MAE 586 Final report

Finite element analysis on orthodontic bracket by ANSYS

Adviser:
Dr. Hsiao-Yin Shadow Huang

Student:
Pei-Hua Lin
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**Introduction**

In recent years, more people are concerned about the appearance of their face. The demand for orthodontic treatment increases dramatically. Thus, it is important to make a good assessment of the effect of orthodontic brackets. A better understanding of the stress and deformation on dentin will yield improved treatment for the patients. Dr. Ching-Chang Ko and his group at the University of North Carolina at Chapel hill has examined this topic for several years. They used a model built by micro-computed tomography (micro CT) to simulate the movement and deformation of part of the dentin and its environment, which consists of bone, soft tissue and enamel. All of these will be influenced by the orthodontic load produced by the orthodontic bracket.

Among these components, periodontal ligament (PDL) plays a role as a soft but elastic cushion between the tooth and bone, which are relatively stiffer than PDL. Therefore, several research projects focused on the material properties of PDL in order to get more realistic results from finite element analysis. From the beginning, many researchers assumed PDL to be linear elastic or bilinear elastic. Then, some researchers found that PDL had viscoelastic property. Recently, others insisted the PDL should be considered hyperelastic, because of the knowledge about collagen fiber. Based on Dr. Ko’s previous model, I am going to determine the material property of PDL by a solid mechanics testing experiment and discover whether hyperelasticity is a proper model and try to find the effect of the different material properties model.

**Background review**

**Dentin model**

![Figure 1: The actual structure of a tooth and its surrounding ligament. In our model, we will have different kinds of material properties for enamel, dentin, pulp, periodontal ligament, alveolar bone and cortical bone. Each has a different Young’s modulus and Poisson ratio. [11]](image)
Figure 1 shows the structure of a tooth. However, each tooth has different geometry and material properties. The material properties even vary with location of each tooth. Therefore, it is difficult to assign the exact material properties to certain components. Thus, we will choose an average value to represent them instead. Further details of our experimental settings will be introduced in “Experiment” section.

**Nonlinearity**

In reality, all structures are usually nonlinear to some degree. Generally speaking, nonlinear simulations are much more complex than linear simulations. They not only take more computing time, but sometimes fail to find a solution (i.e., solution doesn’t converge). There are lots of parameters that are set to control the results of nonlinear solutions. To derive an accurate simulating solution of nonlinear structures, we need to have enough knowledge about these parameters. By slightly modifying them, it is possible to reduce the computing time and even succeed in finding a convergent solution.

Structural nonlinearities come from three sources: large deformation, change of connectivity, and nonlinear stress-strain relations. Nonlinearity due to large deformation is called geometry nonlinearity. Nonlinearity due to the change of connectivity is called topology nonlinearity, which includes failure of structural components, and change of contact status. Nonlinearity due to nonlinear stress-strain relations is called material nonlinearity. ANSYS is able to automatically detect and control the topology nonlinearity. Thus for this project, only geometry non-linearity and material non-linearity must be addressed. Following is a brief introduction of these two issues.

➢ Geometry nonlinearity

Geometry nonlinearity comes from large deformation of structures. The global stiffness matrix is composed of local element stiffness, and each local element stiffness is a function of the element’s material properties as well as geometry. Different from the linear case, local element stiffness is no longer a constant but varies with nodal displacement. Therefore, when the deformation of structure is so large that the global stiffness matrix will change substantially, geometry nonlinearity must be considered. Among the three sources of nonlinearity, geometry nonlinearity causes the fewest troubles in convergence; reducing the time step or refining the mesh quality is usually useful to improve the convergence

\[ [K(D)]\{D\} = \{F\} \]

\([K(D)]:\text{stiffness matrix, function of nodal displacement or external force.}\)

\(\{D\}:\text{nodal displacement} , \{F\}:\text{External forces}\)
Material nonlinearity

When the stress-strain curve is not linear (i.e., it cannot be described by Hooke’s law), this material is nonlinear. In these cases, we need other ways to describe the relation between stress and strain. The slope of stress-strain curve is the important element, because it represents Young’s modulus. A mathematical model used to describe a stress-strain relation is called a material model. A material model is usually a mathematics form with some material constants; these constants are usually determined by experimental test data fitting. Although almost all biological materials have nonlinear stress-strain relationships, in this project, I am only focusing on the material nonlinearity in PDL. Figure 2 shows a typical nonlinear testing result except its x-axis is stretched (i.e., \( \lambda (stretch) = 1 + \varepsilon (strain) \)) in the longitudinal direction.

![Figure 2: Stress versus longitudinal stretch curves, analytical (continuous line) and experimental (dotted line) results for uni-axial loading of the PDL samples: (a) tension branch; (b) compression branch. [6]](image-url)
Material property of periodontal ligament

Periodontal ligament is a soft biological tissue, which connects the tooth and the surrounding alveolar bone. It plays an important role in tooth movement under physiological loads produced by a bracket. Therefore, it is useful to understand the material properties of the PDL, which determines its deformation and stress-strain response in a loading process.

