Biomechanical Analysis of Orthodontic Aligners made of Smart Polymers

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Dedication

I would like to dedicate this thesis to the memory of my grandfather, to my father and mother, and to my beloved siblings; Nada, Ghada, and Yasser.

Tarek Elshazly

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List of Abbreviations

1D	One Dimension
3D	Three Dimensions
3PB	Three Point Bending
4D	Four Dimensions
FEM	Finite Element Method
OMSS	Orthodontic Measurement and Simulation System
PDL	Periodontal Ligaments
PETG	Polyethylene Terephthalate Glycol
PU	Polyurethane
PVC	Poly-vinyl Chloride
SMPs	Shape Memory Polymers
Tetra 10	10-noded Tetrahedrons Elements
Tetra 4	4-noded Tetrahedral Elements
T_g	Glass Transition Temperature
T_m	Melting Temperature
T_{Trans}	Transition Temperature

1. Abstract

Objective: The aim was to assess the biomechanical behavior of orthodontic aligners, experimentally and numerically, to test the applicability of shape memory polymers (SMPs). **Materials and methods:** Experimentally, the design of the first study was to achieve 1.9 mm correction movement of a maxillary central incisor (Tooth 21) on a typodont using thermoformed aligners made of SMP material (ClearX) after appropriate activation steps. ClearX aligners were tested for repositioning of tooth 21 in the typodont model. The typodont was scanned after each step and the corrective movement was measured through the superimposition of scans. In the second experimental study, printed aligners made of SMPs were used (4D technology). The movement of tooth 21 on the typodont also was measured. Three point bending test (3PB) was carried out under standardized conditions and at different ambient temperatures, including 37 °C. An Orthodontic Measurement and Simulation System (OMSS) was used to measure force/deflection and torque/rotation relationships on tooth 21. Numerically, our typodont was scanned to produce a 3D digital model, which was imported into 3-matic software for designing of aligners with 4 different thicknesses: 0.4, 0.5, 0.6, 0.7 mm. The model was then exported to Marc/Mentat finite element (FE) software. A series of sensitivity analyses was performed to get the suitable parameters for FE simulation. **Results:** The thermoformed SMP aligners could initiate a 1.76 mm movement, and the 4D aligners showed a movement of 2.5 mm. The maximum deflection forces were (0.5 - 3.8) N. Forces delivered on lingual displacement of tooth 21 were (0.2 - 0.7) N. Numerically, the resultant maximum forces generated on facio-lingual translation of tooth 21 were within the range of (1.3 - 18.3) N. The force was direction-dependent and was increasing with increasing the thickness. The contact normal stress map showed uneven distribution of stresses all over the facial surface and concentration at specific points. **Conclusion**: Aligners made of SMPs could move a tooth by biocompatible orthodontic forces, after a suitable thermal stimulus within the oral temperature range. Additionally, a validated FE model could facilitate understanding the force systems of clear aligners and performing better treatment planning.

Keywords: Orthodontics; Tooth Movement; Biomechanics; Shape Memory Polymers; Clear Aligners; Removable Plastic Appliance.

2. Introduction and Aims with References

2.1 Introduction

Clear aligners are a series of thin, clear, custom-made, removable, plastic splints, which are created to effectively move teeth into their desired position. Besides their esthetical appearance, they showed to be comfortable and better for oral hygiene than fixed braces [1]. In addition, they need shorter dental appointments and seem to be ideal for orthodontic retreatment cases [2]. As well, they improve the bad parafunctional habits during treatment, like bruxism, and disarticulation of the teeth may also be beneficial for patients with TMJ problems. Moreover, they are much easier to handle in every-day practice than lingual appliances technical-wise [3]. Aligners can be made of different polymers [4], such as polyvinyl material, poly-vinyl chloride (PVC), polyethylene terephthalate glycol (PETG) [1], polypropylene, polyester, and polyurethane [5]. Clear aligners are worn for about 20 hours per day and are changed approximately every two weeks [1]. Each aligner will move the teeth by around 0.2 to 0.3 mm for translations and 1 to 3° for rotations per tooth [3], [5]. A poor patient compliance to dentist's instructions can lengthen treatment time and increase the cost, and also can affect the quality of the final result [1].

One of the important drawbacks of an aligner treatment is the aligner change regime (14 days) due to the rate-limiting step. Therefore, investigators are working on doing improvements to aligner materials, force systems, staging of tooth movements, and treatment planning [6]. One of these trails of improvement is the incorporation of shape memory polymers (SMPs), a type of important stimuli-responsive smart polymers, which can recover their original shape upon exposure to external stimuli. Many academic reviews have been published on SMPs [7] especially thermal responsive SMPs. Few of them reported about their application in the orthodontic field [8]. In our current study, we have tried to use the thermal responsive SMPs in fabrication of aligners and use the changing of their shape on change of temperature from room temperature to oral temperature to move the teeth after setting its original shape to the desired alignment and programming the shape recovery to suit the kinetics of periodontal tissues [9, 10].

Biomechanically, there are few studies that are relating the force levels in aligners and that are addressing deformation of aligners in the mouth over time and their effect on tooth movement [11]. Moreover, tooth movements by clear aligners are more complex compared to fixed appliances and many parameters are involved in determining the clinical outcome [12]. However, using the finite element method (FEM) enables the investigators to understand the biomechanics of orthodontic devices as it allows the estimation of stresses, strains, and deformations in different tissue structures during treatment [13]. FEM is a modern tool for structural analysis that is applicable to solids of irregular geometry which contain heterogeneous material properties. It yields a better understanding of the reactions and interactions of individual tissues. The structure is divided into so called “elements” connected through “nodes” [14]. By choosing the appropriate mathematical model, element type and degree of subdivision, we can obtain accurate solutions. Stresses and strains are calculated in each element [15]. This makes it possible to adequately model the tooth, the periodontal structure, the bone and the aligner [16]. Most researchers worked on fixed orthodontic appliances and only few studies focused on the study of clear aligners and their behavior in delivering forces [17], [12]. In our current study, we developed a finite element model that can be used to study the biomechanical behavior of clear aligners [18].

2.2 Aim of the Study

The aim of the current study was to:

1. Characterize whether several novel shape memory materials could be used for fabrication of the aligners and select the appropriate one.
2. Measure force/deflection behavior of the individually produced aligners from the tested materials.
3. Develop a numerical 3D finite element model that can be used to study the biomechanical behavior of clear aligners.
4. Compare experimental results and numerical simulations to validate the finite element model.

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3. Publications

3.1 Study 1

Primary Evaluation of Shape Recovery of Orthodontic Aligners Fabricated from Shape Memory Polymer (A Typodont Study)

Tarek M. Elshazly, Ludger Keilig, Yasmine Alkabani, Ahmed Ghoneima, Moosa Abuzayda, Sameh Talaat, Christoph P. Bourauel

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Article

Primary Evaluation of Shape Recovery of Orthodontic Aligners Fabricated from Shape Memory Polymer (A Typodont Study)

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Abstract: As an innovative approach to overcome the rate-limiting staging of conventional aligners, using shape memory polymers (SMPs) as aligners' materials was investigated in this in vitro study. The ability of SMPs to shape recover and consequently move tooth, upon appropriate stimuli, was evaluated on a typodont model before clinical application. The study design was to achieve 1.9 mm correction movement of an upper central incisor by one aligner after multiple steps/activation. A custom-made aligned typodont model with a movable upper central incisor was scanned. Using an orthodontic software and a 3D printer, resin-models were generated. Seven aligners of ClearX sheets (SMPs) were fabricated by thermoforming on the resin aligned model. Each aligner was tested for repositioning of the central incisor in the typodont model. The model was scanned after each step and the corrective movement was measured through the superimposition of scans. Results showed that the total correction efficiency of the SMPs' aligner was ≈93% (1.76 mm). The corrective movement was 0.94 ± 0.04 mm after the reforming step, 0.66 ± 0.07 mm after the first activation step, and 0.15 ± 0.10 mm after the second activation step. It was concluded that aligners made of SMPs could have a promising future-use in orthodontic aesthetic treatment.

