Comparative analysis of adhesive failure of orthodontic resins: An *in vitro* mechanical test with the finite element method

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ABSTRACT

Objective: The purpose of this study was to validate finite element (FE) method as a reliable adhesive shear strength test method by investigating and comparing the results from *in vitro* mechanical tests and 3-D FE simulations. **Materials and Methods:** Four groups of teeth (n=15) using Transbond XT (3M Unitek, Monrovia, CA) and Enlight Ormco (Glendora, CA) with metallic and ceramic brackets (Twin-Edge and InVu, TP Orthodontics, Inc., La Porte, IN) were obtained and submitted to shear bond strength tests. Subsequently, an equivalent geometric model was subjected to FE modeling analysis. ANOVA tests indicated a statistically significant difference (P<0.05) between the shear bond strength of the two bracket types regardless of the resin, and there was no interaction between the resin and bracket type. **Results:** FE analysis showed the stress distribution in the adhesive layer and revealed an increased stress distribution in the ceramic brackets. These results were consistent with *in vitro* detachment experiments. **Conclusions:** This study establishes that FE sub-modeling can be used to simulate adhesive resistance.

Key words

Adhesive failure, brackets, finite element method

INTRODUCTION

The technique of direct dental surface bonding emerged when Buonocore proposed the use of acid to alter the surface of the enamel.^[1] Since then, shear bond strength tests of composite resins on these surfaces have been performed.^[2]

Immediate adhesive strength is of particular interest to the orthodontist and adequate bond strength should allow safe re-bonding, although not permitting adhesive failure, because it delays orthodontic movement, extends clinical time due to the re-bonding procedure^[3] and also becomes an inconvenience for the patient.^[4] With adequate shear bond strength, the tooth should be able to resist masticatory forces and avoid superficial enamel damage during re-bonding.^[3,5-7] It is necessary to select

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the best bonding technique and material, for promoting the desired dental movement. [8]

New base designs have been made to improve mechanical retention. [3] Unfortunately, the development of these orthodontic resin designs has been based on relatively imprecise experiments, which measured only one component of the system: The resin. [9]

Studies utilizing *in vitro* strength assessments of adhesion systems have been subject to variables^[3,10,11] that increase the difficulty of comparing the results of two studies and can cause their conclusions to be compromised.^[4,12,13] Due to the aforementioned variations, these tests should only be used to compare one system with another to determine the effect of the alteration of some of the variables within the same system.^[14] Almost all of the possible test variables have a significant influence; therefore, the values of shear bond strength are responsible for the incoherencies in the results.^[15,16]

The finite element (FE) method is an analytical tool of mathematics that permits to apply an array of forces on any site and in any direction, thereby providing a source of information about the displacement and the degree of stress/strain caused by the application of these forces on the analyzed structure.[17]

In our case, the system includes three components: The bracket, the resin, and the enamel. [15,18,19] Although there is evidence regarding the performance of this group, the few studies that are relevant are limited to justifying the utilization of numerical models to assess orthodontic bonding [15] with the goal of reducing the need for laboratory experiments. [18]

The shear bond strength of orthodontic resins with both metallic and ceramic brackets was verified *in vitro* and the stress/strain values as functions of both the type of resin and the type of bracket were evaluated by FE, and the deformation patterns of the resin layer determined. The results of the computerized numerical simulation were compared with those obtained from the *in vitro* mechanical shear bond strength test.

MATERIALS AND METHODS

Shear bond strength test

Sixty human teeth were used, and the sample was composed of maxillary central incisors with integrated vestibular surfaces that were free of carious lesions, restorations, cracks, and fractures. All of the procedures during samples and shear bond strength process followed the protocol established by International Organization of Standardization (IOS/TS 11405),^[20] of method recommendations. The teeth were separated into four groups, as shown in Table 1.

Characterization of the orthodontic resins – three-point flexion test

The three-point flexion test is a test that attempts to determine the flexural elasticity of the material. This test was performed on both the Transbond XT and Enlight orthodontic resins after they were placed in relative moisture for 24 h. Testing was performed based on the recommendations found in the guideline ISO 10477. [21] The Poisson coefficient of the composite resins was taken from the literature.