➢ Structure

According to Dorow’s report [4], PDL consists mostly of collagen fibers (50%-75%), which form several fiber bundles. Therefore, the mechanical properties of PDL are dependent on these fiber bundles. Furthermore, not only the density of fiber bundles has an important influence on PDL’s mechanical properties but also their spatial configuration. In general, these fiber bundles randomly distribute from the cementum to the alveolar bone in a three-dimensional network. In addition to collagen fibers, there are blood vessels, which are responsible for exchanging blood to supply the PDL and other substances such as water, proteoglycans and glycoproteins.

Figure. 3 shows a histological cross-section of the PDL of an anterior tooth of a pig. Collagen fiber bundles looks like a dense network between the tooth and alveolar bone.

Figure. 3: Lots of collagen fiber bundles connecting between tooth and bone (Left). PDL is a soft and thin layer between tooth and bone. [4]
The PDL is clearly important, but its biomechanical behavior remains unclear. Some previous results related to PDL material properties were introduced in Chih-Han Chang’s report [1]. Toms et al. [3] did a shear test by using a transverse thin specimen of the premolar tooth. They found PDL is anisotropic. Dorow et al. [4] tested the response of the porcine anterior tooth under different strain rates. Their results revealed the viscoelasticity due to hysteresis effect. Natali et al. [6] measured the mini-pig premolar tooth and obtained the nonlinear relation between force and displacement of PDL. In 2009, Tohill et al. [7] determined the relaxation characteristics of the premolar porcine tooth. All of these material characteristics should be considered when choosing a proper analytical model. An analytical model should fit the experimental data.

- **Analytical model**
  There are three typical analytical models used in finite element analysis simulation: (1) linear elastic models, (2) viscoelastic models, and (3) hyperelastic models.

    The linear elastic model was introduced in previous reports for a long time because of its simplicity. However the range of Young’s modulus varied from 0.07 MPa to 1750 MPa. Thus, a bilinear model appeared to replace single linear elastic model. However, some studies indicated that PDL had material nonlinearity. It seems there was a slight inaccuracy with linear or bilinear model. After the revelation of viscoelastic characteristics, viscoelastic model had assumed viscoelastic properties for the PDL such as creep, stress relaxation, and hysteresis phenomenon. However, it is so hard to determine an analytical model that takes viscoelasticity and nonlinear stress-strain relation into account simultaneously. Finally, because the force-displacement relation of the PDL is insufficient, a strain energy-based model was developed and named the “hyperelastic model”.

- **Linear elastic model**
  Linear elastic is the simplest way to represent the stress-strain curve. However, it is obvious that the stress-strain curve is not linear. Therefore, we can use a bilinear model to catch the elasticity in different range of strain. The following result was done by Dorow’s research [4].

    From Figure. 4, we see there are different values of stiffness of PDL under different range of strain. Stress increases exponentially before strain reaches 50%. Besides, before strain reaches 100%, stress is proportional to strain. However, after 100%, it is clear that PDL is broken and not able to resist the increasing stress anymore. We can also say that 100% is the yield point for this PDL sample.

    The stress-strain curve shown in Figure. 4 can be replaced by a bilinear model. Such an approximation is useful because we can simply input two simple constant elasticity values
derived from the slopes of the curve rather than a set of data array to finite element analysis simulation. In Figure 4. The slope E1 of the first straight line is the slope of the tangent line at the origin of the stress-strain curve. The slope E2 of the second straight line corresponds to the linear part of the stress-strain curve. The two straight lines intersect at a strain value of $\epsilon_s$. The values E1, E2 and $\epsilon_s$ can then be used to represent the nonlinear stress-strain curve. The inaccuracy occurs, because it cannot model the exponential part of the data curve.

![Stress-strain curve](image)

**Figure. 4:** Stress-strain curve of a sample which was approximated by bilinear material properties. In this case the exponential part of the curve covered strains up to about 50%, while the yield point was recorded at about 100% strain. [4]

➢ **Viscoelastic model**

Based on Dorow’s research [4-5], we know the periodontal ligament shows viscoelastic characteristic due to the combination of fluid and elastic components. Biological tissue usually has viscoelastic properties, which is characterized by non-linearity, time dependency and loading history. Several mechanical tests in previous research has verified the viscoelastic properties of force relaxation and hysteresis of periodontal ligament tissue, both of which depend on loading history. The viscoelastic properties of the PDL can be explained by the different components composing it and their interaction.

**Stress relaxation:**

The time to complete stress relaxation ranged from a few minutes to several hours. According to Fung [8], the relaxed stress was approximately proportional to the maximum stress, which the sample was subjected. The mean value of the relaxed stress of the 24 samples
was 67.68% of the initial stress value. Figure 5 shows the stress relaxation for three different samples. Figure 6 shows the precondition of a sample, which was loaded by a fixed maximum stress of $0.43 \frac{N}{mm^2}$. It took about three cycles to reach its limiting value. The relaxed stress value was approximately 67% of the maximum stress.

