root. As indicated in Fig 3, maximum principal stresses were below 0.05 MPa at all locations and were highest at the apex. Shear stresses for these linear models were less than 0.06 MPa at all locations and were higher on the buccal than lingual and near zero at the apex (Fig 4).

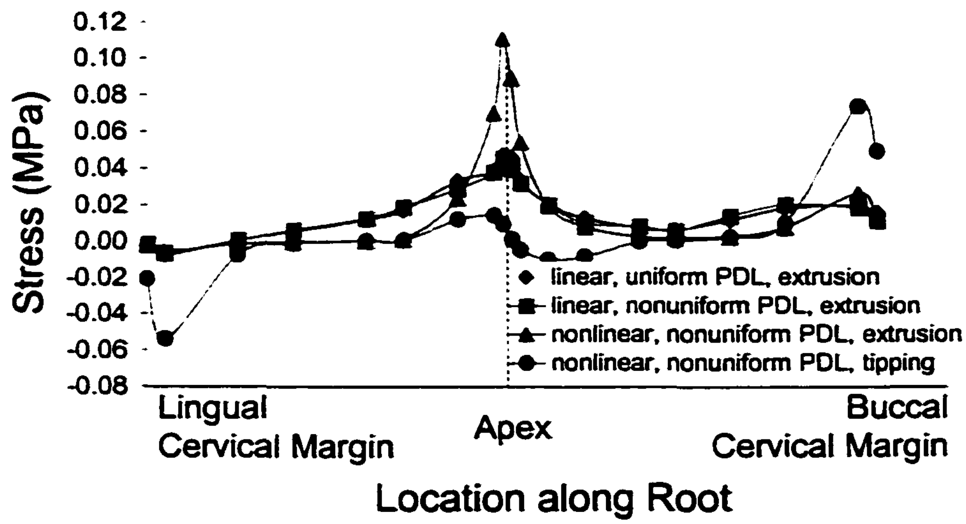

Fig 3. Maximum principal stresses in the PDL predicted by the FE models of a mandibular premolar subject to orthodontic force.

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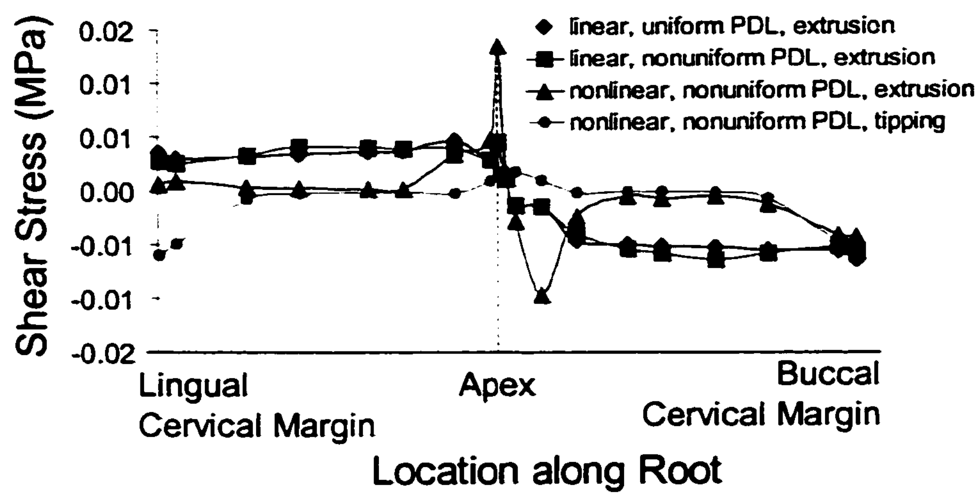

Fig 4. Shear stresses in the PDL predicted by the FE models of a mandibular premolar subject to orthodontic force.

The nonlinear nonuniform model predicted very large maximum principal stresses at the apex (0.111 MPa) but much smaller stresses (< 0.02 MPa) for the midroot and cervical margin locations on both buccal and lingual aspects (Fig 3). Peak shear stresses for this nonlinear model were adjacent to the apex on the lingual side (0.014 MPa). Midroot shear stresses were very near zero and increased to 0.004 MPa on the buccal cervical margin (Fig 4).

The nonlinear nonuniform model with a tipping load predicted the greatest maximum principal stresses at the cervical margin locations, which were slightly higher in magnitude (0.07 MPa) on the buccal than on the lingual (0.06 MPa). Likewise, shear stresses for this tipping model were greatest at the cervical margins (0.006 MPa) and reduced to near zero for midroot and apex regions.

