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Authors: **S. Barone, A. Paoli, A. V. Razionale, R. Savignano**

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Computer aided modelling to simulate the biomechanical behaviour of customised orthodontic removable appliances

S.Barone, A. Paoli, A. V. Razionale, R. Savignano

Abstract

In the field of orthodontics, the use of Removable Thermoplastic Appliances (RTAs) to treat moderate malocclusion problems is progressively replacing traditional fixed brackets. Generally, these orthodontic devices are designed on the basis of individual anatomies and customised requirements. However, many elements may affect the effectiveness of a RTA-based therapy: accuracies of anatomical reference models, clinical treatment strategies, shape features and mechanical properties of the appliances. In this paper, a numerical model for customised orthodontic treatments planning is proposed by means of the finite element method. The model integrates individual patient's teeth, periodontal ligaments, bone tissue with structural and geometrical attributes of the appliances. The anatomical tissues are reconstructed by a multi-modality imaging technique, which combines 3D data obtained by an optical scanner (visible tissues) and a computerised tomography system (internal tissues). The mechanical interactions between anatomical shapes and appliance models are simulated through finite element analyses. The numerical approach allows a practitioner to predict how the RTA attributes affect tooth movements. In this work, treatments considering rotation movements for a maxillary incisor and a maxillary canine have been analysed by using multi-tooth models.

Keywords: orthodontic tooth movement, removable thermoplastic appliance, anatomical modelling, numerical analysis

1 Introduction

Orthodontics is the branch of dentistry dealing with diagnosis and care of irregular bites. In the last few years, the interest for adult orthodontic corrections has raised the requirement of aesthetic alternatives to conventional fixed devices. In this context, the use of Removable Thermoplastic Appliances (RTAs) [1] is becoming increasingly common for minimally invasive treatments.

A clinical RTA-based treatment [2] consists of a set of thermoformed templates that are sequentially worn by patient. The system of forces and moments to correct malocclusions is generated by the difference between the appliance shape and the dentition geometries. A single template is able to perform only a small part (from 0.15 to 0.25 mm for translations and no more than 2 degrees for rotations) [1,3] of the complete tooth movement. Therefore, a full treatment consists of a set of templates with varying shapes from the initial anatomical geometry to the target tooth positions. The number of appliances depends on the amount of the desired movements, as well as on the individual biological response. Usually, each template needs about two weeks to exert its specific mechanical function.

In clinical practice, the conventional approach to orthodontic diagnoses and treatment planning processes relies on the use of plaster models of the patient's mouth. Dental technicians manually analyse and modify plaster dentitions in order to simulate and plan corrective interventions. The appliances are then created by using proper physical set-ups for every desired tooth movement. These procedures require labour intensive and time-consuming efforts, which are mainly restricted to experienced technicians. Nowadays, the developments of Computer-Aided Design (CAD) methodologies have made the orthodontic treatment planning faster and more accurate through the use of virtual 3D models of patients' dentitions [4].

Even if RTA-based orthodontic treatments are becoming an effective solution for moderate to complex malocclusions [3], most of the technical literature is focused on case reports and system descriptions. There have been few evidence-based attempts to describe the RTA behaviour in delivering forces able to produce specific tooth movements. The ability to make an accurate treatment prediction has long been a challenge for orthodontists, since many parameters may affect the clinical outcome. In these circumstances, a better understanding of how tooth movements are achieved would allow the design of optimised appliances leading to more efficient orthodontic treatments.

The present paper aims at developing a simulation model to be used during the design phase of a RTA-based orthodontic treatment. In particular, a patient-specific 3D finite element method (FEM) model has been created to investigate the influence of both RTA geometrical and structural attributes on the correction of mal-positioned teeth. This model encompasses individual patient's teeth, including root geometries, periodontal ligaments (PDL), alveolar bone and the thermoplastic appliance. The patient's anatomical model is created by integrating multi-modality data captured by independent imaging sensors. An optical scanner, based on a structured light approach, is used to reconstruct tooth crowns and oral soft tissues while Cone Beam Computed Tomography (CBCT) imaging is used to obtain tooth roots and the alveolar bone geometry. A customized multi-body orthodontic model, composed of teeth, oral soft tissues and bone structures can then be created. An orthodontic appliance is modelled by exploiting boolean operation through a CAD software, in order to replicate the appliance manufacturing process. The interactions between anatomical tissues and appliance structures are simulated through finite element analyses. The virtual model allows geometrical and mechanical appliance attributes to be tuned in order to obtain the target tooth movements. The approach detailed in the paper is based on an enhanced interaction between the RTA designer and the patient anatomy, through an extensive use of virtual and numerical models, with the aim at customize and optimize the appliance's behaviour. The present study can be seen as a first step towards the development of a fully interactive modelling tool for the real-time planning of customised orthodontic treatments by using removable appliances. In this paper, some case studies including rotations for a maxillary incisor and a maxillary canine have been analysed to evidence how different design choices affect the tooth movements.

2 RTA-based orthodontics

Nowadays, design and manufacturing of RTAs for orthodontic applications are generally based on an extensive integration (Figure 1) between patient's anatomy reconstruction, CAD tools and Rapid Prototyping (RP) techniques [4,5]. The digital reconstruction of an actual patient's dentition can be carried out by optically scanning a plaster model or directly the patient's mouth. Segmentation tools are used on the 3D mouth model to separate the individual tooth shapes from the soft tissue representation. A 3D virtual planning of the treatment is then carried out by specialized technicians, who plan tooth movements, within a CAD system, according to clinician's prescriptions. 3D tools allow geometrical (i.e., available space) and functional constraints (i.e., occlusion condition) to be verified, thus guiding the technician during the tooth re-positioning process performed by shifting or tilting movements. The whole treatment is finally partitioned into smaller sequential movements of the teeth over the course of the treatment: from the initial actual condition to the final expected outcome. A 3D physical mould of the teeth is then manufactured by RP methodologies for each single step of the sequence. The custom appliances are then produced from the prototyped moulds by a vacuum thermoforming process. A single thermoplastic polymer resin sheet (about 0.75 mm thick) is stretched over each prototyped mould and trimmed to extract the final configuration.
Actually, the orthodontic treatment design is made on the basis of geometrical considerations about the tooth crown position, almost neglecting root movements. However, this simplification can bring to erroneous predictions about the real treatment outcomes, since the estimation of the tooth centre of resistance cannot exclude tooth root geometries. Moreover, possible collisions between adjacent roots should be monitored, since root movements can be significant, even for small crown displacements.
Another crucial aspect of a RTA treatment concerns the use of auxiliary elements, such as attachments, divots and power ridges. These elements facilitate the load transfer between the appliance and the dentition. Figure 2 shows an example of digital dentition model including prismatic attachments. Disposition, shape and number of the attachments are usually settled by practical experiences, without an optimisation analysis of these attributes and an identification of the RTA limits when the correction of complex malocclusions must be faced. Nowadays, numerical methodologies would allow a reliable simulation of orthodontic behaviours, even for individual clinical cases. However, the research activities have been mainly focused on the analysis of the

traditional orthodontics (i.e., fixed brackets), whereas few attempts have been made for the biomechanical modelling of RTA-based treatments.

