Biomechanical Analysis of Orthodontic Appliances Through 3D Computer Aided Engineering

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1 STAGE OF THE RESEARCH

In the field of dental health care, misaligned teeth can cause aesthetic and functional problems for the patients. Different appliances have been developed to correct malocclusions, first of all the classic fixed wire appliance. In the last decades, however, research in the orthodontic field has focused not only on the effectiveness of the appliances on correcting teeth position, but also on the fulfilment of comfort issues during the treatment. For this reason, many new orthodontic appliances have been developed with the aim at being minimally invasive for the patients. In particular, lingual brackets, which are less visible than vestibular brackets and clear removable aligners, made of transparent thermoplastic material and then almost invisible, raised a growing interest.

Treatments based on clear aligners are composed of a set of thermoformed templates (Figure 1), having different shapes, which are sequentially worn by the patient (Kesling, 1943). Each aligner is shaped a bit different than the real teeth position in the mouth in order to force teeth to move in the correct position. The shape of the last aligner corresponds to the desired position of the teeth at the end of the treatment. When the dentition have reached the position imposed by the aligner, the patient can wear the following aligner which continues to move the teeth. A set of distinct templates is usually required to achieve the final desired outcome since each aligner can perform only a limited rotation and/or translation. Usually, each aligner needs about two weeks to completely exert its specific function. When the dental technician started to produce the first aligners, about 70 years ago, they were made designing manually each of them. The technician used a plaster cast of the mouth and moved the teeth in the desired position for the creation of the first aligner, then he had to repeat the process until the last aligner of the treatment. Nowadays through the increase of CAD systems the design process has become faster and has changed the market of these appliances. The aligner's producers have changed from small local laboratories to industries which can serve a large amount of patient all over the world. (Beers, Choi, and Pavlovskaia, 2003).

Figure 1: Example of a thermoplastic aligner.

The production process of these appliances is composed of 3 distinct steps:

- Creation of a digital model of the patient's mouth
- Design: The shape of each aligner is defined by a technician through CAD software tools. The technician designs the aligners starting from the teeth position in the mouth obtained by the digitalization process. Then following doctor's prescription which indicates the desired teeth position at the end of the treatment with the aligners the technician designs the aligners.
- Aligner production.

Actually, the design is made mainly through geometrical consideration about the teeth's crown position almost neglecting the roots. This simplification can bring to erroneous prediction about the real treatment outcome. Roots can have interferences between them during the treatment causing an undesired final teeth position. Their shape also influences very much the way how the teeth move into the alveolar region.

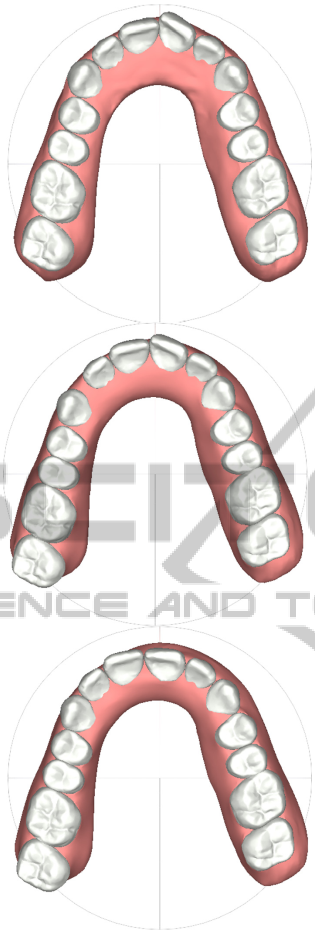

Figure 2: Virtual designed treatment. Initial teeth position (upper), half-treatment (center), end of the treatment (lower).

During the design phase, the technician can suggest to the physician the application of attachments, having particular shapes, onto some teeth in order to facilitate the load transfer between the aligner and the dentition. (Figure 3). A typical attachment consists of dental composite material which is polymerized onto the tooth surface.