The center of rotation (CR) for the linear model was located on the midline of the tooth approximately 4.3 mm from the apex and did not move during load application (Fig

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5). The CR for the nonlinear extrusively loaded model started at this point but was displaced off the midline 0.0025 mm to the buccal side and 1 mm toward the apex during load application at load increment 7. Additional loading redirected the CR back to the midline of the root but to a more apical location. The nonlinear model subjected to a tipping force predicted movement of the CR from the midline to the lingual side of the root during load application, approximately 3.8 mm from the apex (Fig 6).

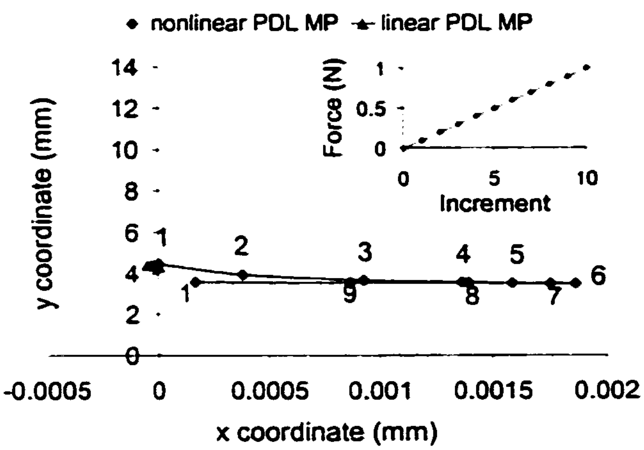

Fig 5. Instantaneous center of rotation of a mandibular premolar during application of 1 N extrusive loading in 0.1 N increments (inset) assuming linear and nonlinear material properties (MP) of PDL. The tooth is approximately 24 mm in length, and the root tip is at the origin. The center of rotation deviates from the long axis of the tooth when nonlinear MP are used for PDL. The center of rotation is stationary when linear material properties are used.

Discussion

As hypothesized, stresses predicted in PDL by computer simulations were dependent on assigned material properties. When a sophisticated description of elastic modulus was employed stresses were substantially higher than for the linear model. In

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addition, a uniform thickness PDL was adequate to predict stresses in the soft tissue due to extrusion.

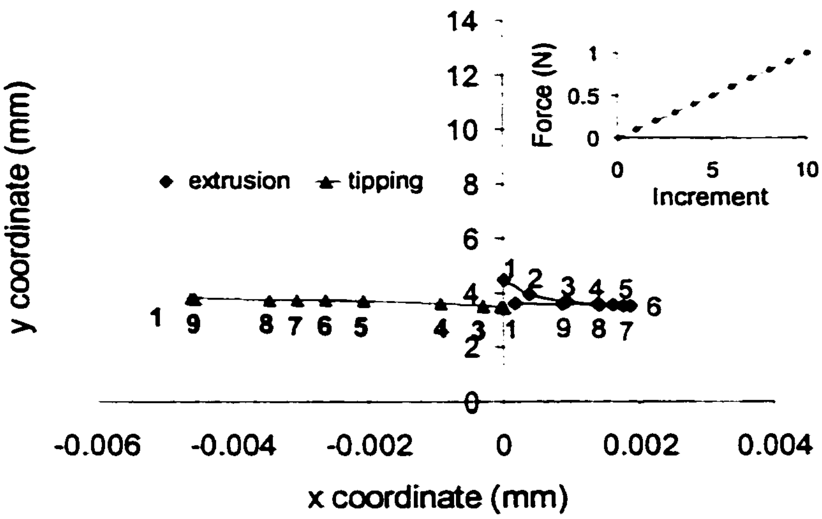

Fig 6. Instantaneous center of rotation of a mandibular premolar during application of 1 N extrusive and tipping forces in 0.1 N increments (inset), assuming nonlinear material properties for PDL. The tooth is approximately 24 mm in length, and the root tip is at the origin. Data points are numbered according to load increment. The center of rotation deviates from the long axis of the tooth during load application.

Maximum principal stress in the PDL for the uniform linear model was highest in magnitude at the apex and tapered to zero at the lingual cervical margin and to 0.01 MPa on the buccal cervical margin. An asymetrical stress pattern about the long axis of the root was also observed for a three-dimensional linearly elastic PDL model of a maxillary canine in extrusion.[14] The similar predictions in maximum principal and shear stresses comparing the uniform and nonuniform models suggest that a PDL of uniform 0.25 mm thickness is adequate and that incorporation of a more biofidelic hourglass[15,16] shape of the PDL is unnecessary in the computer models.