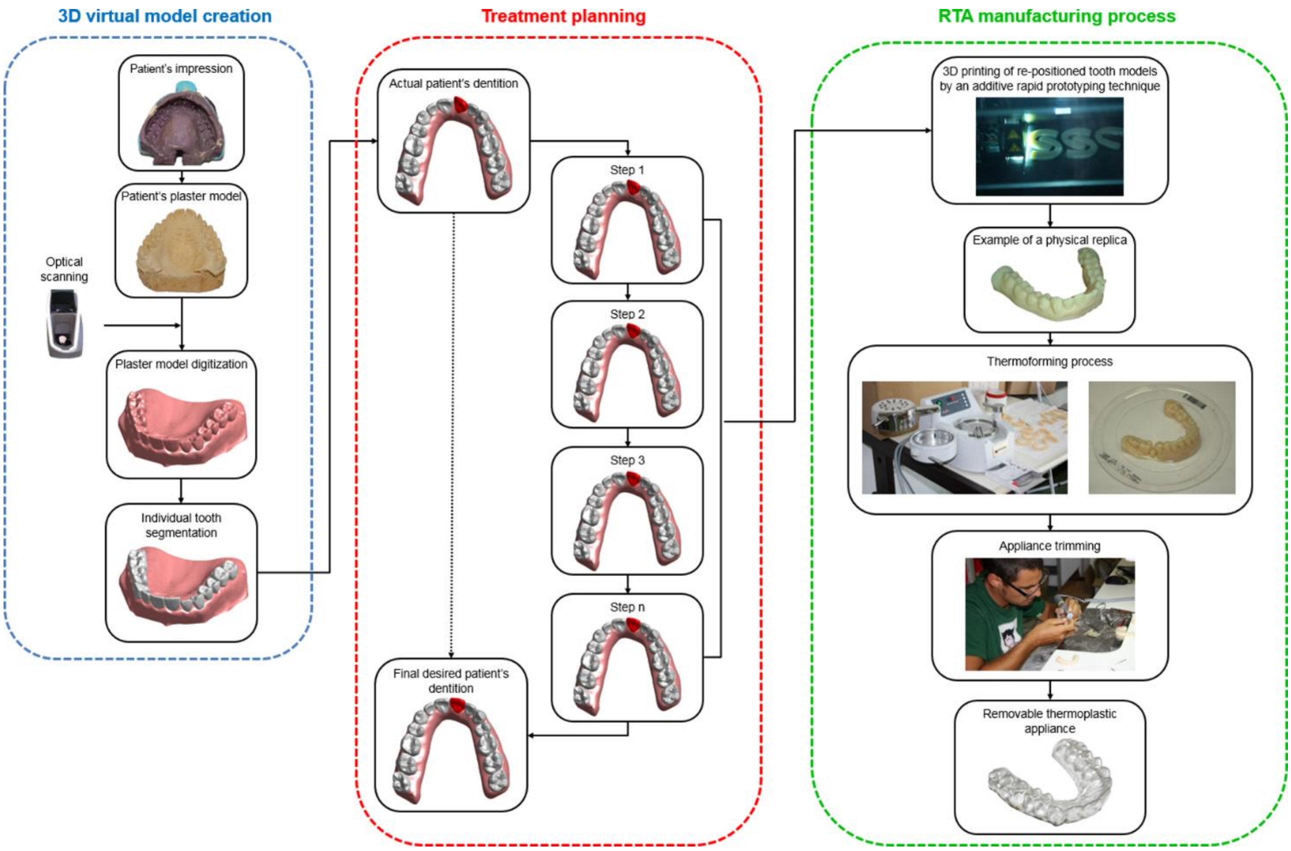


Figure 1 – Flowchart of a typical manufacturing process for the production of customised orthodontic removable thermoplastic appliances.

Figure 2 – Prismatic attachments (highlighted with an orange colour) positioned on the two upper canines teeth to be rotated.

3 Experimental and numerical methods in orthodontics

There is a wide literature addressing the use of numerical methods in orthodontics. Current research trends can be catalogued into three different categories: 1) creation of reliable orthodontic FEM models, 2) characterization of PDL mechanical properties, and 3) evaluation of the effectiveness of RTA for orthodontic tooth movements.

The use of finite element analysis (FEA) approaches for the simulation of orthodontic treatments is a research field that has attracted many authors, each of them looking at the issue from a different point of view. Most of the existent papers, however, concern with treatments performed by fixed wires [6-10], whose modelling process greatly differs from that occurring when RTA are used. The main difference can be ascribed to the load application area. When fixed wires are used, the imparted forces can be simplified as concentrated in pre-determined points, thus allowing the wire geometry to be disregarded. Instead, a different behaviour has to be modelled using a thermoformed appliance. In particular, geometries and materials are responsible for the forces transferred through the overall tooth contact surface. In the last few years, FEA results have been reported by considering single tooth models with either concentrated loads [7] or more complex multi-tooth models which also accounted for orthodontic wires modelling [8].

The mechanical properties of dental structures have been thoroughly evaluated and researchers have mainly modelled biological tissues by using linear elastic constitutive models. This choice is well accepted for what concerns hard tissues (bone and tooth), but it does not represent the best solution to describe the mechanical response of the most deformable constituent, i.e. the periodontal ligament [11]. The PDL is a dense, fibrous, connective tissue that surrounds the tooth root and connects the tooth to the alveolus. It is generally accepted that the functional role of the PDL is primarily tooth support. The PDL is constituted of a bundle of fibres immersed in a fluid and its mechanical behaviour is hard to be understood and modelled due to its complex structure. Research in PDL biomechanics has essentially focused on four specific types of structured constitutive modelling approaches: linear elastic models, bilinear elastic models, multiphase models and viscoelastic models [12]. The last two models are more complex than the others, but they seem to better approximate the PDL behaviour. Regarding the linear elastic models, there is a great difference in the Elastic modulus evaluated by the researchers. Typical values for the PDL Modulus of Elasticity (E) vary from 0.059 MPa to 1750 MPa [12]. This great difference is mainly due to the different assumptions and the different environmental conditions considered for each test case. Some of the experiments have been performed for masticatory load simulations [13], whereas others for orthodontic simulations [7]. Moreover, discrepancies may be ascribed to the biological difference between the subjects considered within each research activity. The PDL is the main responsible for the orthodontic movement. When a load is applied to the teeth, it is transferred to the ligaments that incur in compression and tension. The bone necrosis process is initialized in correspondence of the compression side while the osteogenesis process is initialized on the tension side. It has been established that these two actions only begin if the stress along the PDL's fibres exceeds the pressure value inside the blood capillary vessels in the alveolar region (0.0026 MPa) [7]. Stress values into ligaments must be taken into account also in order to foresee the root resorption process, which seems to be generated by combinations of root and PDL stresses [14].