**Figure. 5:** Stress relaxation of three samples. The stress relaxed within 15 minutes to 68.6%, 70.9% and 73.9% respectively of the initial value. Relaxation of the third sample was completed after approximately 2 minutes, whereas the stress relaxation of the other two samples took approximately 1 hour. [5]

**Figure. 6:** Precondition of the relaxation of a sample. The limit of stress relaxation decreased from one measurement to another until it reached a limit at approximately 67% of the maximum stress value. [5]
Hysteresis:

To examine hysteresis a sample is stretched to a certain length and then the applied load is removed to allow the sample to return to its original length. If the sample cannot return completely to its original length, hysteresis occurred. Hysteresis can be explained by the loss of internal energy due to internal friction during stretching and releasing. Hysteresis behavior can be determined by the shape of hysteresis curve and the level of hysteresis (i.e., The area enclosed by the hysteresis curve). In addition, different loading history and loading velocity applied on the same sample will lead to different hysteresis behavior.

Figure. 7 shows the hysteresis of two samples that had different thicknesses. The hysteresis effect of two samples was much different. Obviously, sample 2 lost less energy than sample 1 (area between loading and release curves). Figure. 8 shows the response of samples (assumed to have same geometry) subjected to very different loading velocities.

With lower loading velocity, there was a higher hysteresis level (i.e., the area enclosed by hysteresis curve is larger). Similar to stress relaxation, we have to do some preconditioning before we start to test the hysteresis effect (Repeating the same loading and releasing process to make the sample reach the limit status). Figure. 9 shows the preconditioning of a sample. The maximum force value and the hysteresis decreased to approximately 50% of the values recorded in the first measurement after the preconditioning process.

![Hysteresis Curves](image)

**Figure. 7:** Hysteresis curves of two samples with differing shapes and enclosed areas. [5]
Figure 8: Hysteresis curves of a sample that was measured at different loading velocities. [4]

Figure 9: Precondition of the hysteresis of one sample. It took 13 cycles to make the maximum stress and the hysteresis reached a limit at approximately 50% of the value recorded in the initial experiment. [5]
Hyperelastic model

Based on Natali’s research [4], for more realistic result in finite element analysis, we have to consider the mechanical characteristics of different components in the PDL. In general, PDL is made up of other substances and elastin.

Ground substance includes water, proteoglycans and glycoproteins, which have significant influence on periodontal ligament’s stiffness in compression and results in viscoelastic characteristics because it has large amount of liquid state components. On the other hand, elastin is randomly made up of networked collagen fiber structures, which contributes to stiffness in tensile. Because of the random distribution, PDL also shows anisotropic behavior. Figure. 10 shows the random distribution of collagen fibers.

Figure. 10: In general, several single fibers will bind together as a bundle and most of fiber bundles have radial direction, which will endure compressive or tensile stress resulted from tooth translocation. [5]
Due to the above characteristics of the PDL components and experimental evidence that indicated the relationship of stress and strain is nonlinear, we can describe PDL by a hyperelastic constitutive model, which can properly present nonlinear relationship and anisotropic characteristics. There are many different kinds of hyperelastic models. Most of them are derived by strain energy and contain several unknown constants, which have to be determined by experimental data. Table 1 lists some hyperelastic models and their applied strain range. Table 2 lists their numeric formulations.

<table>
<thead>
<tr>
<th>Model</th>
<th>Applied strain range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neo-Hookean</td>
<td>30%</td>
</tr>
<tr>
<td>Mooney-Rivlin</td>
<td>30%~200%</td>
</tr>
<tr>
<td>Polynomial</td>
<td>Up to 700%</td>
</tr>
</tbody>
</table>

**Table 1**: Hyperelastic models and their applied strain range.

<table>
<thead>
<tr>
<th>Model</th>
<th>Applied strain range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neo-Hookean</td>
<td>$\psi = \frac{\mu}{2} (I_1 - 3) + \frac{1}{d} (J - 1)^2$</td>
</tr>
<tr>
<td>Mooney-Rivlin General form</td>
<td>$\psi = \sum_{mn=0}^\infty C_{mn} (I_1 - 3)^m (I_2 - 3)^n + \frac{1}{d} (J - 1)^2$</td>
</tr>
<tr>
<td>2-parameter</td>
<td>$\psi = C_{10} (I_1 - 3) + C_{01} (I_2 - 3) + \frac{1}{d} (J - 1)^2$</td>
</tr>
<tr>
<td>3-parameter</td>
<td>$\psi = C_{10} (I_1 - 3) + C_{01} (I_2 - 3) + C_{11} (I_1 - 3)(I_2 - 3) + \frac{1}{d} (J - 1)^2$</td>
</tr>
<tr>
<td>Polynomial</td>
<td>$\psi = \sum_{mn=1}^{N} C_{mn} (I_1 - 3)^m (I_2 - 3)^n + \sum_{k=1}^{N} \frac{1}{d_k} (J - 1)^{2k}$</td>
</tr>
<tr>
<td>Ogden</td>
<td>$\psi = \frac{\mu_i}{\alpha_i} (\lambda_1^{-\alpha_1} + \lambda_2^{-\alpha_2} + \lambda_3^{-\alpha_3} - 3) + \frac{1}{d_i} (J - 1)^2$</td>
</tr>
</tbody>
</table>

$\psi$: Strain energy  
$I_1$: Deviatoric first principal invariant  
$I_2$: Deviatoric second principal invariant  
$\lambda_k$: Deviatoric principal stretches of the left-Cauchy-Green tensor  
$C_{mn}$: material constants  
$J$: Jacobian  
$\mu$: initial shear modulus  
$d$: incompressibility parameter

**Table 2**: Model numeric formulations.
Experiment

Method

From the beginning, the PDL was assumed to be a hyperelastic material. Fifty-two samples (Figure. 11) were obtained from mandibular bovine lower jaw incisors. Samples were cut in longitudinal locations (apical and mid-root) and circumferential locations (mesial, distal, facial and lingual) (Figure. 12). Utilizing a dynamic mechanical analyzer. (DMA), the properties of the samples were evaluated in an uniaxial tension test at a ramp force of 0.5N/min to 0.5N (Figure. 13) Stress-strain data were further used to fit into the Mooney-Rivlin hyperelastic model. The process of operating the DMA can be found in Appendix 1.