Keywords: orthodontics; smart polymers; clear aligners; orthodontic appliance; typodont; 3D printers; dentistry; digital workflow

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1. Introduction

Conventional orthodontic treatment by fixed appliances, such as braces and wires, is the backbone of orthodontic treatment. However, patients complain from many problems such as: mucosal irritation, soreness of the teeth, in addition to the difficulty of keep good oral hygiene. Moreover, due to the poor aesthetic appearance, some patients refuse having buccal braces, especially the adult ones [1–3]. Alternative treatment options have been introduced by many investigators to satisfy the high demand of an aesthetic orthodontic treatment; on top of these alternatives are ceramic or composite braces, lingual braces, and clear orthodontic aligners [4].

Clear aligners are a series of thin, clear, custom-made, removable, plastic aligners, which are created to effectively move teeth into their desired position. They should be worn for at least 20 h per day and changed approximately every two weeks [5]. Each aligner can limitedly move the teeth by around 0.2 to 0.3 mm for translations and 1° to

3° for rotations per tooth [6]. Clear aligners can be made of different polymers [7], such as polyethylene terephthalate glycol (PETG) [5] and polyurethane [8]. Clear orthodontic aligners have shown a reduced treatment period and shortened chair time in mild-to-moderate cases [9] and they have been proven to be an efficient and a feasible alternative to fixed braces [10,11]. However, still the rate-limiting staging of conventional aligners is limiting their use [5,6,9,12]. Therefore, investigators are working on improvements of aligner materials, force systems, staging of tooth movements, and treatment planning [13].

The aim of many recent interdisciplinary research studies is to introduce novel materials that can play an active role in the appliances [14]. These materials are called smart materials or stimuli-responsive materials which are able to react suitably with external stimuli, such as thermal, electrical, or magnetic input, producing a predictable repeatable output [15]. Shape memory materials are subcategory of smart materials which have the ability of changing their macroscopic shape upon a proper stimulus. Unlike shape changing materials, shape memory materials have the capacity to maintain a stable temporary shape until they are appropriately activated to recover their original shape [16,17].

Shape memory polymers (SMPs), also called actively moving polymers, are a type of smart shape memory material [17,18]. The shape memory mechanism of SMPs depends on presence of two pre-requites: a stable polymer network determines the original shape, and a reversible switching polymer responsible for fixing the temporary shape [19,20]. SMPs possess great attractiveness due to their significant elastic deformation ability, low cost, low density, ease of production, flexible programming, tailorable physical properties, excellent chemical stability, and high biocompatibility [21]. Because of these various advantages, SMPs may have great potential to penetrate virtually in several applications such as biomedical devices [22].

Specifically, thermo-responsive SMPs may have high potential as a novel orthodontic material, from functional and aesthetic point of views. Together with their relatively transparent and aesthetically satisfactory appearance, they have the advantage over the conventional aligner materials by possessing an intrinsic shape recovery property. Hence, application of SMPs to orthodontics can provide the aligners with considerable self-shape-recovery forces which may facilitate their operability and functionality [14,23].

In a primary study by Jung et al. [23], they used orthodontic wires made of shape memory polyurethane. After heating above transition temperature (50 °C), the teeth were corrected within one hour on a typodont model. Although there are some patents [24–26] that propose using smart polymers in fabrication of orthodontic aligners, there are still lack of studies investigating this innovation before being clinically applied [14].

The current study is a preliminary in vitro investigation of a type of orthodontic aligners made from thermal-responsive SMPs. The shape recovery forces generated upon appropriate thermal stimuli was used to move a tooth on a typodont. The aim was to overcome the rate-limiting staging of conventional aligner materials and show the possibility of using one shape memory aligner instead of three subsequent conventional aligners; in order to decrease the number of aligners used per treatment, saving money and time, reducing plastic consumption, and consequently decreasing the total cost.

2. Material and Methods

2.1. Specimens' Preparation

Before establishing the following study design, a series of sensitivity tests were performed. Preliminary experiments were conducted to determine the best parameters especially with respect to temperature and pressure of deep-drawing (thermoforming) and reforming of the material sheets, as well as shape recovery. Furthermore, best parameters were determined for processing time which could end up in optimal results within the limitations of the used material. This means that every step of the following study design was preceded by several initial trials to adjust the optimal parameters that yield optimal results.

A custom-made typodont model (model T) was fabricated from acrylic teeth (Frasaco, Teltnag, Germany) and resin (Technovit 4004, Kulzer, Wehrheim, Germany). The movable acrylic upper left central incisor tooth was embedded in pink wax (Set up dental wax, Cavex, Harleem, the Netherlands), placed in the model, while the other typodont teeth were fixed by resin (Figure 1). The fully aligned model was then scanned (scan 0) using a 3D lab-scanner (D2000, 3Shape, Copenhagen, Denmark). After that, the model was segmented using Ortho System software (Ortho Analyzer v. 2012-1, 3Shape, Copenhagen, Denmark). Using the software, a palatal mal-alignment of 1.9 mm for the upper left central incisor tooth was designed, additionally, an intermediate model was also prepared with 1.2 mm mal-alignment (i.e., a correction of 0.7 mm) (Table 1).

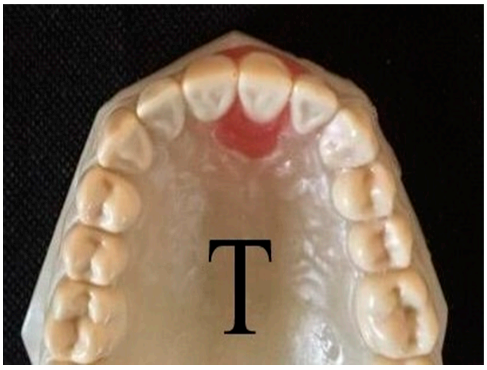

Figure 1. A custom-made typodont upper arch model with a movable left central incisor (Model T).

The three models (two mal-aligned models and one fully aligned model) were exported as STL files. The three models were 3D printed (Figure 2) using a printable resin (Dentona Optiprint model, Dentona AG, Dortmund, Germany) by a 3D Printer (Asiga Max, SCHEU-DENTAL GmbH, Iserlohn, Germany); model 0 (with 1.9 mm mal-alignment, i.e., 0.0 mm correction), model 1 (with 1.2 mm mal-alignment, i.e., 0.7 mm correction), and model 2 (with 0.0 mm mal-alignment, i.e., full 1.9 mm correction). A guiding splint was fabricated from a conventional thermoplastic sheet (Erkodur, Erkodent Erich Kopp, Pfalzgrafenweiler, Germany) with thickness 1.5 mm by thermopressing on model 0, and it was used as an index to ensure re-positioning of the movable typodont central incisor tooth in the same mal-aligned position before repeating the test, and it was made thick to ensure stiffness.

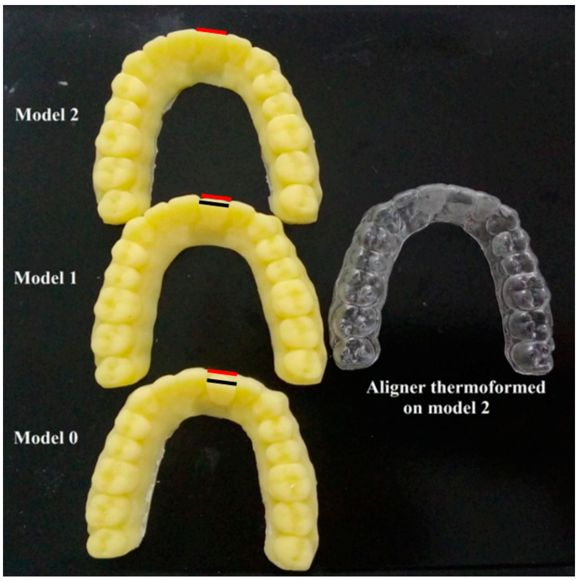

Figure 2. 3D printed models with different mal-alignment of central incisor and a thermoformed aligner of ClearX material.

Table 1. A list of models and scans used in the study.