Only few papers have been published about the behaviour of RTA during orthodontic treatments [15-21]. Some researchers evaluated the forces delivered by the appliances by using strain gauge measurement systems joined with a replicated dental arch [15-17]. However, these in-vitro studies were limited on measuring the forces on a single tooth (the maxillary central incisor) by using custom made force-measuring systems and resin models. An in-vivo experimental study was carried out by [18] in order to measure buccal tipping movements of the upper first premolar through a pressure-sensitive film approach. A film was interposed between dentition and RTA during the treatment in order to obtain measurements of the forces imparted by the appliance. Ryokawa et al. investigated the mechanical properties of the thermoplastic disk after the thermoforming process by replicating the real working environment of the appliance [19]. A further study evaluated the changes of the mechanical properties of a thermoplastic appliance after the thermoforming process [20]. Only a paper considered a FEA approach for an orthodontic treatment carried out by removable appliance by focusing on the structural differences between appliances made with different manufacturing technique [21].

The aim of the present paper is to establish a numerical model, which allows the simulation of patient-specific RTA-based treatments. Numerical analyses, carried out by means of the finite element method, provide a powerful tool for the evaluation of the appliance attributes and can be used for an extended and accurate assessment of orthodontic tooth movements on the basis of individual clinical contexts including anatomical references, biological parameters and orthodontic targets.

4 Computer-aided modelling of RTA-based treatments

4.1 Reconstruction of patient-specific anatomical models

The accurate digital reconstruction of the patient's anatomical tissues (bones, periodontal ligaments, tooth shapes) involved in an orthodontic treatment is a challenging task. In this paper, the reconstruction of bones and teeth has been performed by integrating two different imaging techniques: CBCT scanning and surface structured light scanning [22].

An optical scanner, based on a coded structured light approach, has been used to create an accurate digital model composed of visible dentition structures (tooth crowns) and oral soft tissues. The scanning process is performed onto plaster models created from patient's impressions. The overall surface representing tooth shapes and oral soft tissue is then segmented into disconnected regions, representing the individual crown geometries and the gingiva (Figure 3-a), through a semi-automated procedure, which exploits the curvature of the digital mouth model.

The CBCT data, stored in a sequence of Digital Imaging and Communications in Medicine (DICOM) images (slices), are instead used to reconstruct tooth roots and bone tissues. The optically-scanned crown models are used to guide the segmentation of CBCT images. In particular, tooth roots are individually reconstructed by processing CBCT data sets on the basis of an active contour model in a level set formulation [23]. The 3D individual dental tissues, obtained by the optical scanner and the CBCT sensor, are fused within multi-body models with minimum user interaction. The final dental model (Figure 3-b) includes the most accurate representation for each tissue: i.e., tooth crowns by optical scanning and tooth roots by CBCT imaging.

The alveolar bone is similarly segmented by processing the same CBCT data. For each slice, the regions outlined by the detected tooth contours are subtracted from the area outlined by the extracted bone contour. Tooth shapes are excluded from the alveolar bone model and replaced by the separated segmented tooth models (Figure 3-c). Therefore, each tooth can be independently manipulated within the orthodontic model, thus providing an effective tool for orthodontic simulations and treatment planning processes.

The periodontal ligaments are not discernible with a CBCT exam, due to their low thickness (about 0.2 mm) [11]. Their morphology could be acquired by a micro-CT acquisition, even if a great radiation dose would be absorbed by the patient. For this reason, the PDL has been geometrically created by detecting the intersection area between bone and tooth models to which a 0.2 mm thick shell has been added. The volume shell is then subtracted from the alveolar bone in order to define the PDL volume [24]. Finally, the bone modelling process has been performed by taking into account the division between cancellous and cortical bone, which has a mean thickness value of 0.25 mm around the teeth socket [25]. The bone volume, obtained by segmenting CBCT data, has been divided into two different regions, assuming an external layer with a 0.25 mm thickness as cortical bone and the inner part as cancellous bone (Figure 4).

The appliance geometry has been created by exploiting CAD tools in order to define a layer completely congruent with the tooth crown surfaces. All the individual teeth are firstly joined (Figure 5-a), root geometries are deleted (Figure 5-b) and the undercut volumes manually removed thus creating a unique layer (Figure 5-c). A 0.5 mm thick shell is then modelled on the layer (Figure 5-d). Finally, the original teeth are subtracted from the shell (Figure 5-e) and its external surface is removed (Figure 5-f) in order to outline the inner surface of the appliance. This procedure is carried out to guarantee an optimal fit between the mating surfaces of the tooth crowns and the removable appliance. The RTA is supposed to have a uniform 0.7 mm thickness which originates from the mean thickness of the thermoplastic material disk (0.75 mm thick) before the thermoforming process [19]. This condition will be accounted for during the creation of the FEM model.

The complete 3D model originating from the previous steps is composed of different triangular meshes (StL tessellations) describing the anatomical surfaces. A further step is required since this geometrical description is generally not suitable to perform FEM analyses. The triangular tessellations are approximated by a set of trimmed Non Uniform Rational B-Spline (NURBS) surfaces (Figure 6). The procedure consists of three phases: 1) identification of surface partitioning, 2) creation of patches, 3) surface fitting on the original triangular meshes. The first step can be either user-guided or completely automatic with different results in terms of number and arrangement of the obtained surface’s partition. The user-guided approach allows for a substantial control on both number and distribution of the surface’s parts. This procedure yields a greater accuracy in the reproduction of the original geometry. In this work, a user-guided approach has been used for teeth, RTA and PDL geometries, while an automatic approach has been used for bone geometry. During the patches creation phase, a further subdivision of the partitioned tessellations is performed. A nearly rectangular grid subdivision is defined in order provide a $m \times n$ NURBS patch. The parameters m and n are the number of control points along the principal directions. These control points are chosen with the aim at guaranteeing a trade-off between the required accuracy and the manageability of the model. The last step requires the fitting of the NURBS surface onto the original tessellated mesh. The tolerance between the target surface and the original triangular mesh can be adjusted in order to define the smoothness level of the final surface. In this paper, the selection of the tolerance value has been driven by the boundary conditions required for the finite element analyses (section 4.2.3).

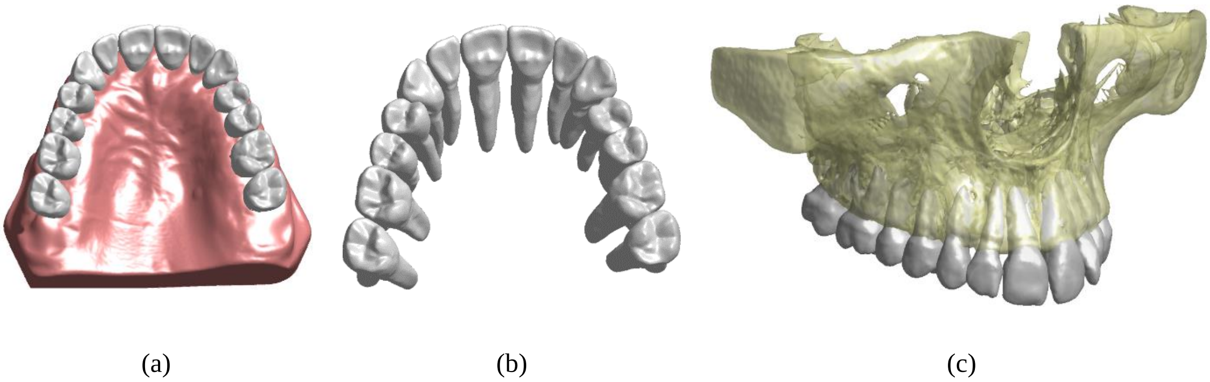


Figure 3 – (a) Crowns segmentation from the digital plaster model, (b) individual tooth anatomies including also root shapes, (c) complete model composed of tooth and jawbone geometries.