Obtaining the computational model

The physical and geometrical quantification of every component was performed [Table 2] in order to develop a valid tridimensional model.^[19]

To characterize the mechanical properties of the enamel, dentine, the metallic (Twin-Edge® Stainless Steel) and ceramic (Invu® Ceramic-Polycrystalline Aluminum) brackets, and the acrylic resin, the Young's modulus of elasticity and the Poisson coefficient were taken from the literature.

In order to, provide a faithful reconstruction, the bracket base dimensions were analyzed using a digital pachymeter (Litz professional, Germany), a digital microscope (model DM-130 U) with a magnification range of $\times 10$ to $\times 200$, and the appropriate measurement software (Miview, China).

Utilizing the same steps, the adhesive layer was modeled according to the base area of the bracket. The thickness of the resin was calculated to be $271\,\mu m$; this measurement was made at its thickest point, as suggested by Knox $\it et~al.^{[19]}$ but varied from one bracket to the next because the angulation of the base. The thickness of the layer that corresponded to the upper edge of both brackets was made to be $130\,\mu m$.

For the enamel, a high-resolution computerized micro-tomograms (micro-CT) device (SkyScan 1172, Foster City, CA) was used to generate micro-CT.

Two tridimensional models composed of the human central incisor, and the resin layer were then created in the Solid Works, version 2010 (Dassault Systems, Solid Works Corp., Concord, MA). The difference between the two models was due to the choice of bracket material and the properties of the resin layer. All of the materials were assumed to be homogeneous, isotropic, and linearly elastic. [15,18,19,22,23] The number of nodes and elements of the metallic bracket model was 541,195 and 344,614, and of the ceramic bracket model was 389,407 nodes and 245,659 elements.

We attempted to follow the *in vitro* procedures exactly for the tridimensional model, resulting in force being applied at the base of the bracket. The force utilized was 23.928 N, which corresponded to the lower mean of the maximum force obtained in Group 1 [Table 1] from the *in vitro* mechanical test (randomly selected only for standardization purposes).

To analyze the normality of the data, the Kolmogorov-Smirnov test was utilized for the elasticity

Table 1: Sample for the adhesive resistance test					
Group	N	Bracket	Base area	Resin	Resin's components
1	15	Twin-Edge® (TP orthodontics)	14,4mm²	Transbond™XT (3M)	Silane treated quartz 70-80%
2	15	InVu® (ORMCO)	15 , 6mm²		Silane treated silica <2%
3	15	Twin-Edge® (TP Orthodontics)	14,4mm²	Enlight® (ORMCO)	Inert mineral fillers, fumed silica, activatorsand preservatives 65%
4	15	InVu® (ORMCO)	15 , 6mm²		

and flexion moduli as well as the shear bonding strength. To test the homogeneity of the variance within these same variables, the Levene test for homogeneity of variance was used. The Analysis of Variance test (Two-Way ANOVA for Independent or Correlated Samples) was applied to two criteria for a complete factorial model of the analysis of the results. Once a difference was observed within the groups, and the data demonstrated homogeneity of variance, the identification of the differing groups was performed using the Tukey Honestly Significant Difference multiple parameter comparison test of homogeneous variances.

The statistical software Statistical Package for Social Sciences version 16.0 (SPSS, SPSS Inc., Chicago, IL) was used to tabulate and analyze the data.

RESULTS

For the three-point flexion test, Student's *t*-test for the comparison of independent samples was performed [Table 3]. For the shear bonding test, considering that the sample size was less than 30 (*n*=15), the ANOVA test was applied to two complete factorial models [Table 4].

Table 2: Physical properties of all components							
Three-dimensional model structure	Poisson's ratio	Young modulus (Gigapascal-GPa)					
Enamel	0.3	46.89					
Dentin	0.31	18.6					
Metalic bracket	0.3	210000					
Ceramic bracket	0.19	380000					
Acrylic resin	0.4	2979					
Transbond™XT	0.21	10.7					
Enlight®	0.21	7.6					

Gpa – Gigapascal

Table 3: Two-way ANOVA test, complete factorial model							
	Sum of squares	df	Mean	F	P		
Resin	20.886	1	20.886	2.542	NS		
Bracket	66.992	1	66.992	8.154	*		
Resin X bracket	6.534	1	6.534	0.795	NS		
Error	460.037	56	8.214				
Total corrected	554-45	59					

ANONA – Analysis of variance; NS – Not significant; *Significant at the o.o5 level

Table 4: Maximum principal stress for each grou	р
Group	Мра
1	3.743
2	4.428
3	4
4	4.356

Mpa – Maximum principal stress

The values of the maximum principal tension for the four groups of resin with bracket combinations were obtained together with a color scale. The color scale allows for the visualization within the adhesive layer and the two interfaces resin/bracket [Figures 1a-d], and enamel/resin [Figures 2a-d].