Even if orthodontic treatments based on the use of clear aligners are commonly used in clinical practice there is no technical literature describing how the loads are transferred from the thermoformed aligner to the patient dentition. Since both design and production processes involves many clinical and technological skills (knowledge), the optimisation of aligners features represents one of the most challenging aspects of this kind of orthodontic treatments. The design of customised and optimised

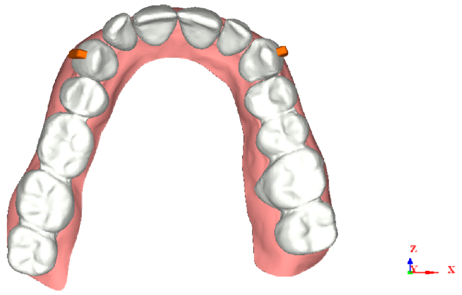

Figure 3: Attachments (orange) positioned on the two upper canines teeth that have to be rotated.

templates would be of utmost importance to obtain more effective treatment plans and accurate prediction of the achievable results.

2 OUTLINE OF OBJECTIVES

The aim of the present research consists in the development of a simulation model to be used in the design of an orthodontic treatment by using thermoformed aligners. Demanding problems are given by the understanding on how each aligner works on teeth, how load are transmitted from the aligner to the teeth and what are the effects that can be observed on the surrounding dental structures. The objective of this research is to understand limits and real effectiveness of clear aligners by using FEM simulations.

Some of the characteristics which have to be investigated and then optimised are:

- Composite attachments shape and dimensions with the aim at facilitating teeth movements;
- Aligner thickness;
- Aligner material properties;
- Treatment strategies.
- Production process
- Model verification

3 RESEARCH PROBLEMS

Concerns encountered in the first part of the study can be catalogued into three categories:

- Creation of an accurate 3D patient mouth model;
- Estimation of the mechanical properties characterising the involved dental structures;
- Contact modelling between teeth and aligner;

3.1 Geometry Creation

The creation of a customised 3D digital mouth model represents the starting point for each simulation. This model should accurately reproduce both bone and dental structures of the patient. Recent developments in digital imaging techniques have allowed a wide spread of three-dimensional methodologies based on capturing anatomical tissues by different approaches, such as CBCT, three-dimensional photography and surface scanning. (Barone et al., 2013b). Figure 4 shows an example of a patient model composed of maxillary bone and teeth with their roots . Combining optical and radiographic technologies (CBCT, Orthopantomography) allows the evaluation of roots morphology that usually is not available while designing an orthodontic treatment with clear aligners.

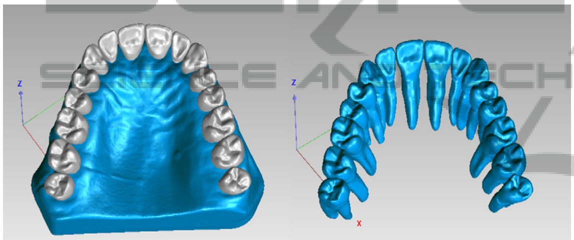

Figure 4: Reconstructed geometry of maxillary bone and teeth(left) and teeth with roots reproduction.

A further problem is related to the aligner modelling. The aligner is supposed to have a constant thickness of 0.7 mm originating from the mean thickness of the thermoplastic material disk (having 0.75 mm thickness) after the thermoforming process (Ryokawa, Miyazaki, Fujishima, & Maki, 2006).

However, possible thickness variations may occur after the thermoforming process and should be taken into account. Discontinuities in the aligner thickness could modify its mechanical behaviour during the orthodontic treatment.

3.2 Material Properties

Material properties must be correctly assigned to each component of the model. Scientific literature has been used to identify teeth and bone properties (i.e.: Young's modulus and Poisson's ratio).

Periodontal ligaments properties are rather characterised by different values and theories which vary from linear elastic models to multiphase models through literature (Fill, Toogood, Major, and Carey, 2012). Also for the aligner and the attachments the material properties have to be appropriately assigned. About the aligner the properties changes due to the production process must be taken into account.