Type	Name	Description	Use
Models	Model T	The typodont.	Scanned with fully aligned teeth (Scan 0, which was used for software manipulation). The movable central incisor tooth was used for showing the amount of movement achieved by the shape memory recovery of the aligner.
	Model 0	The 3D printed resin model with full mal-alignment (1.9 mm)	Used for fabrication of a guiding splint used for repositioning of the typodont movable central incisor tooth to the zero position.
	Model 1	The 3D printed resin model with partial mal-alignment (1.2 mm), i.e., partial correction (0.7 mm)	Used for reforming of the aligners.
	Model 2	The 3D printed resin model with full correction (1.9 mm)	Used for thermoforming of the aligners.
Scans	Scan 0	A scan of the fully aligned typodont model.	Used for software manipulation and production of models 0, 1, and 2.
	Scan 1	A scan of the typodont model after using the guiding splint to move the central incisor tooth to the fully mal-aligned position.	Ideally should correspond to Model 0 shape.
	Scan 2	A scan of the typodont model after the movement of the central incisor tooth by using the reformed aligner.	Used for superimposition of the scans and measurement of amount of the tooth movement.
	Scan 3	A scan of the typodont model after the movement of the central incisor tooth by using the activated aligner received the first activation cycle.	Used for superimposition of the scans and measurement of amount of the tooth movement.
	Scan 4	A scan of the typodont model after the movement of the central incisor tooth by using the activated aligner received the second activation cycle.	Used for superimposition of the scans and measurement of amount of the tooth movement.

In order to achieve a correction of 1.9 mm mal-alignment by only one aligner instead of three subsequent aligners, steps of thermoforming, reforming, and two activation cycles should be followed, respectively. A clear aligner was fabricated on the fully aligned model (model 2) using a shape memory sheet (ClearX) supplied by (Kline-Europe GmbH, Düsseldorf, Germany). The (0.76 mm thick) sheet was thermo-pressed by using a thermoforming device (Ministar, SCHEU-DENTAL GmbH, Iserlohn, Germany), by heating at 120 °C for 30 s, followed by pressing over the model at a 4 bar pressure (the recommended instructions provided by the supplier). Each aligner was then removed from the models, trimmed and finished. It was reformed on model 1 (with partial correction); where the reforming is a ClearX manufacturing step (introduced by Kline Europe, Düsseldorf, Germany) which is done to reshape the aligner on the previous step of the treatment plan (which has less tooth correction). Hence, in the current study, the thermoformed aligner on model 2 was reformed on the partially corrected model 1 (Figure 3). That was done by utilizing wet heating of the aligner in a warm water bath at 85 °C for 20 s followed by immediate pressure and heat adaptation on model 1 using the thermoforming device used earlier for the thermoforming step. So, basically, the aligner was heated once for the thermoforming step (to give it the original shape) and another time for the reforming step (to give it a temporary shape).

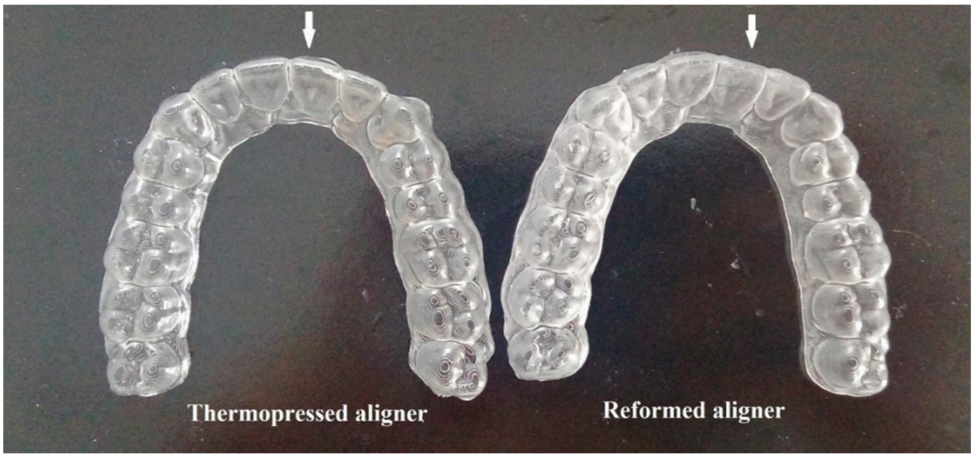

Figure 3. Thermopressed aligner on model 2 and reformed aligner on model 1.

2.2. Testing of Shape Memory Correction on the Typodont Model

The wax around the upper left central incisor tooth in model T was softened. The guiding splint was used for positioning of the tooth in model T to be equally positioned as model 0. The model T was then placed in a 5 °C water bath for 10 min, to ensure that the wax is no longer soft and can withstand aligner placement without getting distorted [8]. Model T was then scanned (scan 1). The reformed aligner was then placed on model T, and together, they were placed in a hot water bath of 50 °C for 10 min. The model was placed on its base in a hot water basin and the water volume was adjusted to be at the level of the wax just below the aligner margin, to avoid, as much as possible, activation of the shape memory recovery of the aligner by the elevated temperature, meanwhile the wax was softened by hot water to allow the imbedded tooth to move. At the end, the model was replaced again in a water bath of 5 °C for 10 min to ensure wax hardening before aligner removal. After that, the model was scanned again (scan 2).

Afterwards, and to initiate the shape memory recovery, the aligner received the first activation cycle by placing it in an activation device (ClearX aligner booster v. 2.1, Kline-Europe GmbH, Düsseldorf, Germany). The ClearX aligner booster (Figure 4) is a programmed electric device, wirelessly connected and controlled by a mobile application (ClearX Mobil App. v. 1.1.4, Kline-Europe GmbH, Düsseldorf, Germany) (available on both Apple and Google store), was developed to provide the necessary medium for the shape memory aligner to regain its original shape through heating the aligner for a certain period of time in a hot water of certain temperature. The activation was done by keeping the aligner within the container of the device submerged in a hot water at 67 °C for 10 min. The activated aligner was then placed on model T, then they were placed together in a hot water bath of 50 °C for 10 min. Again, the water volume was adjusted to be at the level of the wax just below the aligner margin. After that, the model T was scanned (scan 3). Afterwards, the aligner received its second activation cycle, then the activated aligner was then placed on model T, and together, they were placed in a hot water bath of 50 °C for 10 min in the same way it was done before, and the model T was rescanned (scan 4).

This experiment was repeated 7 times, i.e., a total of 7 aligners were used in the study (n = 7), each time a new aligner was used to ensure the repeatability and the consistency of the results. Additionally, new wax was used each time to ensure that its properties were not altered by repeated heating and cooling cycles. In addition, the initial mal-aligned position was rescanned (scan 1), after using the guiding splint to re-position the typodont upper left central incisor tooth, and before using each new aligner to avoid any reading errors.

Figure 4. ClearX booster device controlled by a mobile application used for programmed activation of the ClearX aligners.

2.3. Analysis of Digital Models

For each aligner, four 3D digital scans of Model T were obtained after different steps (Figure 5), which were: one scan after using the guiding splint for the initial 1.9 mm mal-aligned model (scan 1), a second scan after using the reformed aligner (scan 2), a third scan after using the aligner with first activation cycle (scan 3), and a fourth scan after using the aligner with second activation cycle (scan 4).

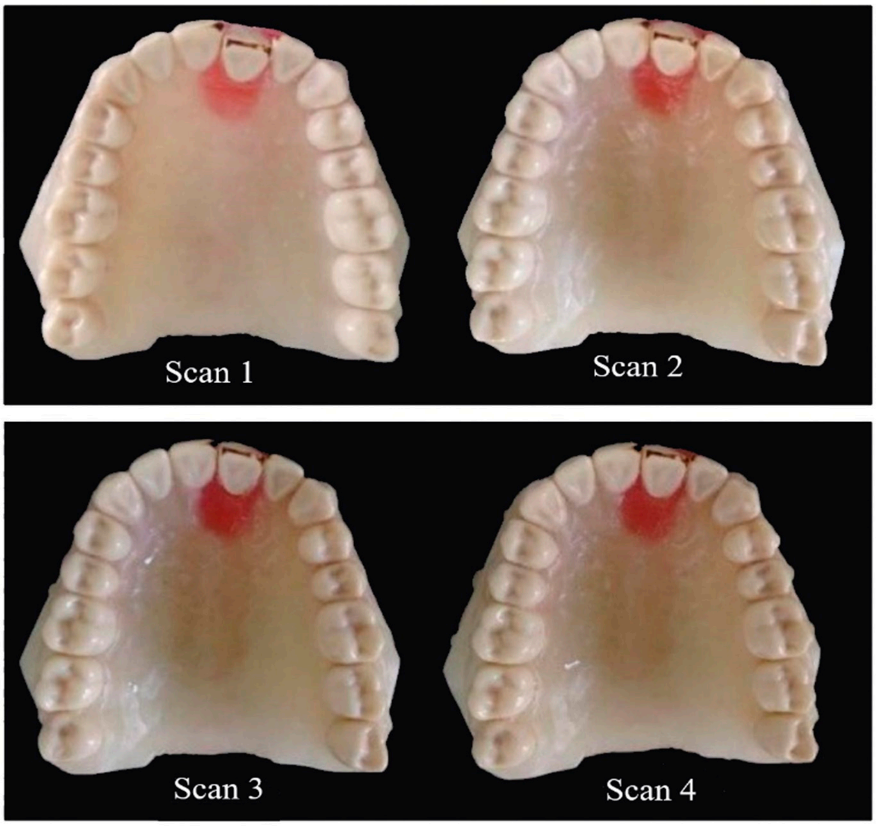

Figure 5. Model T before scanning at the different stages of treatment.