<table>
<thead>
<tr>
<th>PDL Dimensions</th>
<th>Length (mm)</th>
<th>Width (mm)</th>
<th>Thickness (mm)</th>
<th>PDL Length (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>52 Samples</td>
<td>7.11 ± 1.60</td>
<td>2.28 ± 0.45</td>
<td>1.28 ± 0.30</td>
<td>1.63 ± 0.39</td>
</tr>
</tbody>
</table>

Figure. 11: The way to obtain 52 samples from bovine lower jaw incisor and the average dimension of samples.

Figure. 12: The locations of the tooth. ‘M’ is mesial, ‘F’ is facial, ‘D’ is distal, ‘L’ is lingual.
**Experiment result**

The Young’s modulus was measured from the linear elastic model of the PDL. It was approximately 37% greater for apical samples than the middle regions of roots (p<0.05). Mean (SD) Young’s modulus were 0.55(0.09) GPa, 0.83(0.10) GPa, 0.77(0.11) GPa, and 0.89(0.09) GPa for mesial, distal, lingual and facial surfaces, respectively. The Mooney-Rivlin hyperelastic model fitted well the non-linear stress-strain curve of PDL (r=0.99), which could be further utilized to accurately predict tooth movement in a computer simulation. Table. 3 lists Young’s modulus at each location of the tooth and the mean value of the two locations.

<table>
<thead>
<tr>
<th></th>
<th>Mean Modulus +/- std (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Apical</td>
</tr>
<tr>
<td>Mesial</td>
<td>0.82</td>
</tr>
<tr>
<td>Distal</td>
<td>1.46</td>
</tr>
<tr>
<td>Facial</td>
<td>0.62</td>
</tr>
<tr>
<td>Lingual</td>
<td>0.91</td>
</tr>
<tr>
<td>Mean</td>
<td>0.92 ± 0.39</td>
</tr>
</tbody>
</table>

**Table. 3**: Mean modulus for circumferential samples sorted by their respective longitudinal locations (apical and mid root).

**Data processing**

After the experiment, we had to process the data. First, the data was arranged by order of tooth. There were four teeth used in this experiment. **R1**: Right central incisor, **R2**: Right lateral incisor, **L1**: Left central incisor and **L2**: Left lateral incisor. Second, the data was arranged by order of longitudinal location of the tooth (**mid-root, apical**). Third, the data was arranged by order of circumferential location of the tooth (**facial, lingual, mesial, distal**). After re-arranging the experimental data, the data was compared in order to determine any similarities within the sets. Several observations from the majority of several samples in similar location were made.

- Central Incisors (**L1, R1**) are similar and lateral incisors (**L2, R2**) are similar respectively in geometry and material properties.
- In mid-root location, PDL has lower stiffness. The range of strain is from 0 to 0.7, The range of stress is from 0 to 0.2MPa
In apical location, PDL has larger stiffness. The range of strain is from 0 to 0.2, The range of stress is from 0 to 0.15MPa.

Based on the above observations data, which did not match the observations, were eliminated, and regression lines (polynomial) were derived to represent data of different circumferential location of the tooth (Figure 14). Finally, the conclusion was made that the difference in PDL properties was more dominated by the longitudinal location. This means the PDL property was similar in the circumferential location (Figure 14), but not similar in longitudinal location (Figure 15). According to the conclusion, the whole PDL data was separated into two parts. One was the mid-root part and the other one was the apical part. Each has different material properties but both of them were hyperelastic. Next, the experiment uniaxial stretching data was added to ANSYS to produce a user-defined material by curve-fitting.

![Circumferential Comparison: L1R1](image1)

**Figure 14:** Circumferential stress vs. strain comparison for apical incisor location.

![Longitudinal Comparison: L1R1](image2)

**Figure 15:** Longitudinal stress vs. strain comparison for mid-root vs. apical location.
Simulation

Determine material properties for PDL

Mooney-Rivlin hyperelastic model:

The Mooney-Rivlin model is developed from the Neo-Hookean model. It has several forms, which consist of different numbers of parameter. The usually used forms are 2-parameter, 3-parameter, 5-parameter and 9-parameter. Typically one begins with the 2-parameter form and move to more parameters forms gradually. You can also choose the form by inspecting the stress-strain curve. For example, if the stress-strain curve has only one curvature, 2-parameter form is suitable. Moreover, if there are one inflection and two inflection points, we may need to use 5-parameter and 9-parameter forms respectively.