3.3 Tooth-aligner Interface

A complex problem is related to the contact conditions between the aligner and the teeth. In particular, the interface between aligner and tooth must be modelled. When simulations concerning fixed orthodontic wires have to be performed, loads can be supposed as concentrated and transferred through a single point of the tooth crown. In many cases, the wire can be neglected since not meaningful for the simulation results except when the aim of the study is to investigate the stress generated along the wire (Penedo, Elias, Pacheco, and de Gouvêa, 2010). When a clear aligner is used, the transferring interface is represented by the overall tooth crown geometry and the load distribution over the contact surfaces is unknown. The aligner could be disregarded within the model in order to have faster simulations. This could be possible only if the load distribution would be known. However, the exact formulation of this distribution represents a difficult task due to the high irregular and patient-specific shape of the dentition.

4 STATE OF THE ART

Several studies about orthodontic biomechanics have been performed by considering the problem from different point of views. In the last few years, some researchers have reported results of orthodontic FEM simulations, starting from single tooth models (Penedo, Elias, Pacheco and de Gouvêa, 2010) to more complex multi-teeth models (Field, et al., 2009). However, the majority of the presented models refer to fixed orthodontic appliances and only few studies focused on the study of orthodontic treatments through clear aligners by using FEM models (Martorelli, Gerbino, Giudice and Ausiello, 2013). Some recent experimental studies have been focused on the measurement of load and torques applied by an aligner onto the dentition model using electronic devices based on strain gauges which are connected to a replicated teeth arch (Hahn, et al., 2010). Other studies used a pressure measurement film in order to evaluate the force transferred by the aligner to the teeth. (Barbagallo, Shen, Jones, Swain, Petocz and Darendeliler, 2008). Useful studies have been published about the material properties of some different thermoformed aligners and can probably help us in the research development (Kohda, Iijima, Muguruma, Brantley, Ahluwalia, and Mizoguchi, 2013). Some studies are related to the material properties before thermoforming while others investigate the mechanical properties after thermoforming and trying to replicate the real working environment of the aligner (Ryokawa, Miyazaki, Fujishima, and Maki, 2006).The mechanical properties of the dental structures have been well studied and the properties of tooth and bone structures are almost the same in most of the papers, but there is a different situation regarding the periodontal ligament.

A lot of literature regards the periodontal ligament mechanical properties. However, it is really hard to investigate its in-vivo properties due to its small dimensions (about 0.2 mm thickness). For this reason, the majority of the available papers investigated the mechanical properties of the periodontal ligament through experimental analyses.

Typical values for the periodontal ligament Young Modulus (E) vary from 0,059 MPa to 1750 Mpa (Fill et al., 2012). This great difference is due to the different assumptions and the different environments considered in each research. Some of the experiments have been performed during masticatory load simulation (Natali, Pavan and Scarpa, 2004)while some others during orthodontic simulation (Penedo, Elias, Pacheco, & de Gouvêa, 2010). Another reason of this results are the biological differences between the subjects considered in each research. All the assumption made by researchers caused a great variability of the properties estimated for the periodontal ligament.

5 METHODOLOGY

5.1 Geometry Creation

In the present study, dental data, captured by independent imaging sensors, are fused to create multi-body orthodontic models composed of teeth, oral soft tissues and alveolar bone structures. The methodology is based on integrating CBCT and surface structured light scanning (Barone et al., 2013a). An optical scanner is used to reconstruct tooth crowns and soft tissues (visible surfaces) through the digitalization of plaster casts. These data are also used to guide the segmentation of internal dental tissues (tooth roots) by processing CBCT data sets. The 3D individual dental tissues obtained by the optical scanner and the CBCT sensor are fused within multi-body orthodontic models with minimum user interaction. The final orthodontic model is provided by the fusion of the multi-modal data sets including the most accurate representation for each tissue: i.e., tooth crowns and gingiva by optical scanning and tooth roots and alveolar bone by CBCT imaging. The created anatomical geometry is converted into "*Iges*" models in order to be imported within a Finite Element modeller software (Ansys® 14). The periodontal ligament has been modelled as an uniform 0.2 mm thickness shell between tooth and bone (Figure 5).