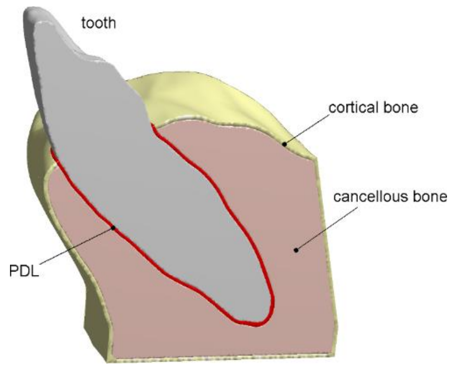


Figure 4 – Results of the PDL and bone modelling processes.

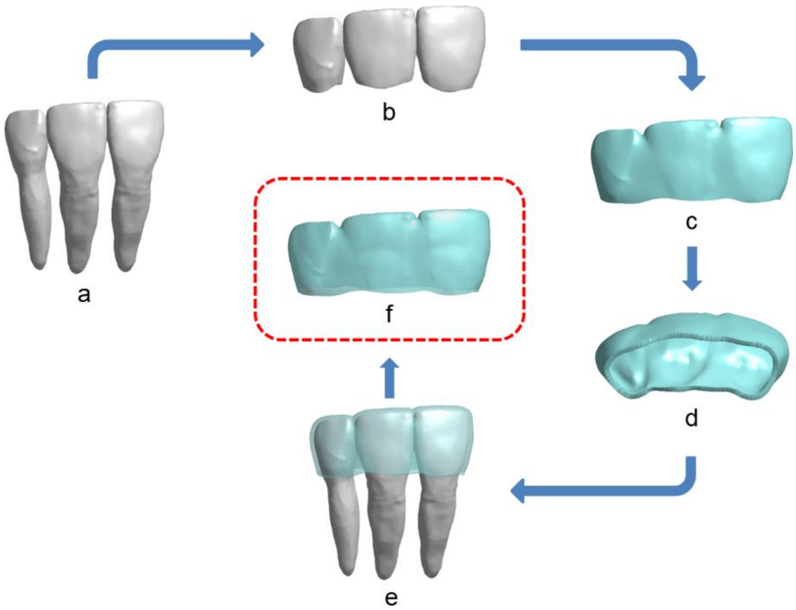


Figure 5 – Design process of the RTA geometry.

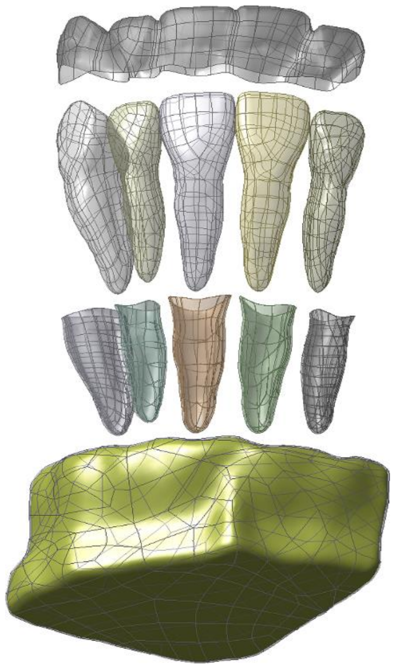


Figure 6 – Final NURBS surface models of the geometries obtained from the modelling process of bone tissue, periodontal ligaments, tooth shapes and relative RTA by considering five teeth.

4.2 Definition of the FEM model

The reconstructed surface models have been imported within the finite element modeller (Ansys® 14). All the different bodies, except for the RTA, have been meshed by using quadratic 10-node tetrahedral elements (SOLID187). These elements have been used since well suited to model irregular shapes as those characterizing the reconstructed patient-specific anatomical models which have been obtained by combining multi-modality imaging techniques. The RTA has been meshed as a shell body with a 0.7 mm thickness by using four-noded elements (SHELL181). The use of single-tooth models is not appropriate to simulate RTA treatments since neighbouring (*non-target*) teeth may affect the amount of the resulting displacement. Proper grip points, able to generate forces on the dentition anatomy, can be obtained by using at least a three-tooth model. In this paper different multi-tooth models, composed of three, five and seven teeth, have been taken into account. Moreover, the influence of attachments has been simulated by introducing prismatic elements (4.5 mm × 1.5 mm × 1 mm, *height* × *depth* × *width*) placed on the middle of the vestibular surface of the target tooth along the principal axis (Figure 7). This allows the functional simulation of composite attachments, which are typically polymerized onto the tooth surface.

The interpenetration between teeth and appliance is the main responsible of the simulation's results. Therefore, the meshing process must preserve the ideal desired interpenetration within a certain tolerance range. In this work, an initial interpenetration tolerance of ± 0.01 mm has been accepted and controlled by a mesh refinement in correspondence of the tooth cusps, preserving the higher curvature geometries. The mesh refinement allows to better approximate the computational domain geometry which primarily influence the interaction between appliance and dentition. Figure 8-b evidences the areas where the mesh enhancement has been applied while

Figures 8-a and 8-c show the two meshes before and after the refinement process, respectively. Figures 9 shows the overall different meshed models used for the simulations of three-tooth (Figure 9-a), five-tooth (Figure 9-b), seven-tooth (Figure 9-c) dentitions along with a RTA without attachments. Figures 10 show the meshed models used for the simulation of the maxillary incisor rotation (Figures 10-a and 10-b) and the maxillary canine rotation (Figures 10-c and 10-d) without and with a prismatic attachment, respectively. Table 1 summarizes the corresponding numbers of elements and nodes for the three-tooth (3TM), five-tooth (5TM), seven-tooth (7TM) models.

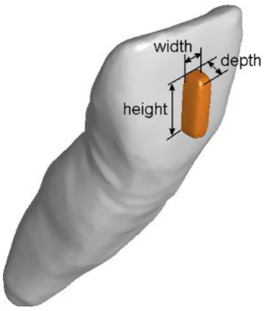


Figure 7 – Example of a prismatic attachment positioned onto a central incisor indicating the characterizing sizes.