Visual fit and the error norm/residual value are two useful methods to determine whether the result is acceptable or not. Plotting the curves and visually assessing the result is usually the best indication. Error norm value helps you determine the quality of curve fitting and whether to accept the results, but are not always the best indicator of a valid curve fit.
From our experimental data, not all had a single curvature. Some of them had one inflection. Therefore, the analysis began with the 3-parameter form. The strain energy function for the 3–parameter model is,

$$\varphi = C_{10}(T_1 - 3) + C_{01}(T_2 - 3) + C_{11}(T_1 - 3)(T_2 - 3) + \frac{1}{d} (J - 1)^2$$

where the required input parameters $C_{10}, C_{01}, C_{11}$ are material constants. $d$ is material incompressibility parameter. The initial shear modulus is defined as: $\mu = 2(C_{10} + C_{01})$ and the initial bulk modulus is defined as:

$$k = \frac{2}{d}.$$

$T_1, T_2, T_3$ are first, second and third deviatoric principal invariants.

**Curve-fitting by ANSYS**

To do curve-fitting in ANSYS, the experimental data was inputed into ANSYS. First, an Analysis System was selected. A “Static structural”, which was used to measure the response (reaction stress or strain and deformation) of static structure to arbitrary loading (pressure, point force and gravity) (Step 1), was used. Then, a new material whose material properties were determined by previous experimental data was produced. Thus “Engineering Data” had to be opened (Step 2). A new material was added (Step 3) and curve-fitting wa performed in “Engineering Data”.

After the name was assigned (Step 4) to the newly created material, “Uniaxial Test Data” in the “Hyperelastic Experimental Data” was selected (Step 5). Then the testing temperature was entered (Step 6) and the experimental data was inputted (Step 7). The graph of all input data would show in the right-bottom screen (Step 8).

Next, the hyperelastic model to use to for curve-fitting was determined. Choose “Mooney-Rivlin 3 Parameter” in the “Hyperelastic” (Step 9). Right click “Curve Fitting” and select “Solve Curve Fit” (Step 10). Choose “Normalized Error” for “Error Norm for Fit” to get better fitting results. (Step 11) The unknown “Material constants” and “Residual error” will be found automatically by curve-fitting (Step 12). The results of curve-fitting graph will show in the right-bottom screen (Step 13). Finally, right click “Curve Fitting” as in step 10 and choose “Copy Calculated Values To property” (Step 14).
After curve fitting for first incisor, the following results were obtained.

<table>
<thead>
<tr>
<th>Hyper elastic model</th>
<th>Residual/error norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neo-Hookean</td>
<td>136.4</td>
</tr>
<tr>
<td>Polynomial 3(^{rd}) order</td>
<td>43.782</td>
</tr>
<tr>
<td>Yeoh 3(^{rd}) order</td>
<td>45.802</td>
</tr>
<tr>
<td>2 parameter</td>
<td>53.555</td>
</tr>
<tr>
<td>3 parameter</td>
<td>45.799</td>
</tr>
<tr>
<td>5 parameter</td>
<td>45.522</td>
</tr>
<tr>
<td>9 parameter</td>
<td>43.781</td>
</tr>
</tbody>
</table>

**Table 4:** Residual/error norm for different hyperelastic models.

Obviously, the Mooney Rivlin model with 9-parameters has the least error norm. However, there is not a huge difference from the 3-parameter form. Thus, the 3-parameter form was chosen to do curve-fitting and the following result were obtained for the first incisor.

<table>
<thead>
<tr>
<th>First incisor</th>
<th>(C_{10})</th>
<th>(C_{01})</th>
<th>(C_{11})</th>
<th>(d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Longitudinal</td>
<td>Mid-root</td>
<td>0.0098242</td>
<td>0.0044069</td>
<td>0.042671</td>
</tr>
<tr>
<td></td>
<td>Apex</td>
<td>0.26534</td>
<td>0.2342</td>
<td>0.25378</td>
</tr>
</tbody>
</table>

**Table 5:** The PDL property of mid-root and apical location can be determined by these material constants obtained by curve-fitting.
Finite element analysis model

The finite element analysis model used in the simulation was created by micro computed tomography. The model included the first incisor, lateral incisor, canine, first premolar, cortical bone, trabecular bone, PDL, and an orthodontic bracket and wire. Figure 120 shows the front view and cross section view of the model. Each tooth was composed of dentin, enamel and pulp. All had different material properties. Except for PDL, all of the components were assumed to be isotropic linear elastic and had fixed Young’s modulus and Poisson ratio. Table 6 lists three main properties of these material.
Table 6: Density, Young’s modulus and Poisson ratio of each component in our model. Enamel has highest Young’s modulus in the dentin. Structural Steel is used to build orthodontic bracket.