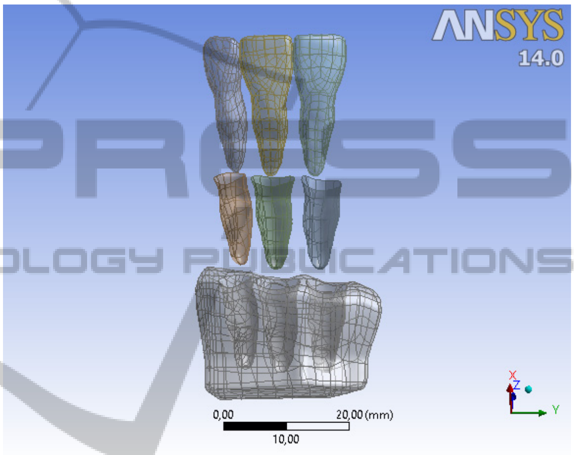

Figure 5: View of the model with three teeth with their periodontal ligaments and underlying bone.

The aligners are always created by thermoforming a disc of thermoplastic material on a cast obtained by a rapid prototyping machine. The disc thickness can vary depending on the producer, but an often used thickness is 0.75 mm, so has been decided to start the study using this value. To simulate the aligner creation the teeth have been combined and the resulting object has been cut manually over the gingival margin to obtain a thin object (0.7 mm) that wears well on teeth surfaces. Assuming a constant thickness for the aligner is a simplification that can bring to some errors in the simulation results, so an alternative way can be to create the model for the aligners using an optical scanner to acquire the aligner geometry and then to create the geometry readable by the finite element modeller in order to have a more realistic model.

5.2 FEM Simulation

The bodies have been meshed dividing them into solid and shell bodies. The teeth, bone and the

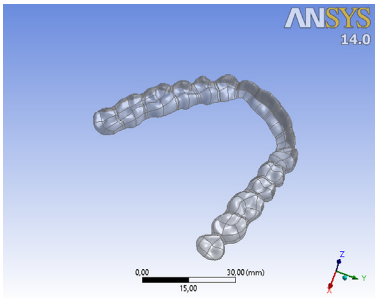

Figure 6: Model of the orthodontic aligner.

attachment have been modelled as solid bodies using tetrahedrons. The periodontal ligaments and the aligner have been modelled as shell bodies due to their small thickness.

The simulation phase started with the creation of a single tooth model, then the complexity has been increased in order to obtain a more complete and realistic simulation.

For the single tooth model has been used an upper central incisor. The single tooth model has been used only in the first time while trying to replicate a well working model for orthodontic simulation with brackets (Penedo, Elias, Pacheco, & de Gouvêa, 2010). Couldn't be used the single tooth model while simulating the treatment with the removable aligner because is not possible to model the mesial and distal extremity of the aligners. Cutting the aligner at the mesial and distal side brought to an erroneous result because the aligners completely followed the tooth while not having any grip point. Also closing the aligner on the mesial and distal sides brought to the same problems, so has been used this model to simulate a torque movement and to "validate" the chosen model.

With three teeth the aligner has the right grip point to generate forces on the teeth. The three teeth model comprised the upper central incisor and the two neighbours teeth. The first simulation was related to a 2° clockwise rotation of the upper central incisor. The simulation was performed using three different appliances features. In the first case was used a common clear aligner, in the second case has been added a composite attachment on the tooth that is commonly used to help this kind of tooth movement. In the third case we used an aligner with an introflection on the lingual surface and an introflection on the vestibular surface that are positioned in order to concentrate the force on the tooth and are supposed to help achieving a better result.

The idea for the next phases of the research is to perform the simulation using a full dental arch to have a more realistic situation and simulating different shape and dimensions of the composite attachments and different aligner thickness to find the best configuration for the different teeth movements. Then could be simulated a complete treatment of a set of aligners that involves bone remodelling evaluations (Qian, Fan, Liu and Zhang, 2008).