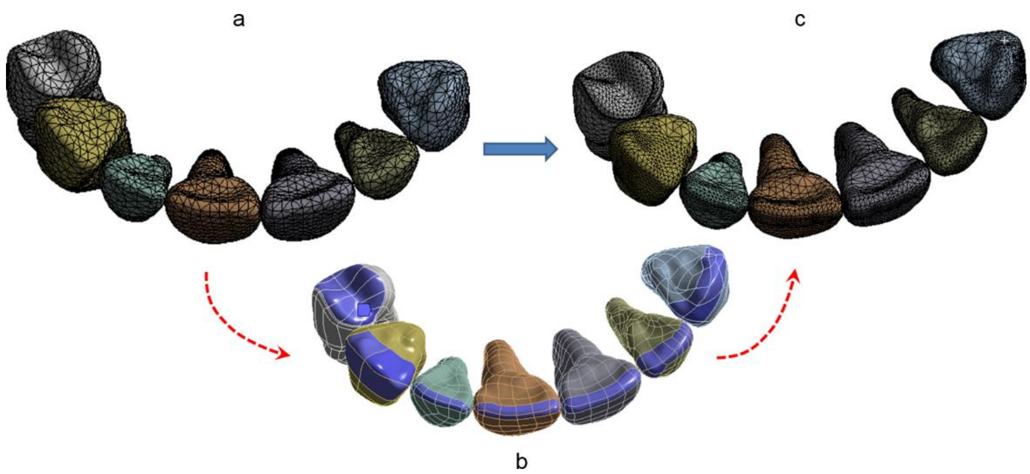
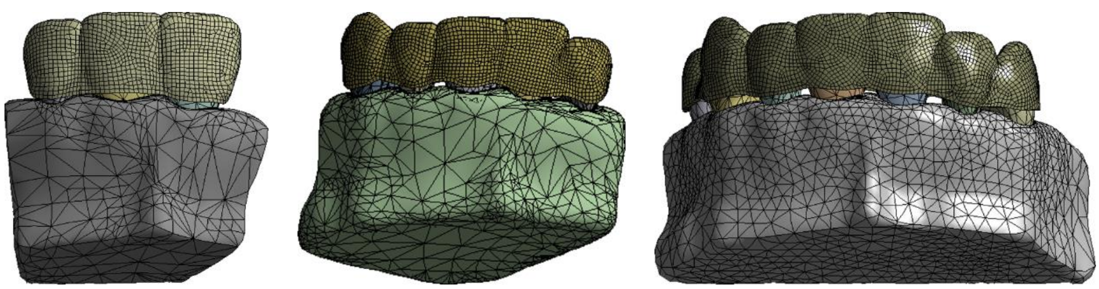
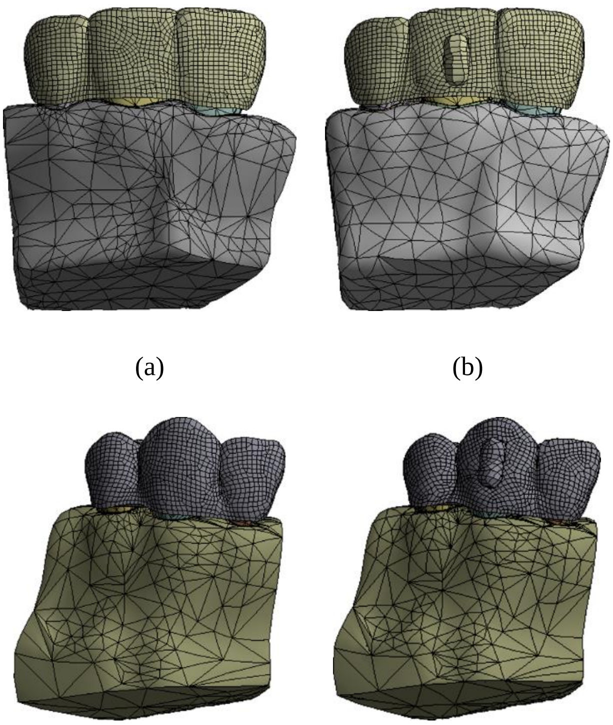


Figure 8 – Mesh before (a) and after (c) the refinement process in correspondence of the tooth cusps (areas highlighted with a blue colour (b)).



(a) (b) (c)

Figure 9 – Meshed models used for the simulations; (a) three-tooth model (3TM), (b) five-tooth model (5TM), (c) seven-tooth model (7TM), without attachments.



(a) (b)

(c) (d)

Figure 10 – (a,b) meshed models used for the simulation of the maxillary incisor rotation without (a) and with (b) a prismatic attachment; (c,d) meshed models used for the simulation of the maxillary canine rotation without (c) and with (d) a prismatic attachment.

Table 1 – Number of elements and nodes for each FEM model.

	Maxillary incisor				**Maxillary canine**	
	3TM	**3TM with attachment**	**5TM**	**7TM**	**3TM**	**3TM with attachment**
elements	107309	118540	172700	298909	141228	147993
nodes	77040	80731	122035	212840	96209	101037

4.2.1 Mechanical properties

The mechanical response of cortical bone, cancellous bone, teeth, attachments and RTA has been described by using a linear elastic constitutive model (Table 2). Dental tissue has been modelled has a uniform body without taking into account the division into dentin, enamel and pulp [7,10,11,13]. In technical literature, different biomechanical models have been proposed to simulate the PDL properties [12]. Even if the linear elastic model demonstrated to provide satisfying results for the simulation of the initial phase of the orthodontic movement [7], the adoption of a more complex model guarantees more realistic results. In this paper, the volumetric finite strain viscoelastic model has been implemented as proposed by [26]. The viscoelastic parameters were obtained through an inverse parameter identification process. Starting from a generic viscoelastic constitutive equation, parameters were optimized by exploiting a finite element analysis in order to replicate Ross experiment [27]. For each simulation, values obtained by FEA were compared with the experimental data and updated until the parameter's convergence was obtained.

The removable appliances have been simulated as made of a polyethylene terephthalate glycol-modified (PETG) thermoplastic disc, whose mechanical properties are reported in Table 2. The auxiliary attachments have been supposed to be made of the same tooth material (Table 2).

Table 2 – Material properties with reference to the adopted linear elastic models.

	E [MPa]	Poisson's ratio
Tooth	20000	0.3
Cortical Bone	13800	0.3
Cancellous Bone	1370	0.3
RTA	2050	0.3
Attachment	20000	0.3

4.2.2 Analysis settings

Simulations have been carried out in order to evaluate the behaviour of the orthodontic appliance under different conditions. In particular, two different treatments have been analysed:

- 1 degree rotation around the *x*-axis for a maxillary central incisor;
- 1 degree rotation around the *x*-axis for a maxillary canine.

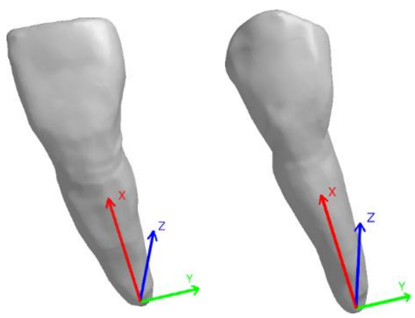
Distinct local coordinate systems have been defined for the maxillary central incisor and the maxillary canine as illustrated in Figures 11-a and 11-b, respectively. The positive *x*-axes are oriented in order to describe extrusive forces and movements parallel to the long axis of the tooth. Horizontal forces and movements are rather described in the *y*-axes and *z*-axes. For both the maxillary incisor and canine, the positive *y*-axis has been oriented in order to describe mesial movements, while the positive *z*-axis is oriented in order to describe palatal movements.