The scans were superimposed using the Ortho Analyzer software, and the amount of tooth movement was measured in mm for each step, compared to the initial position in scan 1 and also compared to the position in the previous step (Figure 6). A list of all models and scans used in this study is illustrated in Table 1. A schematic diagram illustrating the main steps of ClearX method is shown in Figure 7.

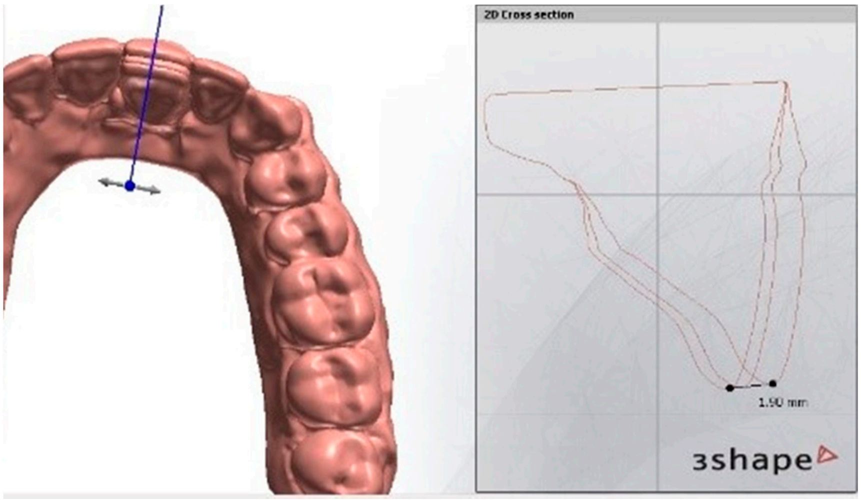

Figure 6. Superimposition of the typodont's scans using 3Shape Ortho System software (Ortho Analyzer) and the amount of tooth movement was measured for each step.

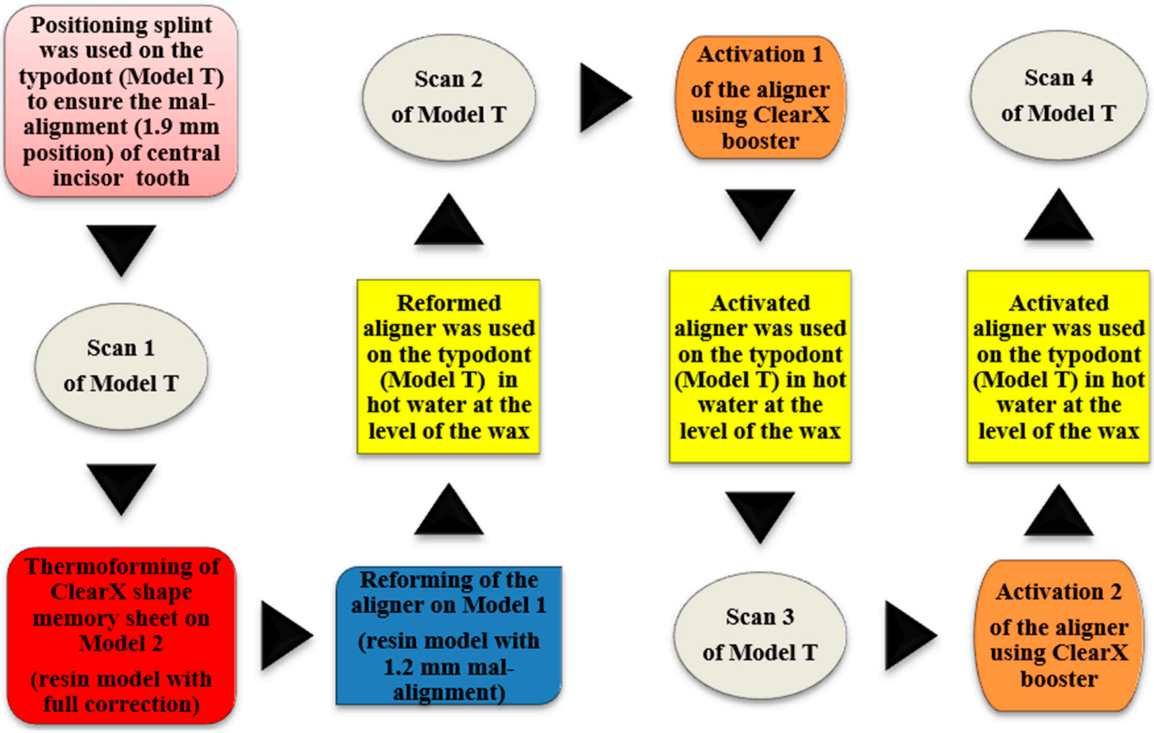

Figure 7. A schematic diagram illustrating the main steps of ClearX method.

3. Results

Considerable corrective repositioning movements of the upper left central incisor tooth on the typodont were observed after each step. The added corrective movement after using the reformed aligner was 0.94 ± 0.04 mm to give an average correction of 49.47% of the total movement (scan 2 compared to scan 1), while after the first activation was 0.66 ± 0.07 mm to give an average added correction of 34.74% from the total planned movement (scan 3 compared to scan 2), and for the second activation was 0.15 ± 0.10 mm to give an average added correction of 7.89% of the total planned movement (scan 4 compared to scan 3). Results are shown in Tables 2 and 3, as well as Figure 8.

Table 2. Mean and standard deviation (SD) of the total cumulative correction (TC) of the position of the upper left central incisor tooth after superimposition of each step's scan over the scan of the initial mal-position, the added correction (AC) after superimposition of each step's scan over its predecessor step's scan, and the percentage of correction efficiency by the ClearX aligner.

	Scan 1 vs. 2		**Scan 1 vs. 3**		**Scan 1 vs. 4**	
	TC	**AC**	**TC**	**AC**	**TC**	**AC**
Planned movement	0.70	0.70	1.50	0.80	1.90	0.40
Aligner 1	0.94	0.94	1.65	0.71	1.76	0.11
Aligner 2	0.98	0.98	1.64	0.66	1.70	0.06
Aligner 3	0.96	0.96	1.61	0.65	1.72	0.11
Aligner 4	0.95	0.95	1.60	0.65	1.70	0.10
Aligner 5	0.87	0.87	1.65	0.78	1.74	0.09
Aligner 6	0.97	0.97	1.52	0.55	1.83	0.31
Aligner 7	0.90	0.90	1.55	0.65	1.84	0.29
Mean (mm)	0.94	0.94	1.60	0.66	1.76	0.15
SD	0.04	0.04	0.07	0.07	0.10	0.10
Correction % (divided by 1.9 mm total movement)	49.47%	49.47%	84.21%	34.74%	92.63%	7.59%

Table 3. Numerical values and percentages of shape memory recovery components.