<table>
<thead>
<tr>
<th>Component</th>
<th>Density (kg/m³)</th>
<th>Young’s modulus</th>
<th>Poisson ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trabecular bone</td>
<td>1400</td>
<td>1.37×10⁹</td>
<td>0.3</td>
</tr>
<tr>
<td>Cortical bone</td>
<td>1600</td>
<td>1.37×10¹⁰</td>
<td>0.31</td>
</tr>
<tr>
<td>Enamel</td>
<td>2000</td>
<td>8×10¹⁰</td>
<td>0.41</td>
</tr>
<tr>
<td>Dentin</td>
<td>1600</td>
<td>1.8×10¹⁰</td>
<td>0.31</td>
</tr>
<tr>
<td>Pulp</td>
<td>1000</td>
<td>1.75×10⁸</td>
<td>0.3</td>
</tr>
<tr>
<td>Structural Steel</td>
<td>7850</td>
<td>2×10¹¹</td>
<td>0.3</td>
</tr>
</tbody>
</table>

It is also important to consider the environmental condition. The top and lateral surfaces of cortical bone and trabecular bone were fixed because of their high Young’s modulus. In addition, a pin support was assigned (restricted in displacement but free in rotation) on both ends of the bracket wire. Figure 21 shows the environmental condition in our model.

Figure 20: Front view (left) and cross section view (right) of a part of dentin.

Figure 21: Fixed support on cortical bone and trabecular bone (left). Pin support on two ends of wire (right).
After a solid geometry was obtained of our model and the environmental condition was
defined, a suitable mesh needed to be created. The basic concept of finite element analysis is to
break a body into several small elements. Then, governing equation are used to do the
calculation. Once the result of each element was obtained, they are summed to represent the
result of whole body.

ANSYS is able to generate mesh automatically. Sometimes meshing not only influences
the accuracy of result but also has an impact on convergence problems. Therefore, in order to
get a more accurate and convergent result, some modification on meshing were made. For the
brackets and wire, 0.2 (mm) was assigned as the mesh size elements and 0.8 (mm) size
elements were assigned to both the bones and the tooth. Tetrahedron was used as a basic
element except for the wire. Wire had simpler geometry so a hexahedron could be used as its
basic element which is easier to get a convergent solution.

Figure. 22: Meshing of the whole model. Small size hexahedron elements of bracket and wire. Meshing element
Split PDL into middle and apical part

In order to assign different material properties to middle and apical parts of the PDL, the PDL was split into two parts. It is possible to modify the geometry of model in ANSYS directly. Before using the split method, cutting planes which were used to split PDL, had to be defined. Two planes were defined, which would approximately cut the PDL through its middle part. Table. 8 lists how these cutting planes were chosen. Noted that because an originally continuous PDL was cut into two parts, it resulted in geometry nonlinearity and made solutions hard to converge. Therefore, the contact areas had to be carefully controlled to reduce the initial gap and penetration effect.

<table>
<thead>
<tr>
<th>Name</th>
<th>Assignment</th>
<th>Volume (mm$^3$)</th>
<th>Mass (Kg)</th>
<th>Nodes</th>
<th>Elements</th>
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<tbody>
<tr>
<td>1 Dentin</td>
<td>Dentin</td>
<td>540.2</td>
<td>8.64E-04</td>
<td>15835</td>
<td>10323</td>
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<td>Enamel</td>
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<td>2.83E-04</td>
<td>9813</td>
<td>5390</td>
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<td>8.1927</td>
<td>6.43E-05</td>
<td>18696</td>
<td>10982</td>
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<td>6.44E-05</td>
<td>6701</td>
<td>3282</td>
</tr>
<tr>
<td>1 Pulp</td>
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<td>1.48E-05</td>
<td>935</td>
<td>377</td>
</tr>
<tr>
<td>2 Dentin</td>
<td>Dentin</td>
<td>292.46</td>
<td>4.68E-04</td>
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<tr>
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<td>1.90E-04</td>
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<td>4602</td>
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<td>2 Fa Bracket</td>
<td>Structural Steel</td>
<td>11.223</td>
<td>8.81E-05</td>
<td>22631</td>
<td>14031</td>
</tr>
<tr>
<td>2 PDL apex</td>
<td>PDL</td>
<td>19.976</td>
<td>2.00E-05</td>
<td>2396</td>
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<tr>
<td>2 PDL middle</td>
<td>PDL</td>
<td>31.228</td>
<td>3.12E-05</td>
<td>2904</td>
<td>1379</td>
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<tr>
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<td>Pulp Chamber</td>
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<td>2.20E-05</td>
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<td>416</td>
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<td>9254</td>
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<td>3.53E-04</td>
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<td>19.468</td>
<td>1.95E-05</td>
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<td>1360</td>
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<td>Cortical Bone</td>
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<td>897.6</td>
<td>1.44E-03</td>
<td>25194</td>
<td>12328</td>
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<tr>
<td>Fa Wire New</td>
<td>Structural Steel</td>
<td>11.305</td>
<td>8.87E-05</td>
<td>13683</td>
<td>2304</td>
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<tr>
<td>Trabecular Bone</td>
<td>Trabecular</td>
<td>5055.1</td>
<td>7.08E-03</td>
<td>14662</td>
<td>8779</td>
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</table>

Table. 7 Meshing information

<table>
<thead>
<tr>
<th>Offset in Z direction</th>
<th>Rotate about X axis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plane 1</td>
<td>15.5 mm</td>
</tr>
<tr>
<td>Plane 2</td>
<td>14.5 mm</td>
</tr>
</tbody>
</table>
Table. 8 Cut original PDL into middle and apical Define the plane to cut in the central of original PDL. Plane 1, plane 2 were used to cut first incisor, lateral incisor respectively.

Figure 23: PDL of first incisor and lateral incisor were sliced to apical and middle parts. PDL of canine and first premolar had continuous geometry.