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Incorporation of nonlinear material properties for the PDL resulted in a dramatic departure from the stresses predicted by the two linear models. Apical maximum principal stresses in the nonlinear model were 2.4 times higher than those calculated by the linear models. Maximum principal stresses in the midroot regions were lower for the nonlinear model than the linear model. These data suggest that linear models may, in general, underestimate PDL maximum principal stresses at the apex and overestimate them in the midroot locations. Similar underestimations are indicated by the shear stress data. Some have suggested that a linear, homogeneous representation of PDL is adequate for very low force; however, our data imply that a more sophisticated representation based on experimental data is required for accurate FE predictions. Others demonstrated for a root tip subjected to a tipping load that predicted stresses in PDL with nonlinear material properties were substantially higher than those based on linear material properties.[17]

The CR predicted by the linear elastic model is located on the long axis of the root approximately 4.3 mm from the apex and was stationary during load application. In contrast, the CR moved during load application for both the extrusive and tipping nonlinear models. To our knowledge, this is the first report of movement of the CR within a tooth under orthodontic loading. Since the model is two dimensional, a three-dimensional biofidelic rendering of a premolar may provide a better prediction of the motion of the CR.

The current parametric FE study offers unique information about the importance of PDL material properties in predicting PDL stresses and tooth motion under orthodontic loading. Although the two dimensional plain strain model cannot accurately represent all aspects of a complex three dimensional dental structure, it suggests that behavior of the

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dental structures under low force is strongly dependent on the material properties of the periodontal ligament.

Summary

The following conclusions were made from this parametric FEA of a mandibular premolar subjected to tipping and extrusive orthodontic forces.

1. Nonlinear material properties are required for the PDL for accurate predictions of stresses in PDL.

2. A PDL of uniform thickness in the computer model is adequate for accurate predictions of stress in the PDL.

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DISCUSSION AND CONCLUSION

In an effort to better understand the biomechanics of periodontal ligament, we tested cadaveric specimens of mandibular premolar teeth and subjected the ligaments to intrusive and extrusive loading. We applied quasi-linear viscoelasticity (QLV) theory to derive mathematical descriptions of nonlinear time-dependent mechanical behavior of the ligament. In addition, we used the experimental data as input to a two-dimensional finite element model of the tooth/ligament/bone to predict stresses in the ligament for an orthodontic loading scenario. As a result of these studies, a more complete picture of periodontal ligament biomechanics under orthodontic loading has been developed.

Testing of Hypotheses

Hypothesis 1 stated that the periodontal ligament could be described mathematically by the quasi-linear viscoelastic model. The experimental data demonstrated that the theory accurately predicted peak stresses of PDL during cyclic extrusive ramp loading, using derived equations of stress relaxation and nonlinear stress-strain. The findings support the use of QLV to characterize PDL stress-strain behavior for the many complex loading scenarios encountered in dentistry.

Hypothesis 2 stated that material properties of the periodontal ligament are nonlinear and anisotropic. Stress-strain curves for transverse sections of specimens for both intrusion and extrusion had distinct linear and toe regions, demonstrating nonlinearity. Stiffness of the ligament was found to be higher for intrusion than

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extrusion, suggesting anisotropic ligament properties. Optimal orthodontic forces for intrusive and extrusive tooth displacements were found to be different.

Hypothesis 3 stated that the stress distribution in the periodontal ligament is complex and not constant along the root for intrusive and extrusive loads. Average linear shear modulus in extrusion was higher for cervical margin and apex regions than for midroot regions. In addition, the average size of the toe region was smaller for intrusion than extrusion.

Hypothesis 4 stated that FE-predicted stresses in the PDL would differ substantially when comparing linear and nonlinear material properties of the ligament. The two-dimensional parametric study of a mandibular premolar subjected to tipping and extrusive orthodontic forces indicated that the incorporation of nonlinear material properties of the ligament resulted in substantially different predicted maximum principal and shear stresses. In addition, PDL stresses and tooth center of rotation were affected by PDL properties. Of clinical interest is that the center of rotation moved away from the long axis of the tooth when nonlinear material properties were assigned to the PDL.

Future work

The QLV experiment demonstrated that the theory mathematically described temporal and nonlinear elastic behavior of periodontal ligament but was limited by the very small sample size and donor ages of the mandibular premolars. Presently the behavior has been shown to depend on donor age, anatomical location, and force direction. Thus additional testing is required to build a database of stress-strain behavior from which average QLV equations can be derived. Testing would include all classes of teeth

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(incisors, premolars, canines, and molars from maxillary and mandibular arches) from young and elderly populations.

Elastic behavior of the ligament for intrusive and extrusive loading was quantified for a small sample of young and elderly donors; however, rotation was not investigated. This loading direction is important in orthodontic biomechanics where correction of rotated teeth is a frequent requirement. The test apparatus would need to be adjusted to accommodate the new loading direction.