Recovery	Added Movement	% Recovery of Shape Memory Component Per Step (Divided by Total 1.2 mm)	% Recovery of Activated Shape Memory Component Per Step (Divided by Total 0.96 mm)
Spontaneous	0.24 mm	20%	
First activation	0.66 mm	55%	68.75%
Second activation	0.15 mm	12.5%	15.63%

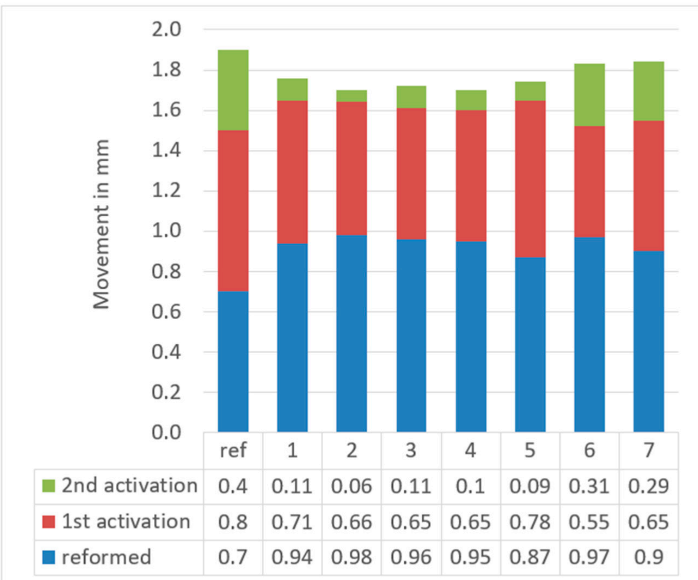

Figure 8. Amount of correction of the position of the upper left central incisor tooth on a typodont model per step by seven ClearX aligners.

4. Discussion

The aim of all optimizations, innovations, or advances in the orthodontic aligner field is mainly to facilitate the fabrication and treatment process, as well as to reduce time and cost of the treatment. The introduction of digital technology in fabrication of orthodontic aligners has been one of the most noteworthy orthodontic advances in this century [1,3]. Introduction of new materials for aligner fabrication pull the attention of some researchers [24–26]. It is always difficult when it comes to favor a suitable material, especially when it is a must to consider the biocompatibility and biomechanical behavior. Moreover, it was a challenge to introduce a clinically applicable method to evaluate the shape memory property of the material. For these reasons, full investigation of the used material and several in vitro studies should be done first before any clinical application. In the current study, it was proposed to use smart polymers in fabrication of orthodontics aligners, particularly thermo-responsive SMPs, which have the ability to keep two or more shapes and recover their permanent shape upon exposure to an appropriate thermal stimulus, or a series of stimuli [27].

ClearX system sheets, which were introduced by Kline Europe GmbH, are claimed to be a thermo-responsive shape memory polyurethane-based thermoplastic material. It is claimed that the material has the ability to recover to its original thermoformed shape after a reforming step, by a process of thermal activation at specific temperature for a certain period of time. Due to the stepwise shape changing property, this material was proposed to be used for the fabrication of orthodontic aligners, as it may successfully be used to overcome the rate-limiting staging of conventional aligners, in a way that one aligner may be able to replace three subsequent conventional aligners. Consequently, the number of aligners used per treatment could be reduced, beside saving money and time, especially for long and more complex therapies such as molar distalization and severe open/deep bite correction that are frequently performed nowadays [28–30].

Additionally, the method tested in the present investigation is easily linkable with CAD/CAM systems, which registered a constantly increasing use in many fields of dentistry, such as restorative dentistry, prosthodontics, and orthodontics. CAD/CAM technology allows a completely digital workflow, from impression to final framework, with clinical reliability [31] and good patients feedback [32].

It was found that nearly 92.63% of total correction efficiency could be reached on a typodont through one step of reforming and two steps of activation, i.e., three steps of treatment. The shape recovery behavior of the material is not only influenced by the chemical structure and composition of the polymer molecules, but also by the processing conditions. Controlling these conditions is important for controlling the properties of the material in practical applications [33]. Therefore, the whole study has been set up after performing a series of sensitivity tests. Several changeable parameters could control the result and determine the success of sufficient shape recovery. Temperature, moisture, and time of each step were the main governing parameters. Starting from the thermoforming step, passing by the reforming step, and ending with the activation step, all have showed high sensitivity. The activation of the shape memory property was done by the booster system (Figure 4). The appropriate parameters, required to accomplish the optimal shape recovery of the material by using the booster, were reached, after the sensitivity testing, in a way that the first activation cycle was found to initiate an average of 65% shape memory recovery in the aligner and the second cycle was found to initiate an average of 35% shape memory recovery.

The fundamental mechanism of shape memory effect in SMPs is the presence of a two-domain system with two different glass transition/melting temperatures. Hence, at an ambient temperature, one domain is being hard/elastic, while the other domain is soft/ductile [34]. In other words, the shape memory mechanism in thermal-responsive SMPs is a reversible activation and inactivation of polymer-chain motion in the switching segments respectively above and below certain temperature called transition temperature (T_{trans}). T_{trans} could be either glass transition temperature (T_g) or melting temperature

(T_m) [14,20,35]. So, once the T_{trans} is reached, the deformed shape memory material displays an elastic property and return to its original shape; this shape recovery generates forces that may be able to move a tooth [36].

SMPs could have more than one temporary shape, because they have a wider shape recovery temperature range and a much higher recoverable strain [19,27]. Shape memory polyurethane resins consist of both polar and non-polar molecules which segregate into micro domains of hard and soft segments. By combining hard and soft molecular domains, the material could achieve both high strength (from the hard regions) and high toughness (from the soft regions), in a way that enables fabrication of durable orthodontic aligners which can move the tooth over longer period of time [33,37]. Additionally, the polyurethane resin is resistant to accumulation of deposits and stains, allowing it to stay clean in oral conditions for longer time, however, it shows sensitivity to moisture due to presence of hydrogen bonding [37–39]. That could explain why the moisture was a governing factor at the reforming and activation steps of ClearX aligners.

Ideally speaking, the reformed aligner should make a 0.7 mm corrective movement, while the first activation should result in an average of 55–65% shape recovery, and the second activation should result in an average 25–35% recovery, depending on the type and amount of the planned movement. However, the results of the present study showed an average movement of 0.94 mm for the reformed aligners, which is higher than the planned 0.7 mm movement (Table 2, and Figure 8). This could be attributed to a spontaneous recovery occurring during stress release, or, could be in part triggered by a partial shape memory recovery caused by the heat generated by the 50 °C water bath used in this study to soften the wax. Thus, an average of 0.24 mm extra movement was achieved by the reformed aligner (20% of the total shape memory component of the movement).

Upon first activation, the aligners gave an average 0.66 mm added movement, which compromise 55% of the planned shaped memory movement, and thus give an average total movement of 1.6 mm (84.2% of the total planned movement of 1.9 mm). The second activation gave an average added movement of 0.15 mm which corresponds to 12.5% of the total planned shape memory movement, and thus giving an average total movement of 1.75 mm (92.63% of the total planned movement).

In the ClearX system, the manufacturer claimed that the slight unrecovered residual part of movement (≈7–8%) should be achieved using the next aligner before activation, which the company refers to as recurrent aligner, this also gives another chance to any lagging orthodontic movement. Thus, the next aligner should be first used to confirm that full movement of the previous aligner is achieved and then it is activated to deliver additional movements, and so on.

The comparable results between specimens showed a consistent behavior of the material. Although the results are promising, this study could only be considered as a proof of concept and it still has many limitations. It is just a preliminary in vitro study on a typodont. In the typodont studies, the wax substitutes the periodontium. However, the bone modeling due to orthodontic forces is a complicated biological process resulting from a complex biomechanical reaction of the biological tissues of the periodontium [40]. Additionally, an idealized movable single tooth movement was conducted, while the other teeth were fixed in the resin of the typodont model, yet, such situation is not clinically related. Moreover, within the range of activations' temperature, it was neglected that in the clinical situation, the hot foods and/or drinks can affect the whole treatment process, as they can activate the aligner in between and distort the whole design of treatment. Furthermore, the mechanical behavior of the aligner should be thoroughly studied and the delivered forces by the shape memory recovery should be measured. Such investigations and limitations will be considered in further upcoming studies.

5. Conclusions

Experimentally, tooth movement could be conducted on a typodont model by using clear aligners made of shape memory polymers (SMPs). The aligner, however, should undergo different steps of special heat treatment above its transition temperature in order to initiate its shape memory recovery. Consequently, aligners made of SMPs could be a promising future choice for orthodontic aesthetic treatment.

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3.2 Study 2

Potential Application of 4D Technology in Fabrication of Orthodontic Aligners

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Potential Application of 4D Technology in Fabrication of Orthodontic Aligners

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Objectives: To investigate and quantify forces generated by three-dimensional-printed aligners made of shape memory polymers (four-dimensional [4D] aligner).