Simulations related to the first treatment, were performed by considering a three-tooth model, a five-tooth model and a seven-tooth model, without using any attachment, in order to account for the influence of neighbouring teeth onto the results. Then, both treatments have been simulated by using a three-tooth model with and without attachments.

A complex problem to be faced is related to the contact conditions occurring between the appliance and the dental anatomy. In particular, when a RTA is used, the transferring interface is represented by the overall tooth crown geometry, and the load distribution over the contact surface is unknown. This interface should be modelled in order to disregard the RTA geometry within the model and provide faster simulations. This could be possible 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, which makes unfeasible the application of external loads. For this reason, loads are introduced by rotating the target tooth by 1° around its longitudinal axis (*x*-axis) with the aim at creating an initial interpenetration between the designed RTA and the tooth anatomy. Actually, this condition is the opposite with respect to the real clinical treatment, which considers the RTA thermoformed onto the prototyped model with the target tooth already rotated. However, the resulting loading condition is formally the same with the advantage that the RTA must be modelled only once, and different orthodontic tooth movements can be analysed by simply varying the amount of tooth displacement.

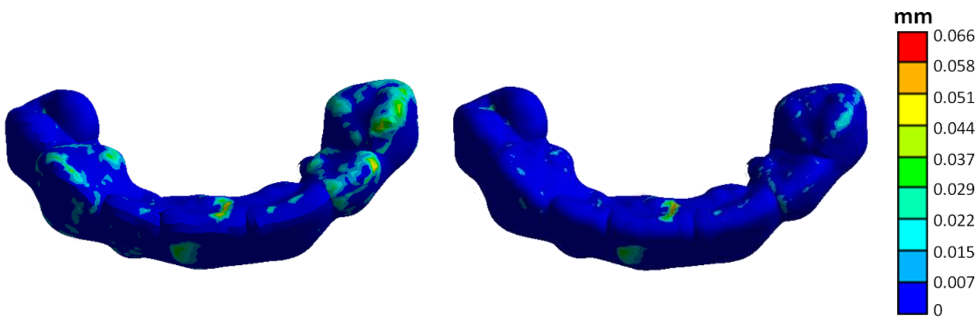
Figure 12-a shows the geometrical interpenetration between RTA and crown geometries, before the numerical simulation, obtained by rotating the maxillary incisor using the non-refined mesh model of Figure 8-a, and Figure 12-b shows the interpenetration obtained by using the refined mesh model illustrated in Figure 8-c. In practice, the mesh sizes have been iteratively refined, in correspondence of high curvature regions (i.e., tooth cusps), in order to avoid undesired interpenetration between RTA and dentition. The use of a non-refined mesh model indeed determines a considerable undesired interpenetration also on non-target neighbouring teeth (see Figure 12-a). This rough initial condition imparts forces also on teeth different from the target tooth, thus influencing the final teeth displacements.

The adopted approach allows the definition of a model, which is particularly sensitive to patient-specific geometries.



(a) (b)

Figure 11 – Tooth axes definition for the maxillary central incisor (a) and the maxillary canine (b).



(a) (b)

Figure 12 – Initial interpenetration between the RTA and the crown geometries obtained by rotating the maxillary incisor using the non-refined (a) and refined (b) mesh models. The full-field interpenetration maps are shown on the RTA geometry.

4.2.3 Boundary conditions

The bone extremities have been fixed in all directions. An augmented Lagrangian formulation has been used to simulate contact. Bonded contact surfaces have been considered between cortical bone and cancellous bone, between cancellous bone and PDL and between PDL and teeth. Corresponding nodes cannot separate each other and a perfect adhesion between contact surfaces, without mutual sliding or separation, can be assumed.
The interface between RTA and teeth, which represents the most important contact surface since responsible for the loading condition, has been rather modelled by using a frictionless model. This is a reasonable choice due to the existent dissimilarity between the appliance thermoplastic material and the dentition biological tissue taking also into account the presence of saliva.
The non-linear problem has been solved by using the Newton-Raphson residuals method based on the force and moment convergence values. The number of initial sub-steps for each simulation has been set as 100 while the contact stiffness is automatically updated at each iteration. During the Newton-Raphson iterations, the contact penetration is checked with respect to a maximum allowable penetration tolerance value, which has been defined as 0.01 mm. This value has been determined by considering that higher values significantly affect the end-result while lower values increase convergence time without entailing significant changes in the final rotations. The pinball region has been manually set to 0.1 mm in order to include all the existing interpenetration between the bodies.

5 Results and discussion

5.1 Numerical results

Initially, different simulations have been performed in order to evaluate the rotations obtained for a maxillary incisor by using multi-tooth models composed of three, five and seven teeth. All the numerical simulations have been performed by using an Intel® Xeon CPU E3-1245 v3 (3.4 GHz), 16 GB RAM test machine. Simulation time processing has been in the order of 60, 120 and 180 minutes for three-tooth models, five-tooth models and seven-tooth models, respectively. The comparison between the final rotation values points out that adding neighbouring teeth to the moving tooth does not significantly affect the simulation results (Table 3). Variations in the final rotation value (from 0.48° to 0.52°) obtained with the three models can be considered negligible.
Hereinafter, the three-tooth models have been used to simulate the attachment behaviours on both maxillary incisor and maxillary canine rotations. In particular, the numerical analyses have been performed with and without prismatic attachments in order to assess their influence on target orthodontic movements. Figures 13 show the full-field maps of the resulting tooth displacements obtained rotating the maxillary incisor with (Figure 13-a) and without (Figure 13-b) attachment and the maxillary canine with (Figure 13-c) and without (Figure 13-d) the attachment. Table 4 summarises the rotation values around the *x*-axis. The numerical results point out that the use of attachments increases the amount of the final tooth rotations for both incisor and