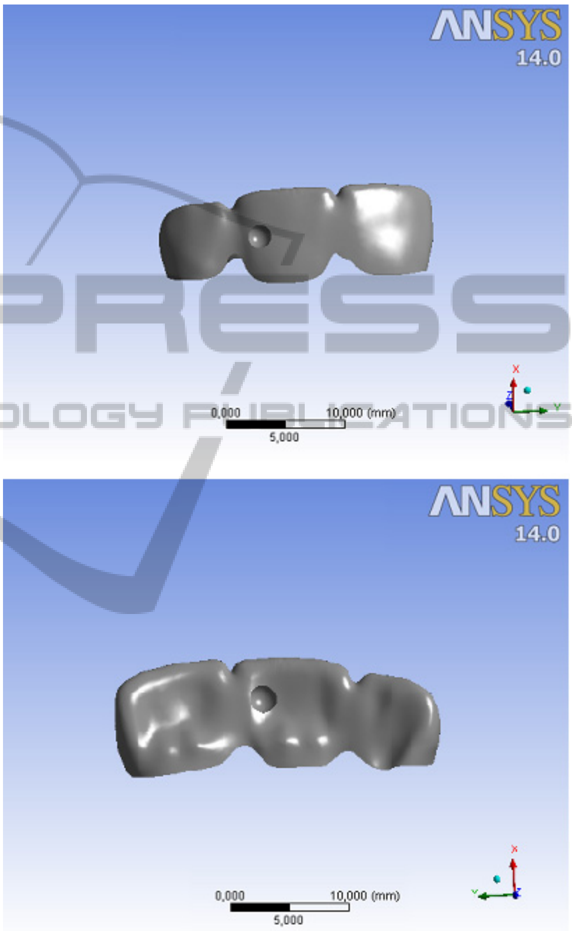

Figure 7: Introflection on vestibular and lingual surfaces.

5.2.1 Material Properties

Data have been then transferred to the finite element modeller (Ansys® 14). The structures of the mouth have been distinguished in three different parts:

- Bone;
- Teeth;
- Periodontal ligaments.

There is no distinction between Cancellous and Cortical bone, because of the very higher stiffness of the second one. For the same reason also the teeth are not divided into: Dentin, Enamel, Pulp, but each tooth is considered a homogeneous body .This

simplification has been made in previous studies (Penedo, Elias, Pacheco and de Gouvêa, 2010) to save computational time without losing many information if the aim of the research it's not to study the single part, but as in this case to evaluate the effects of the treatment in a more macroscopic way.
The material properties that have been used are:

Table 1: Material properties.

	Young's Modulus [MPa]	Poisson's Ratio
Tooth	20000	0.3
Bone	13800	0.3
Periodontal ligament	0.059	0.49

The most difficult choice regards the model to be used to simulate the ligament properties since many are the biomechanical models available in literature.

Some researchers assumed a viscoelastic model for the periodontal ligament(Su, et al., 2013), which seems to simulate well the time-dipendent properties of the ligaments.

However in this phase of the research, the linear elastic model has been used since the project is more focused on the comparison of the results obtained by using different properties of the appliances rather than on the study of the behaviour of the ligament itself. In a further stage of the research, different assumptions regarding the periodontal ligament model could be introduced in order to refine the investigations.

5.2.2 Boundary Conditions

The tooth and the ligament are joined by a bonded contact which allows only small sliding movements between joined nodes. The same connection has been used to join bone and ligament. The mesial and distal faces of the bone have been fixed to the ground (Figures 8-9).

5.2.3 Creating Teeth-aligner Displacement

The created aligner is completely congruent with teeth. For this reason, a difference between aligner and dentition geometry has been generated in order to simulate a real treatment condition. As a first example, the treatment simulation during the rotation of an upper central incisor has been investigated. This has been done through the finite element modeller by defining the tooth principal axis and clockwise rotating the upper central left incisor by 2° around its axis.

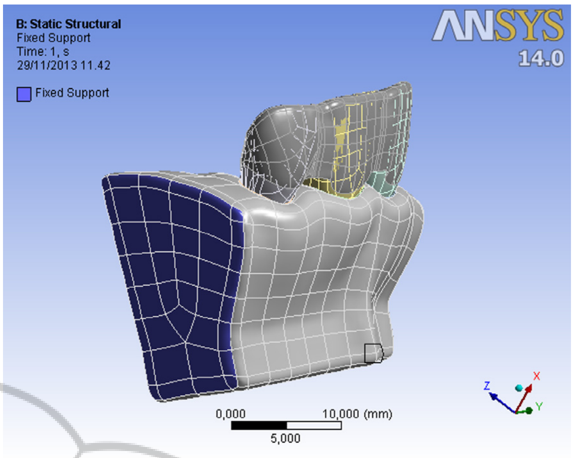

Figure 8: Distal view of the model.