Methods: Clear X v1.1 material was used in this study. On a custom-made typodont model, correction of maxillary central incisor (tooth 21) malposition by 4D aligners with thicknesses of 0.8 and 1.0 mm was measured by superimposition of subsequent scans. Maximum deflection forces generated by foil sheet specimens were measured at different temperatures in three-point bending (3-PB) tests. In a biomechanical system (orthodontic measurement and simulation system [OMSS]), forces generated on movements of tooth 21 by the 4D aligners were measured at different temperatures.

Results: 4D aligners succeeded to achieve a significant tooth movement (2.5 ± 0.5 mm) on the typodont, with insignificant difference between different thicknesses. In the 3-PB test, the maximum deflection forces measured at 20, 30, 37, 45, and 55°C, were 3.8 ± 1.1, 2.5 ± 0.9, 1.7 ± 0.6, 1.0 ± 0.4, and 0.5 ± 0.4 N, respectively. Forces delivered on palatal displacement of tooth 21 at 37, 45, and 55°C by 0.8-mm aligners were 0.3 ± 0.1, 0.2 ± 0.1, and 0.7 ± 0.2 N, respectively, whereas those by 1.0-mm aligners were 0.3 ± 0.1, 0.3 ± 0.1, and 0.6 ± 0.2 N, respectively. A good concordance with movement on the typodont model was shown in OMSS.

Conclusion: An initial study of 4D-printed aligner shows its ability to move a tooth by biocompatible orthodontic forces, after a suitable thermal stimulus within the oral temperature range.

Keywords: clear aligners, shape memory polymers, biomaterial, biomechanics, tooth movement, 4D printing, orthodontics

HIGHLIGHTS

- Rate-limiting staging of conventional aligners consumes time and materials.
- Orthodontic aligners can be made of different polymers.
- Four-dimensional (4D) technology is a three-dimensional printing of polymeric shape memory material.
- Introduction of 4D technology in the field of orthodontic aligners is highly innovative.
- 4D aligners can move teeth by biocompatible forces.

INTRODUCTION

Aesthetics is one of the major demands of patients who seek dental treatment. Major problems facing patients of orthodontic treatment are the bad appearance of metallic orthodontic braces, keeping good oral hygiene, and the long treatment time (Elshazly et al., 2021). In the last decade, treatment by orthodontic aligners has shown growing interest (Ercoli et al., 2014; Ojima and Kau, 2017). The aligners gain great superiority in aesthetic, comfort, and oral hygiene, over fixed braces, even the ceramic and lingual ones, owing to the fact that they are clear and almost invisible, as well as the ability to remove them during eating, brushing, and flossing (Mehta and Mehta, 2014). Additionally, with clear aligners, treatment time and chair time are reduced in nonextraction cases, sometimes by more than the half, compared with fixed braces (Tamer et al., 2019).

Conventional aligners are made from different types of polymers (Ercoli et al., 2014), such as polyvinyl material, polyvinyl chloride, polyethylene terephthalate glycol (Thukral and Gupta, 2015), polypropylene, polyester, and polyurethane (Momtaz, 2016). The functioning principle of such appliances is based on limited movement of each tooth through a programmed deviation between the real tooth position and a setup position. The programmed geometry of the aligner's stent then defines the new tooth position and the amount of movement to be performed (Boyd and Waskalic, 2001). In most of the popular aligner systems in the market, each aligner is designed to move a tooth within the restriction of 0.2 to 0.3 mm for translations and 1° to 3° for rotations, for that it is worn approximately 14 days, and then it should be changed with its successor (Kwon et al., 2008; Thukral and Gupta, 2015; Elkholy et al., 2016). This stepwise staging of conventional aligners leads to time and material consumption and consequently high cost of the treatment (Martorelli et al., 2013; Ercoli et al., 2014; Elshazly et al., 2021).

With the introduction of the technology of digital scanning, three-dimensional (3D) printing, and CAD-CAM, the orthodontic aligner became more precise. Nonetheless, investigators are continuously working on improving the efficiency of the treatment. Many optimizations, innovations, and advances are aiming to facilitate the process and to reduce the time and the cost (Phan and Ling, 2007; Morton et al., 2017; Elshazly et al., 2021). Several researchers are focusing on two main drawbacks: the shortcomings of conventional materials and the biological consideration of tooth movement. Numerous methods have been introduced to biologically accelerate tooth movement (Ojima and Kau, 2017). On the other side, introduction of new aligner material also draws attention (Silverman and Cohen, 1969; Choi and Kim, 2005; Lai and Rule, 2020; Elshazly et al., 2021).

Shape memory polymers (SMPs) are one of the novel materials to be recently introduced into the field of dentistry, particularly for orthodontic applications (Mahmood et al., 2019; Elshazly et al., 2021). They provide great potential for applications in medical materials (Lendlein and Langer, 2002; Zhang et al., 2009; Meng and Li, 2013). In a study by Jung et al. (Jung and Cho, 2010) and another by Nakasima et al. (1991), SMPs were used in fabrication of orthodontic wires. Choi and Kim (2005) registered a patent about a tray-type appliance made of SMPs used for teeth alignment. Also, Lai and Rule (2020) registered another patent about an orthodontic appliance having a continuous shape memory recovery. Through this shape memory property, it can store a large number of geometries throughout the orthodontic treatment. Recently, Elshazly et al. (2021) reported a new orthodontic aligner system based on thermoresponsive shape memory polyurethane-based thermoplastic material, showing the ability of one aligner to recover its shape through three steps of material treatment and consequently conduct stepwise tooth movement in a way that one aligner may be able to replace three subsequent conventional aligners. Despite the mentioned reports, yet, there is lack of data in literature about the application of SMPs in the field of orthodontic aligners.

The technology of four-dimensional printing (4D printing) is based on the 3D printing of shape memory materials. Clearly, 4D-printed parts have the ability to change shape with time (the fourth dimension), upon given environment conditions (Pei et al., 2020). With the continuous development of SMPs, new 4D printing applications within the product design industry are expected to grow (Nam and Pei, 2020). We proposed in our scientific project to introduce the 4D technology in the fabrication of orthodontic aligners.

In this study, on a custom-made typodont model, correction of malposition of tooth 21 by 4D-printed aligners with thicknesses of 0.8 and 1.0 mm was measured by superimposition of obtained and initial scans. Also, forces generated on 2-mm vertical three-point bending (3-PB) tests were measured at different temperatures. Additionally, forces and movements delivered by the 4D aligners were quantified using an orthodontic measurement and simulation system (OMSS).

MATERIALS AND METHODS

Typodont

A custom-made typodont model was fabricated from resin (Technovit 4004; Kulzer, Wehrheim, Germany) and acrylic teeth (Frasaco, Tetnang, Germany). The upper left central incisor (tooth 21) was separated and kept movable by being embedded in pink wax placed in the model, while the other teeth were fixed by the resin (**Figure 1**). The fully aligned model was scanned (scan 0) using a 3D lab scanner (D2000; 3Shape,

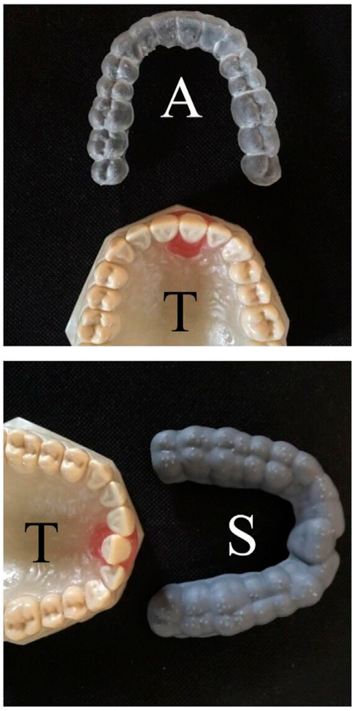

FIGURE 1 | A custom-made typodont (T), a 4D-printed aligner (A), and a gray splint (S).