canine. However, it is worthwhile remarking that only the use of an attachment provides a significant rotation for the canine tooth (0.37°), while the rotation obtained without the attachment is almost negligible (0.16°).
Figures 14 show the full-field map of the von Mises stress values in the PDL obtained by using the three-tooth (Figure 14-a) and the seven-tooth (Figure 14-b) models to simulate the rotation of the maxillary incisor without attachment. Table 5 reports the maximum von Mises stress values obtained in the PDL for the analysed cases. The use of the von Mises equivalent stress value to evaluate the stress state in the PDL, bone, and tooth tissues could be questionable since it is a plastic criteria based on energy principles which involve the yield of ductile materials as metals. However, the von Mises stress criterion is often cited in biologic studies [6,8,10] and its use is usually demanded for comparison purposes.
Research works proposed in literature works [7] demonstrated that the minimum PDL stress value which originates the re-modelling bone process is 0.0026 MPa. If this threshold is not exceeded, the orthodontic movement is only temporary and the tooth could return into the initial position after removing the load. In this paper, the higher von Mises stress value (0.055 MPa) has been obtained for the rotation of the maxillary central incisor by using a prismatic attachment, thus ensuring the beginning of the bone remodelling process.
The use of three different multi-tooth models has also allowed the assessment of the behaviour of teeth, which have not been moved in the virtual orthodontic plan. The numerical results obtained for the different simulations have shown that a treatment performed by removable appliances could also cause undesired movements to non-target teeth. Figures 15-a, 15-b and 15-c show the full-field maps of these displacements, for a 1° rotation of the maxillary incisor, as obtained with a three-, five- and seven-tooth model, respectively. However, the amounts of displacements are lower if compared to those occurring for the target teeth. Moreover, among the non- target teeth, those adjacent to the targets undergo the higher displacements due to more significant anchorage reactions.
The numerical model also enables the RTA structural characterization. Figures 16-a and 16-b show the full-field maps of the stress occurring to the appliance for a 1° rotation of the maxillary central incisor without and with the use of an attachment, respectively. Figures 16-c and 16-d show similar results obtained for the 1° rotation of the maxillary canine without and with the use of an attachment, respectively. Greatest stress values on the RTA can be observed when attachments are used due to the higher forces and moments transferred in the right movement directions.

Table 3 – Rotation values, around the *x*-axis, obtained for a maxillary incisor by using three different multi-tooth models.

	Maxillary incisor		
	3 TM	**5 TM**	**7 TM**
Rotation around *x*-axis [°]	0.48	0.52	0.49

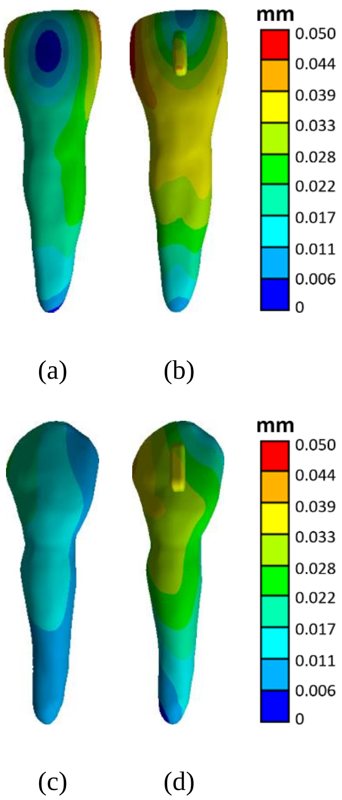


Figure 13 – Full-field maps of the tooth displacements obtained rotating the maxillary incisor with (a) and without (b) attachment and the maxillary canine with (c) and without (d) the attachment.

Table 4 – Rotation results around the *x*-axis for each simulation.

	Maxillary incisor		**Maxillary canine**	
	3 TM	**3 TM with attachment**	**3 TM**	**3 TM with attachment**
Rotation around *x*-axis [°]	0.48	0.56	0.16	0.37

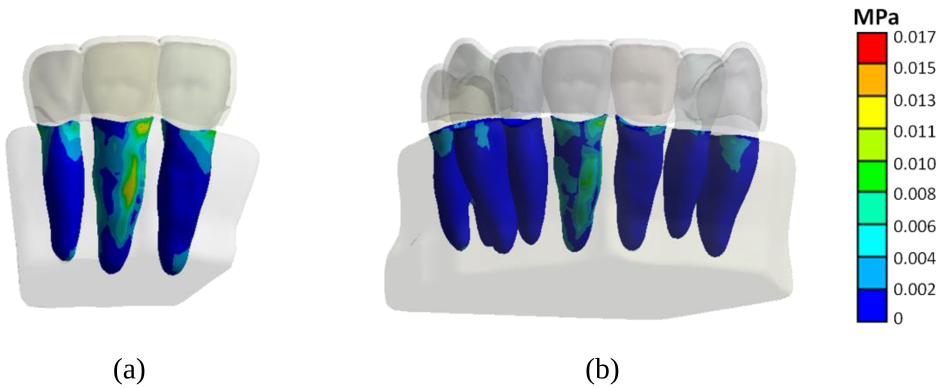


Figure 14 – Full-field maps of the von Mises stress values in the PDL obtained by using the 3TM (a) and 7TM (b) models to simulate the rotation of the maxillary incisor without attachment.

Table 5 – Maximum von Mises stress values measured in the PDL of the target tooth.

	Incisor	**Incisor with attachment**	**Canine**	**Canine with attachment**
PDL von Mises stress values [MPa]	0.017	0.055	0.004	0.046

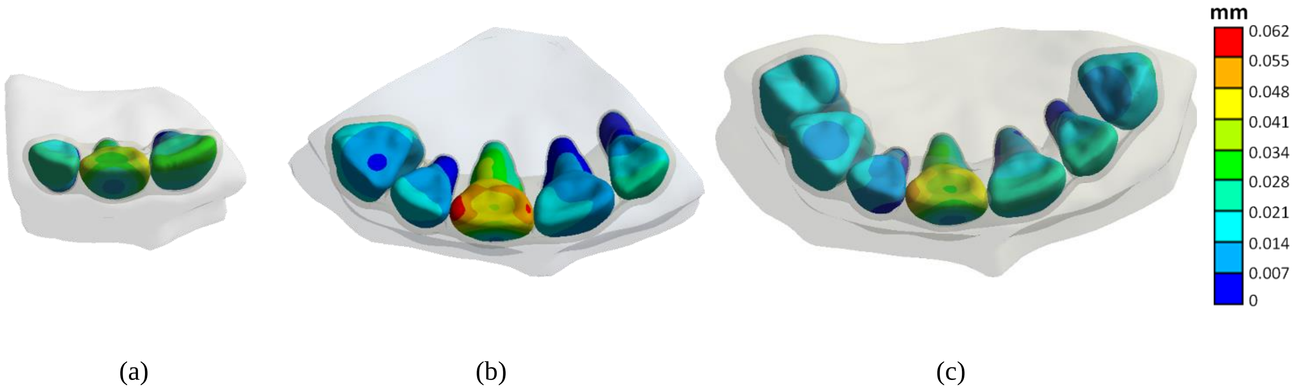


Figure 15 – Displacements occurring to neighboring teeth for a maxillary incisor treatment by considering a three-tooth model (a), a five-tooth model (b) and a seven-tooth model (c).