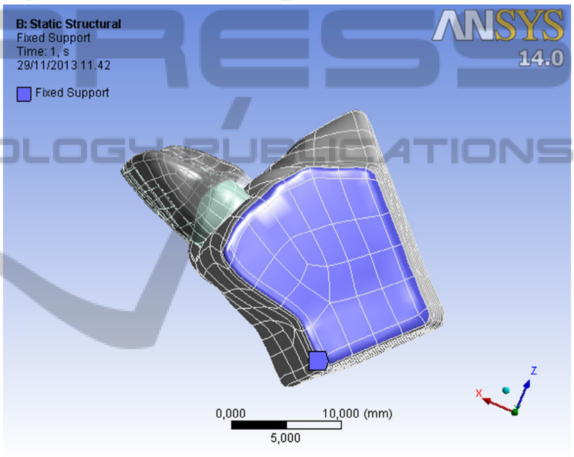

Figure 9: Mesial view of the model.

5.2.4 Analysis Settings

Once the models are created, two are the possible strategies to solve the problem. The first one consists of positioning the aligner onto the dentition and let the software to solve the contact problem in order to obtain a stable condition. In a second strategy, the aligner is positioned over the teeth (Figure 10) and then it is slowly moved until it reaches the contact condition with teeth. This second approach, which needs more computing time, gives further information about the use of the aligners in orthodontic treatments. It is indeed possible to analyse the wearing phase, which is characterised by high and not negligible stresses. Moreover, the evaluation of the stress distribution could allow the prediction of possible aligner fractures.

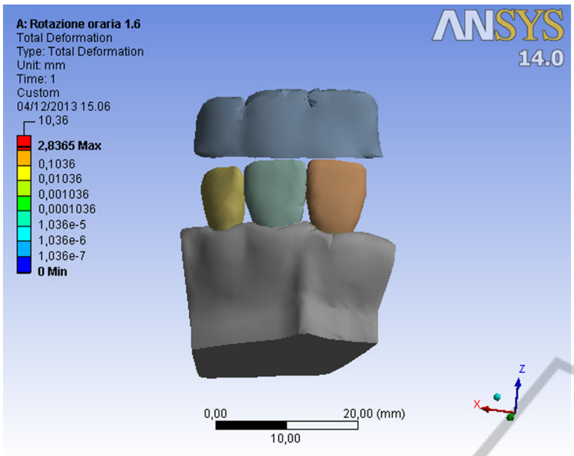

Figure 10: Aligner over the teeth at the starting point of the simulation.

5.3 Model Validation

After obtaining the desired results from the simulations will be performed an experimental validation comparing them with that obtained by other techniques. Some ideas are:

5.3.1 Photoelasticity

Photoelasticity is a full-field technique which directly provides the information of principal stress difference and the orientation of principal stress direction by fringe analysis of components made of birifrangent materials. The thermoplastic material which composes the aligner is transparent and is characterized by having photoelastic properties. The introduction of customized photoelastic analyses for real components would greatly enhance the detection of possible criticalities arising from a challenging application such as the optimisation of removable aligners.

5.3.2 Electronic Measurement Device

Some researchers have developed electronic systems, based on strain gauges, able to measure forces and moments during a simulation of an orthodontic treatment. The comparison between the FEM model with the measurements obtained by the electronic device can give an idea about the accuracy of the model. (Hahn et al., 2010)

5.3.3 Clinical Tests on Real Patients

The best way to validate the model would rely on the comparison of the numerical results with those obtained by clinical tests involving real orthodontic treatments.

6 EXPECTED OUTCOME

The present research project is focused on the study of how the orthodontic aligners work and on the optimization of their design process. The appropriate definition of parameters as shape, dimensions of attachments, thickness and material of the aligner would allow the definition of a more predictable treatment. Moreover, shorter treatment times would be characterized by less discomfort for the patient and lower costs since performed by a lower number of aligners.

The results obtained by this research could be also used to extend the use of invisible aligners to malocclusion problems which are presently treated by different orthodontic appliances, and to improve their production process.

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