Birth-Death technique

In our model, the wire had a 0.45 (mm) bend between the first incisor and canine, which would produce a lift force and a torque to the lateral incisor. In order to put the bended wire into the bracket, two steps had to be set for simulation. In the first step, a negative 0.45 (mm) displacement was assigned on the bent part of the wire to make the wire contact the bracket successfully. In the second step, the bent wire was released to return to its original shape. Birth-Death technique [1] should be used in these two steps. Death process made the lateral incisor bracket disappear during the first step. It could diminish the overlapping effect of the wire and bracket. In addition, it made it possible for the bent wire to initially have a downward movement. The birth process was used to recover the invisible bracket. Then it would endure the force produced by the wire during the second step.

To use Birth-Death technique, a contact surface was assigned between the contact body (bracket) and target body (wire). Then, an APDL commands was added to declare the contact and target body.
Figure 24: Contact surface between the lateral incisor bracket and bended wire. There is initially an overlap between two bodies. After we apply Birth-Death technique, we can ignore the overlapping effect.

Figure 25: APDL command used for Death-Birth technique
Simulation result

Figure 26: Equivalent elastic strain on PDL at the end of first step (1 second)
(1). Front view. (2). Bottom view.
Figure. 26 shows the equivalent elastic strain of PDL. Notice during the first step, the PDL of lateral incisor didn’t show any strain because of the Death process. It makes sense that the PDL of First incisor and canine had more strain because the downward displacement on the bent part of wire (lateral incisor) also influenced its neighboring teeth.

Figure. 27: Equivalent elastic strain on PDL at the end of second step (2 second)
Notice during the second step, the lateral incisor had the most strain because of the birth process. Figure 27 shows the lateral incisor started to endure the force produced by the bent wire. Besides, it is logical that the highest strain appeared on the apical PDL of lateral incisor PDL.

Figure 28 shows the equivalent stress on the wire. During the first step, the bent part of wire was displaced downward to negative 0.45 (mm). It resulted in reaction forces on the bracket of the first incisor and canine. After the wire was released during the second step, the reaction force on the lateral incisor bracket appeared.

Figure 29 shows the deformation of whole model which is exaggerated by 6 times at the end of first and second step. The highest deformation appeared on the lateral incisor bracket.
Here is the link of animation of deformation:

https://www.dropbox.com/s/jk56697ymoso6qa/deformation%20animation.avi?dl=0

**Conclusion**

Many papers indicated that the property of PDL varies with different location. Therefore, it is hard to simulate the effect of orthodontic bracket in reality case. In this project, the PDL of first incisor and lateral incisor was split into two parts and assigned different material properties. The Mooney-Rivlin hyperelastic model was used to curve-fit experimental data. However, because of material nonlinearity, there were still some troubles when simulating in ANSYS. The results became divergent during the second step if different material properties were assigned in the apical and middle part of PDL. The future work should consider some modification in simulation such as refining the mesh near the sliced interface and the contact surface between the bracket and wire, using more sub-steps, modifying the contact situation (bonded or no separation), release the environmental condition or even updating stiffness at contact surface in the each iteration.

![Figure. 30: Force convergence for each iteration.](image-url)
Appendix

I. DMA calibration process

Types of calibration

- Clamp - complete when changing clamps or adding software
- Position - complete when DMA moved or at least once/month
- Instrument - complete when DMA moved or at least once/month

1. Electronics (7 minutes)
   MENU → CALIBRATE → Instrument → Electronics
   i. Must install the shipping bracket before starting
   ii. Press FURNACE button on DMA
   iii. Press CONTINUE Button
   iv. Let it run
   v. Press CONTINUE to end

2. Force (10 minutes)
   MENU → CALIBRATE → Instrument → Force
   i. Remove all clamps
   ii. Press CONTINUE Button
   iii. Let it run (5 minutes)
   iv. Press CONTINUE to move to next part
   v. Place 100g weight on top of drive shaft dovetail- centered and not touching thermocouples
vi. Press FURNACE on DMA
vii. Press CONTINUE
viii. Let it run (5 minutes)
ix. Remove weight
x. Press CONTINUE to end

3. Dynamic (about 1.5 hours)
   MENU → CALIBRATE → Instrument → Dynamic
   i. Install the 35 mm Dual Cantilever Clamp

   ii. Press FURNACE button on DMA
   iii. Press CONTINUE
   iv. Let it run (5 minutes)
   v. Press Continue
   vi. Mount sample
      1. Length: 15mm
      2. Width: 12.803mm
      3. Thickness: 3.147mm
   vii. Press FURNACE on DMA
viii. Press CONTINUE
 ix. Let it run (10 minutes)
 x. Press Continue
 xi. Mount .12mm sample
 xii. Press Furnace on DMA
 xiii. Press Continue
 xiv. Let it run (10 minutes)
 xv. Repeat 3X (10 minutes each) for each size sample
 xvi. Once done press Analyze (30 minutes)