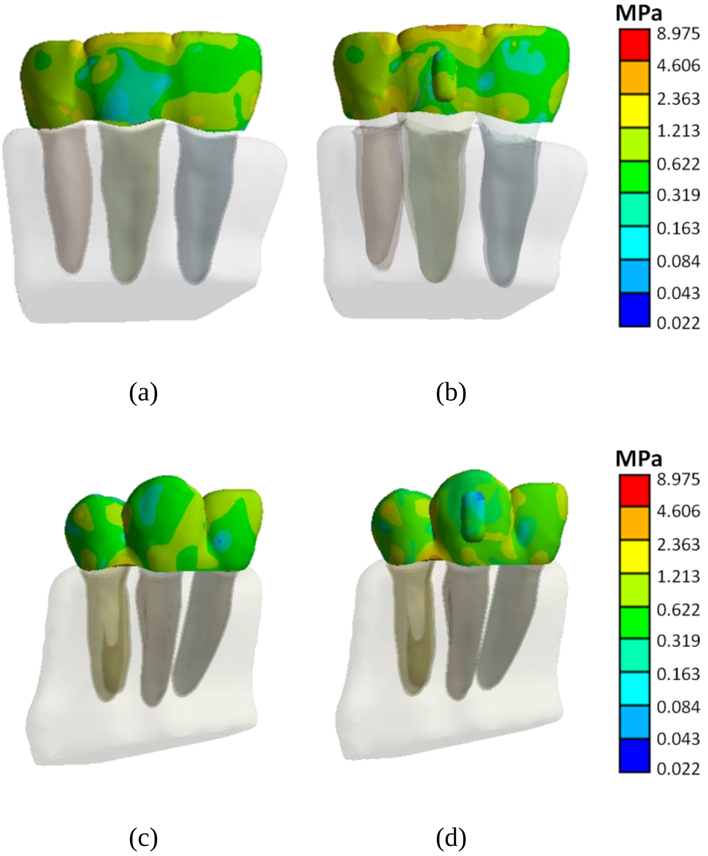


Figure 16 – RTA full-field maps of the von Mises stress values for a 1° rotation of the maxillary incisor (a,b) and the maxillary canine (c,d) without (a,c) and with (b,d) the use of a prismatic attachment.

5.2 Discussion

A supposed restriction regarding the use of RTA in orthodontics relies on the belief that they are not able to transfer an adequate load to provide stable orthodontic movements. However, the numerical analyses have showed that the forces originating from the difference between the appliance shape and the dentition geometry provide stress values in the periodontal ligaments adequate for a bone re-modelling process. Moreover, the use of prismatic attachments increases the amount of achievable rotations, especially for canine teeth. The rotation of cylindrical teeth presents a biomechanical challenge due to the lack of undercut surfaces, which causes the appliance to slip on the crown surface during treatment, making the canine rotation a hardly predictable movement [28]. This result indicates that load transfer from an appliance to a cylindrical tooth without an attachment is possible only to a limited extent. The addition of attachments increases the tooth geometric mass and enhances the interproximal undercuts along the horizontal plane, thus facilitating rotational movements. Moreover, the numerical results obtained are in accordance to those obtained in clinical studies [29], which have compared the amount of predicted tooth movements with that achieved after treatment. In particular, clinical trials have evidenced a mean accuracy of 54.2% for the rotation of a maxillary incisor and a mean accuracy of 32.2% for the rotation of a maxillary canine. The accuracy of canine rotation has resulted significantly lower than the rotation of all other teeth (maxillary canine achieved approximately one third of the predicted rotation versus one-half of the maxillary incisor).

Moreover, the numerical simulations have demonstrated that a three-tooth model can be considered adequate to investigate the accuracy of a single orthodontic tooth movement (i.e., rotation) performed by RTA. This result implies that simplified FEM models can be defined by considering only the target tooth along with the two adjacent teeth operating as anchorage structures.

The FEM simulations have also pointed out that non-target teeth may incur into undesired movements (Figure 15), as also observed in [30]. This result would suggest the use of complete tooth models for the simulation of orthodontic treatments performed by removable appliances. However, the stress distributions in the PDL of non-target teeth do not exceed the values necessary to activate permanent orthodontic movements, as showed in the seven-tooth model of the maxillary incisor without attachment (Figure 14-b).

The amount of the initial interpenetration arising from the loading condition (Figure 12) justifies the use of an accurate optical scanner for the reconstruction of crown geometries. Even small differences from the actual shapes may affect the simulation results. The optical scanning process adopted to acquire dental plaster models guarantees a spatial resolution of 0.1 mm and an overall accuracy of 0.01 mm [22], thus allowing the digitalisation of individual dentitions with the required accuracy.

A final consideration regards the RTA mechanical behaviour. The greatest stress values on the RTA have been obtained by using attachments. However, the obtained maximum value (9 MPa) results lower than the yield strength limit declared by the thermoplastic disc manufacturer (45 MPa). Breaks occurring to the appliances during therapy are mostly related to the wearing phase rather than the working phase due to the manual deformation performed by the patient in order to properly fit the mating surfaces onto the dentition anatomy. Of course, further aspects may influence the appliance behaviour, such as corrosions due to the patient's saliva, geometrical and mechanical effects of the actual thermoforming process, creep phenomena.

6 Conclusions

In the last few years, the use of removable thermoplastic appliances to treat irregular bites has established itself as an aesthetic alternative to fixed labial brackets. However, many variables may influence the efficacy of orthodontic treatments by RTA. Many orthodontists report that a considerable percentage of patients require additional midcourse corrections and/or conversion to fixed appliances before the end of the treatment. In this paper, a methodology to create a patient-specific anatomical model able to predict treatment outcomes has been developed. In particular, a numerical approach by means of the finite element method has been presented with the aim at simulating the behaviour of an orthodontic removable thermoplastic appliance. Numerical simulations have been performed in order to evaluate rotation movements for a maxillary incisor and a maxillary canine by using multi-tooth models, composed of three, five and seven teeth. Information derived from simulation results can be indeed used to change, for example, shape, size, and placement of attachments with the aim at improving the efficacy of the orthodontic treatment. Nonetheless, the developed models are flexible and can be easily adapted to simulate different orthodontic movements (*expansion*, *constriction*, *intrusion*, *extrusion*, *mesiodistal tip*, *labiolingual tip*) on different teeth by simple setting changes. Three-tooth models can be efficiently used to investigate geometrical and structural attributes of the appliance, with the aim at enhancing orthodontic movements. In this paper, the effects of prismatic attachments placed onto crown surfaces, have been studied. Clearly, the combination between shape, size, and placement of attachments greatly influences the movement efficacy of orthodontic treatments. Further studies should be oriented on the definition of optimised shapes, alternative to the prismatic geometry, and locations of attachments in order to enhance various movement typologies.

Moreover, the clinical practice often requires the treatment of malocclusion problems by simultaneously moving several teeth. In these cases, multi-tooth models should be used to represent complete and individual dentitions. In particular, patient-specific anatomical reconstructions, including crowns, roots, bones and ligaments, provide the definition of reliable biomechanical constraints and the customisation of the tooth movement planning. In this paper, a multi-modality imaging approach has been developed by combining an accurate optical scanner and a CBCT sensor. However, technical literature has recently faced the problem of retrieving root anatomies by using panoramic and/or lateral radiographs, without involving tomographic scanning [31,32]. This would bring to the reconstruction of complete tooth models, thus addressing questions regarding root movements, by exploiting minimally invasive imaging modalities, which expose the patients to the minimum radiation doses.

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