DISCUSSION

As stated by Knox *et al.*^[19] there was no way to analyze every element (enamel/resin/bracket) individually in the *in vitro* mechanical test. A representative value of its strength of the resin was obtained, and this is insufficient to understand its clinical performance, as stated by DeHoff *et al.*^[14] and Wiltshire *et al.*^[7] However, it was possible to use FE to obtain information regarding the pattern of failure at the interfaces of the resin with the bracket and with the enamel, as stated by Knox *et al.*^[19] Knox *et al.*^[15] and Viana *et al.*^[24] This was due to the utilization of an accurate geometric model and the characterization of the materials.

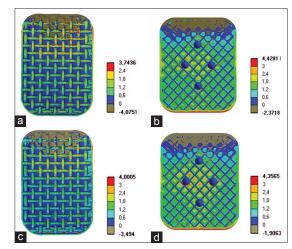


Figure 1: Distribution of the maximum principal stress at the resin/bracket interface for Group 1, Group 2, Group 3 and Group 4

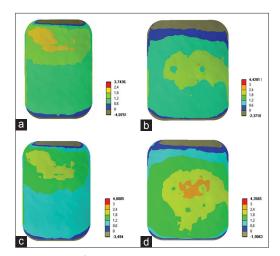


Figure 2: Distribution of the maximum principal stress at the resin/enamel interface, for Group 1, Group 2, Group 3 and Group 4

The *in vitro* shear bonding strengths of TransbondTM XT and Enlight® result were 17.26 and 18.44 MPa, respectively. These results are similar to those obtained by Scougall-Vilchis *et al.*, $^{[25]}$ who also found higher strength using Enlight® resin.

The flexibility of orthodontic resin can also alter its shear bonding strength. [19] Since it is related to the fluidity of the material, [9] as observed in the present study. Enlight® exhibits less strength and elasticity to flexion when compared to Transbond™ XT. This fact gives it better mechanical retention due to the outflow in the mesh size of the base of the bracket, leading to higher shear bonding strength.

Although Viazis *et al.*^[27] refer to the advantage of using ceramic brackets by forming a chemical bond using silane, the producer of the brackets used in this study (TP Orthodontics®) does not recommend the use of chemical bonding agents for any orthodontic resin. Kitahara-Céia *et al.*^[28] and Brantley and Eliades^[11] found that chemical bonding with the bracket is not favorable in orthodontics. Because there may be enamel fractures, during the de-bonding procedure. The shear bonding strength we observed is above what Reynolds *et al.*^[29] found to be the minimum adhesion values (4.9 MPa and 7.85 MPa) and above the minimum acceptable range (8 and 10 MPa) to ensure good bonding of orthodontic brackets.^[30]

The base of the ceramic bracket used in this study had four retainers in the central region but not providing greater retention [Figures 1b and d]. However, they were determinants in the failure reveled by fractography [Figures 2b and d].

Wakabayashi *et al.*^[31] found that ceramic brackets provide better mechanical retention. Applying force would result in cohesive failure^[27] in the resin as well as its interfaces. This occurred in the present study; when force was applied, there was failure at the interface with the bracket as well as with the enamel, However, it was not indicative of greater strength (16.53 MPa and 17.05 MPa) in relation to the values for the metallic bracket groups (17.99 MPa and 19.83 MPa). Other than the square reentries in the ceramic bracket base, its four circular retainers promoted the distribution of traction forces around the center [Figures 2b and d], which caused a failure in the enamel. This did not happen with the metallic bracket, as stated by Kitahara-Céia *et al.*^[28]

Beyond the affirmation of Karamouzos *et al.*,^[32] the difference in this study is due to the different base designs of the brackets used [Figures 1a and c]. As stated by Sharma-Sayal *et al.*,^[9] when the resin penetrates the base, the shear bonding strength also improves, because the bracket with a more retentive mesh size and more fluid resin permitted a better union, and thus, Group 3 (Enlight® + Twin-Edge®) had the highest shear bonding strength (19.83 MPa).