4. Clamp

Install clamp
 i. Raise drive shaft to top and lock using FLOAT/LOCK
 ii. Lower thermocouples to lowest position
 iii. Install splash guard with rim facing up
 iv. Move drive shaft all the way down
 v. Slide dovetail of yoke into drive shaft and lock down with hex wrench
 vi. Install top bar and tighten hex screws

vii. CALIBRATE → CLAMP
 1. Clamp type: select Tension submersion film
 2. Clamp calibration type: select ALL calibrations
 3. Press CONTINUE

viii. Do NOT close furnace
 ix. Press CONTINUE
 x. Let it run (5 Minutes)
 xi. Once done, install rest of clamp
 xii. Remove top bar of yoke and secure fluid container, tighten the four hex screws, but don’t overtighten
 xiii. Put together sample-load assembly
xiv. Secure top bar of yoke to crossbar loading fixture with thumb screws

xv. Sample size: 3.49 mm x 4.560 mm x 0.170mm (if using my attachment, if not then length = 15mm)

xvi. Remove the crossbar loading assembly once set up complete

xvii. Press CONTINUE

xviii. Let it run (1 minute)

5. Position
   a. Remove everything (4:39)
   b. Press CONTINUE
   c. Let it run (1 minute)

When changing clamps- need to recalibrate clamp and position

1. Clamp
   a. Install clamp- tension film clamp (see pic below), add custom jig (small one), jig doesn’t sit flush on clamp so do the best you can to keep it straight and still tighten it.
      i. CALIBRATE→CLAMP
         1. Clamp type: select Tension film clamp
         2. Clamp calibration type: select ALL calibrations
         3. Press CONTINUE
      ii. close furnace
      iii. Press CONTINUE
      iv. Let it run (5 Minutes)

v. Once done, put on offset gauge (clear plastic). Use bottom mark (should measure 3.77 mm- enter this distance for your offset

vi. Offset distance: 3.77 mm (only tighten it to the fixed clamp (top one)

vii. Close furnace
viii. Press CONTINUE
ix. Let it run (1 minute)

2. Clamp Compliance
   a. Lock float to mount sample
   b. L=3.77, W=12.617, T=.760
   c. close furnace
   d. CONTINUE
II. Periodontal ligament DMA protocol

The samples are removed from the -10°C Freezer and allowed to thaw for 1-2 hours. Pour sample onto cell culture dish. Sample length is measured with a micrometer slide (Gaertner Scientific Corporation) with a 10x scope. Measure sample at top, middle, and bottom of the length of the PDL. Average the 3 measurements for final length value of the PDL. Width and thickness are measured with calipers. Fill water bath up with 20mL of saline. Load sample by first securing bone portion to the custom lower clamp. Orient the upper clamp to the lower clamp using the crossbar loading fixture and tighten the thumb screws. Secure the tooth portion to the upper clamp by tightening the set screw on the top bar. Fix the load assembly to the water bath by using the final two thumb screws to align everything and finally by tightening all six screws (2 to the top bar and four to the bath). Remove the crossbar loading fixture. Fill up the remaining bath with saline until almost full (about 20-22mL total to cover sample and a little beyond). See Figure 2 for set up.
Go to TA instrument control program. Make sure the mode is in DMA Controlled Force (Figure 3). Tension: Submersion film. Under the summary tab, enter sample name and data file name. All data is stored under: D:\TA Files\Data\DMA\pdl data\real data. Under the Clamp/Sample portion, clamp type is tension: submersion film and sample shape is rectangular. Enter the dimensions for the sample. Under procedure, the protocol should be preloaded. Press editor to change the protocol. The protocol for this controlled force experiment is:
Ramp 0.5N/min to 0.5N
Ramp 0.5N/min to 0.001N
Isothermal for 2 min
Ramp 1N/min to 1N
Ramp 1N/min to 0.001N
Isothermal for 2 min
Ramp 3N/min to 3N
Ramp 3N/min to 0.001N

Go back to summary tab and hit APPLY, then press RUN.
Figure. A4: TA instrument control software’s experimental view page, summary tab. Purple box outlines where the sample file is names and stored. Red box outlines portion where dimensions should be entered.

Once run is complete, you must go to Universal Analysis and extract data. Go to VIEW\Universal Analysis to open program. Go to OPEN and find the sample data file name under D:\TA Files\Data\DMA\pdl data\real data. Hit OK. Change graph signal setting under GRAPH\SIGNALS: Y1= Stress (Gpa) and X change signal to dimensional change, press OK. Go to GRAPH\UNITS and select Mpa for Modulus. To export, choose VIEW\DATATABLE\SPREADSHEET. Choose low and high range to select for entire X axis and check box for “All data points.” See figure 5 below.
Figure A5: Universal analysis program. Shows pop up menu for extracting data points.

Once you choose OK, an excel spread sheet automatically appears with the data. You must change dimensional change to strain data. Move stress column to "D". In the B column. Add the first value for dimensional change to all values within the column to zero the data. In the C column, divide column B value by initial dimension in microns to get strain. See example below. Now do a scatter plot to confirm data is accurate.

A. B

Figure A6: 6A Shows calculation needed to convert dimensional change to microns and zeroing the first point. 6B shows calculation to calculate strain.
Reference


9. Practical Stress Analysis with Finite Elements By Bryan J. Mac Donald

10. ANSYS "5.1. Hyperelastic Material Curve Fitting"

11. Figure 1: http://www.studiodentaire.com/en/glossary/alveolar_bone.php