This study did not include histologic data to further explain directional differences in stress-strain behavior of PDL. Others have studied the arrangement of PDL fibers at various levels of extrusive loading[7] in the rat model and have correlated the toe regions of stress-strain curves with straightening of the PDL fibers. A similar experiment has not been done for cadaveric teeth.

The current FE study was a two-dimensional prediction of PDL stresses and tooth movement for orthodontic loading, and it was based on assembly of transverse axisymmetric sections of an experimental premolar. A logical next step would be to make a more biofidelic three-dimensional model. This task would require development of three-dimensional models of transverse sections, verification of nonlinear material properties of each section, and assembly of the sections to form a three-dimensional model of the premolar. This task is beyond the capability of COSMOS/M software; however, the University has licenses for more powerful

A limitation of the FE study was that verification of the two-dimensional premolar model with load-displacement data of an experimental tooth was not done. In the future, a valuable experiment would be to capture load-displacement data from an intact

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experimental tooth in several loading directions (pure intrusion, pure extrusion, pure rotation, and tipping) and then section the specimen to get regional material properties. Follow-up FE studies could then be validated by comparing actual experimental data with the FE predictions.

Another limitation of the current FE model is that it models behavior of only one tooth subjected to orthodontic force. In orthodontics, however, forces are applied to many teeth simultaneously and only rarely to just one tooth. The engagement of a wire into an arch of teeth is believed to cause a complex range of forces on the teeth. In addition, movement of the teeth relative to each other (at the time of force application) changes the force distributions. Future models are required to include additional teeth to accurately predict stresses in the PDLs for more realistic orthodontic loading scenarios. A logical step might be to build a model of three teeth in an arch first. To date, no reports of FE predictions of multiple teeth are available.

The biomechanical data acquired in the current study were from cadaveric specimens with healthy periodontium. During orthodontic tooth movement, the periodontium and alveolar bone are being reorganized and remodeled continuously. Biomechanical behavior of PDL undergoing physiologic reorganization is likely different from PDL in a homeostatic physiologic state. Acquisition of PDL undergoing remodeling from a human donor is not possible at this time, but data could potentially be acquired from other animal models and extrapolated to the human case. The rat would be the most likely candidate for experimentation.

This study focused on biomechanics of PDL at very low force (orthodontic). The experimental procedures developed are also suitable for high loading (masticatory) ap-

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plications. The QLV approach in particular is valid for masticatory situations since it describes behavior of the ligament under cyclic loading conditions. A database of stress-strain behavior of PDL at masticatory load magnitudes could allow accurate FE predictions of stress for prosthodontic and periodontic problems.

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APPENDIX

INSTITUTIONAL REVIEW BOARD APROVAL

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THE UNIVERSITY OF ALABAMA AT BIRMINGHAM

Office of the Institutional Review Board for Human Use

Form 4: IRB Approval Form
Identification and Certification of Research
Projects Involving Human Subjects

The Institutional Review Board for Human Use (IRB) has an approved Multiple Project Assurance with the Department of Health and Human Services. The Assurance became effective on February 1, 1994 and the approval period is for five years. The Assurance number is M-1149.

Principal Investigator: STEPHANIE R. TOMS

Protocol Number: E990513003

Protocol Title: The Mechanical Behavior of the Periodontal Ligament and its Influence on Orthodontic Mechanics (Exemption #4)

The IRB reviewed and approved the above named project on 5-13-99. The review was conducted in accordance with UAB's Assurance of Compliance approved by the Department of Health and Human Services.

This project received EXEMPTION review.

Date: 5-13-99

Ferdinand Urthaler, MD

Ferdinand Urthaler, M.D.
Chairman of the Institutional Review Board
for Human Use (IRB)

Investigators please note:

The IRB approved consent form used in the study must contain the IRB approval date and expiration date.

IRB approval is given for one year unless otherwise noted. For projects subject to annual review research activities may not continue past the one year anniversary of the IRB approval date.

Any modifications in the study methodology, protocol and/or consent form must be submitted for review and approval to the IRB prior to implementation.

Adverse Events and/or unanticipated risks to subjects or others at UAB or other participating institutions must be reported promptly to the IRB.

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UNIVERSITY OF ALABAMA AT BIRMINGHAM
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DOCTOR OF PHILOSOPHY

Name of Candidate Stephanie Rose Toms

Graduate Program Biomedical Engineering

Title of Dissertation Biomechanics of Periodontal Ligament Specific to Clinical Orthodontics

I certify that I have read this document and examined the student regarding its content. In my opinion, this dissertation conforms to acceptable standards of scholarly presentation and is adequate in scope and quality, and the attainments of this student are such that she may be recommended for the degree of Doctor of Philosophy.

Dissertation Committee:

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