Copenhagen, Denmark). The model was segmented using an Ortho System software (Ortho Analyzer; 3Shape). Using the appliance designer software (Appliance Designer; 3Shape), two groups of aligners were designed with thicknesses of 0.8 and 1.0 mm and an offset of 0.2 mm, on the fully aligned model. The aligner geometries were then sent for 3D printing, six aligners per each group (n = 6). ClearX v.1.1 3D-printed material (Kline-Europe, Dusseldorf, Germany) was used, reported by the suppliers to have shape memory properties. Afterward, tooth 21 was moved palatally in the software model with a total malalignment of 3 mm. The malaligned model was exported as an STL file and was 3D printed using a 3D-printable resin (Dentona Optiprint model; Dentona AG, Dortmund, Germany). A 3D printer (Asiga Max; SCHEU-DENTAL GmbH, Iserlohn, Germany) was used for the previous printing steps, with 62-µm high-definition print precision.

Three gray splints of thickness 3.0 mm (**Figure 1**) were designed over the malaligned model and were 3D printed (Form 3BL Basic Package; Formlabs, Somerville, MA, USA) using a resin material (Grey Resin 1 L; Formlabs). The first splint was produced over the malaligned model. It was used as an "index" to reposition the typodont (tooth 21) to the exact same malaligned position during testing. The second and third splints were produced over the 3D aligners, one for each different thickness. They were used for reforming and adaptation of the softened aligners to the malaligned models before testing.

The adaptation process was done by immersing the aligner in a hot water bath of 80°C for 30 s to ensure exceeding the glass transition temperature (Tg) of the material, reported by the supplier to be at 30°C, and to ensure enough softening of the material. The aligner was then adapted on the malaligned model by the aid of the corresponding adaptor splint. They were then let together to cool down in a cold water bath of 5°C so that the aligner can maintain its new malaligned shape (malaligned aligner).

The wax around tooth 21 of the typodont model was softened, and the index splint was used to reposition tooth 21 in the typodont model at 3-mm malposition. The typodont was then placed in a 5°C water bath for 10 min to ensure that the wax was no longer soft and could withstand aligner placement without getting distorted. The malaligned typodont model was then scanned (scan 1). Afterward, the malaligned aligner was placed on the malaligned typodont, and both were immersed together for 5 min in a hot water bath of 55°C, which is the activation temperature recommended by the supplier. This initiated the shape memory recovery of the aligner and softened the wax around tooth 21 in the typodont to allow the correction movement of the tooth to happen by the memory recovery of the SMP aligner. Subsequently, they were taken out from the hot water bath and put back in a cold water bath (5°C), so that the wax could get hard at the new position before removing the aligner to avoid distortion. The typodont model was then scanned again (scan 2). Scan 2 was superimposed with scan 1, and the correction was measured by the Ortho Analyzer software (**Figure 2**). The test was repeated six times for each group (0.8 and 1.0 mm), each time new wax and new aligner were used. Using this test, the aligner shape recovery was recorded visually. A schematic diagram illustrating the main steps of ClearX 4D aligner method was added (**Figure 3**).

3-PB Test

The experimental investigation of the force systems generated was performed by a custom-made biomechanical system (OMSS; Drescher et al., 1991) at the University Hospital Bonn in Germany. Six 3D-printed specimens of the 4D ClearX v.1.1 material were produced in dimensions ($50 \times 10 \times 1.0\ mm^3$) and mounted in the biomechanical testing machine (OMSS, **Figure 4**) to perform a 2-mm vertical 3-PB tests under standardized conditions at a rate of 5 mm per minute and at different temperatures of 20°C, 30°C, 35°C, 37°C, 40°C, and 50°C. The force/deflection curves were recorded, and the maximum

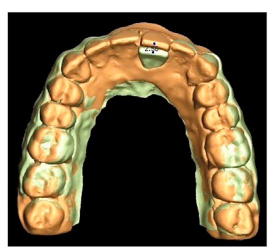

FIGURE 2 | Superimposition of the typodont scans before and after testing of the 4D aligner, scan 1 (before, green) and scan 2 (after, orange).

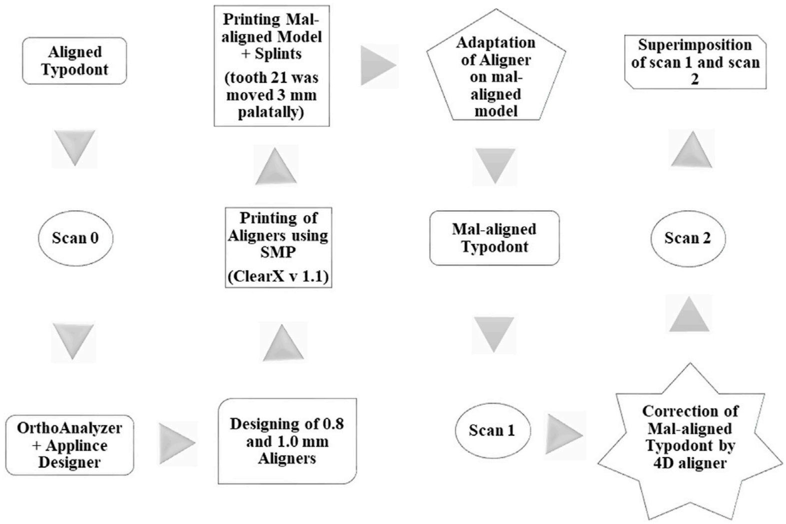

FIGURE 3 | A schematic diagram illustrating the main steps of the ClearX 4D aligner method.

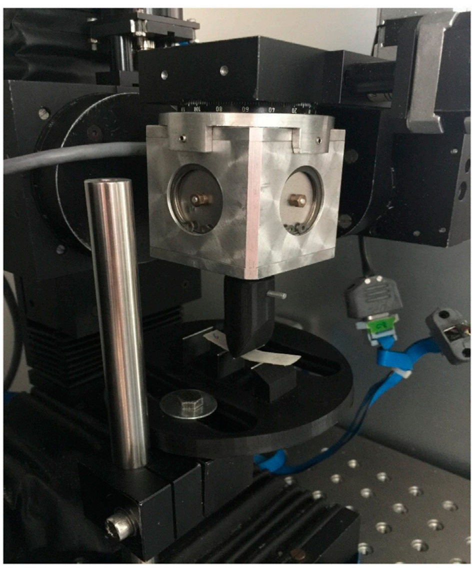

FIGURE 4 | Three-point bending test of a 4D-printed specimen using the orthodontic measurement and simulation system (OMSS) at different temperatures.

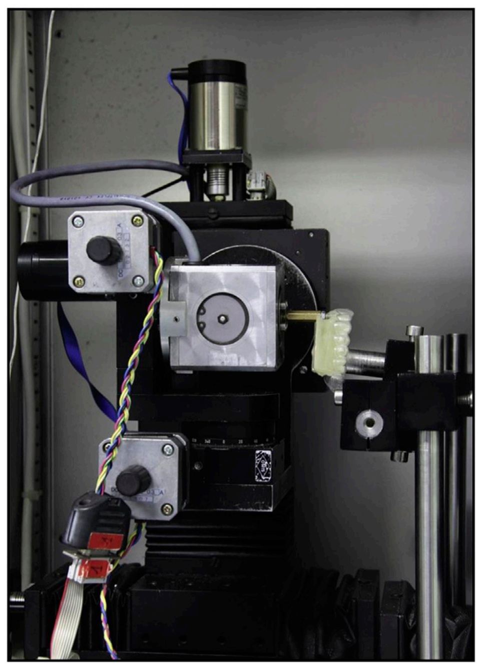

FIGURE 5 | Orthodontic measurement and simulation system (OMSS): a resin replica with a 4D-printed aligner is mounted in the system. Tooth 21 to be analyzed was connected to a computer-controlled 3D sensor. The measured moments and forces are registered, and the motor-driven positioning table simulates the analyzed tooth movement.

generated force was determined. Each cycle was repeated two times with the same specimen.