The greatest changes in the *in vitro* strength and the distribution of tensions recorded by FE were related to the bracket variable [Figures 1 and 2] and force application, since Klocke *et al.*^[33] concluded that there are significant differences in results due to the changing of the site of force application. Loading was performed at the base of the bracket as at *in vitro* experiments.

Liu *et al.*^[34] and Lin *et al.*^[8] utilized a detailed model of the resin/enamel interface. However, in the *in vitro* mechanical test in the current study, we only observed a predominance of adhesive failure with the bracket. Therefore, in the computational numerical analysis, the interface of the resin with the bracket was modeled [Figure 1], as recommended by Viana *et al.*^[24]

Knox *et al.*^[19] predicted the mechanical properties of the mesh size of the bracket base with the resin using homogenization theory.^[35] In our study, specific properties for each component were used to individualize the behavior and thereby determine the exact distribution of stresses and strains in the resin and its interfaces.

The results revealed a concentration of traction stress and strain at the interface of the resin with the enamel [Figure 2], as was also observed by Knox *et al.*^[19] The principal maximum traction stress/strain in the resin was seen when the metallic bracket [Figures 1a and c] was placed close to the site of force application, as stated by Knox *et al.*^[19] and Lin *et al.*^[8] With the ceramic bracket, the stresses and strains were concentrated on the side opposite to where the force was applied.

In the computational simulation of the deformation of the adhesive layer, we observed that with the metallic bracket, greater deformation occurred in the region in which the force was applied [Figures 3a and b]. For the ceramic bracket, although deformations were

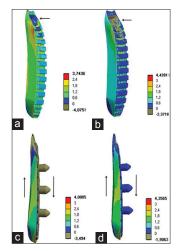


Figure 3: Tendency for deformation in the adhesive layer on an augmented scale (arrows) in the presence of sunken (a and b) metal brackets and (c and d) ceramic brackets

predominant in this same region, they occurred in a more homogeneous manner throughout the resin, with deformations on the outer part of the region opposite the force [Figures 3c and d]. These observations demonstrate that the stresses and strains spread until failure occurs. The peak stress/strain for the metallic bracket was lower, indicating that a greater amount of force was required to cause failure.

When comparing the peak stresses and strains of the FE model with those obtained from the *in vitro* experiment, the differences can be attributed to the calculation. Brackets with identical base dimensions (base and height) could have different areas. Lin *et al.*^[8] found higher principal tension value peaks using a simulation of only the micromechanical retention region of the resin tags on conditioned enamel without considering the mesh size of the bracket base as a variable. This justifies the use of a model that encapsulates all of the components in the present study, corresponding to the results of the *in vitro* mechanical test.

In fragile biomaterials like orthodontic resin, the concentration of stresses and strains on both sides of the interface can be qualitatively related to the most probable sites of initial fracture. [14,16] In FE analysis it was shown through comparison with the *in vitro* mechanical test that there was a prevalence of adhesive failure at the interface of the mechanical union with the bracket. However, it did not show better retention than seen with enamel.

FE method analysis provided an interpretation of the distribution of stresses and strains on the resin layer interface only through comparison with the in vitro mechanical test. Therefore, this was determined to be the interface most susceptible to fracture. To improve computational numerical methodology in the field of orthodontics, studies should be performed to create geometric models for every component. The micromechanical adhesion of the resin with dental enamel is determined by the materials involved, in particular, their shear strength against traction and compression as well as their flexural modulus. Because it has been shown that there is a difference between the different types of brackets, it is necessary to analyze the entire enamel/resin/bracket composite and to not attribute shear strength only to the orthodontic resin.

CONCLUSIONS

- 1. The results of the computational numerical tests agree with those obtained from the *in vitro* tests
- 2. Numerical analysis can contribute to the selection of resins and brackets, and bracket with the more retentive mesh size and the resin that is least resistant to flexion will lead to a better union.

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