Experimental Simulation of Tooth Movement

The typodont without the movable tooth 21 was duplicated using Technovit 4004, and tooth 21 was separated. The resin replica was mounted into OMSS (**Figure 5**). In several articles (Drescher et al., 1991; Simon et al., 2014a), more details of the technical specifications and the software running the experiments of OMSS can be found. The OMSS device consists of sensors that can be used for measuring force and moment vectors in three

TABLE 1 | Mean ± standard deviation (SD) of translation and forces conducted on upper central incisor (tooth 21) by 4D-printed aligners of two thicknesses

	Thickness (mm)	Temperature			*p* value
		37°C	45°C	55°C	
Translation (mean ± SD)	0.8	1.0 ± 0.4^{Ba}	2.4 ± 0.6^{Aa}	2.1 ± 0.5^{Ab}	<0.001*
	1.0	1.1 ± 0.4^{Ba}	1.6 ± 0.2^{Bb}	2.8 ± 0.1^{Aa}	<0.001*
		0.701ns	0.004	0.006	
Force (mean ± SD)	0.8	0.3 ± 0.1^{Ba}	0.2 ± 0.1^{Ba}	0.7 ± 0.2^{Aa}	<0.001*
	1.0	0.3 ± 0.1^{Ba}	0.3 ± 0.1^{Ba}	0.6 ± 0.2^{Aa}	<0.001*
		0.701ns	0.701ns	0.701ns	

Measurement was done at different temperatures in a custom-made biomechanical system (OMSS). Different uppercase and lowercase superscript letters indicate a statistically significant difference within the same horizontal row and vertical columns, respectively.
**Significant (p ≤ 0.05). ns, nonsignificant (p > 0.05).*

dimensions (x, y, and z). Sensors are mounted on a 6-axes motor-driven positioning table, which is able to perform full 3D movements. To describe tooth movements in all three spatial dimensions, a coordinate system was set up. The positive x axis ($+X$) describes extrusive and the negative x axis ($-X$) describes intrusive movements and forces, parallel to the long axis of the tooth. Horizontal forces and movements are described on the y axis and the z axis, where $+Z$ represented the facial movement and force, $-Z$ represented lingual movement and force, $+Y$ represented distal movement and force, and $-Y$ represented mesial movement and force.

The separated tooth 21 was connected to a sensor. Adjustments were made with the index splint so that tooth 21 was passively set in its 3-mm lingual malposition in respect to the other teeth of the resin replica. The whole apparatus was enclosed in a temperature-controlled chamber in order to run the test at different temperatures. Six new aligners for each group of two thicknesses (0.8 and 1.0 mm) were 3D printed on the aligned model. Each aligner was reformed on the malaligned position as described previously at the typodont experiment. The malaligned aligner was mounted on the resin replica, in a way that almost no active forces (zero forces) were transferred to the tooth, whereas the thermal chamber of OMSS is at room temperature (20°C, below Tg). The temperature of the chamber was increased to 37°C, 45°C, and 55°C. By means of continuous measurements of the force systems and simulation of the resulting movement of tooth 21, the force progression generated by an aligner was measured, and the experimentally resulting tooth movement was calculated. For tooth movements in the three dimensions, the measurements were terminated when forces decayed below 0.02 N.

Statistical Analysis

Independent t test was used to compare movement of the typodont tooth with different thicknesses of the aligner. Two-way analysis of variance followed by Bonferroni correction was used to study the effect of different tested variables (temperature and thickness of the aligner) and their interaction on force and translation. The significance level was set at $p \leq 0.05$ within all tests. Statistical analysis was performed using IBM SPSS Statistics version 25 for Windows (IBM Company, Endicott, NY, USA).

TABLE 2 | Mean ± standard deviation (SD) of translation of upper central incisor (tooth 21) by 4D-printed aligners of two thicknesses

Translation (mean ± SD)			*p* value (ns)
Thickness	Typodont	OMSS	
0.8 mm	2.2 ± 0.5^{Aa}	2.1 ± 0.5^{Ab}	0.617*
1.0 mm	2.6 ± 0.5^{Aa}	2.8 ± 0.1^{Aa}	0.257*
p value	0.152ns	0.006*	

Measurement was done at temperature of 55°C on a typodont model and in a custom-made biomechanical system (OMSS). Different uppercase and lowercase superscript letters indicate a statistically significant difference within the same horizontal row and vertical columns, respectively.
**Significant (p ≤ 0.05). ns, nonsignificant (p > 0.05).*

RESULTS

On the typodont, 4D-printed aligners succeeded to achieve a significant tooth movement (2.5 ± 0.5 mm), with insignificant difference between the different thicknesses (**Figure 2** and **Table 2**). In 3-PB test, the maximum forces measured at 20°C, 30°C, 37°C, 45°C, and 55°C were 3.8 ± 1.1, 2.5 ± 0.9, 1.7 ± 0.6, 1.0 ± 0.4, and 0.5 ± 0.4 N, respectively (**Figure 6**).

In OMSS simulations, the forces delivered on palatal displacement of tooth 21 at 37°C, 45°C, and 55°C by 0.8-mm aligners were 0.3 ± 0.1, 0.2 ± 0.1, and 0.7 ± 0.2 N, respectively, whereas those by 1.0-mm aligners were 0.3 ± 0.1, 0.3 ± 0.1, and 0.6 ± 0.2 N, respectively (**Figure 7** and **Table 1**). Varying degrees of temperature had a significant effect on the force, whereas the thickness of the aligner along with its interaction with temperature had no significant effect. Pairwise comparison showed that aligner subjected to 55°C conducted a significantly higher force than those subjected to 37°C and 45°C. A good concordance with movement of tooth 21 in the typodont experiment could be shown in OMSS with insignificant difference between them (**Table 2**). At 55°C, there was a higher significant translation by 1.0-mm aligner than the 0.8-mm one (**Tables 1** and **2**).

DISCUSSION

Although orthodontic aligners have been studied in several aspects and great progress was done in orthodontic treatment by aligners (Bowman, 2017), practitioners still report some

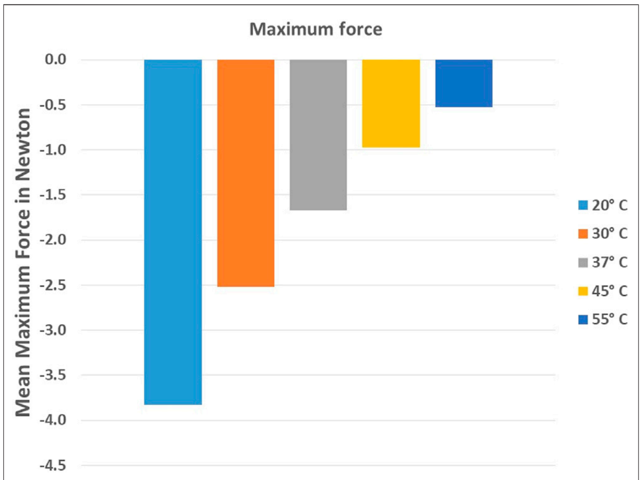

FIGURE 6 | Bar chart showing the mean maximum force generated on a 2-mm vertical three-point bending testing of 3D-printed specimens of ClearX v.1.1 shape memory material at different temperatures.

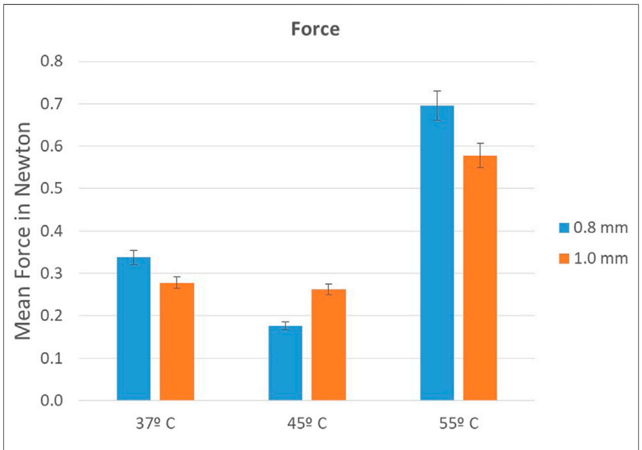

FIGURE 7 | Bar chart showing forces generated by 4D-printed aligners of two different thicknesses; measurement was done at different temperatures in a custom-made biomechanical system (OMSS).

drawbacks to aligner use. On the top of these drawbacks are the limited movement achieved by each single aligner, which leads to use of changing regime through a large series of aligners per treatment (Simon et al., 2014b; Elshazly et al., 2021). Therefore, we believe that if a method could be applied to decrease the number of the aligners per treatment, together with a method to accelerate the biological movement of the teeth, that would be a quantum leap in the field of orthodontics.

The introduction of new aligner materials draws the attention of many researchers. Some of them introduced smart materials, particularly SMPs (Silverman and Cohen, 1969; Choi and Kim, 2005; Lai and Rule, 2020; Elshazly et al., 2021). The idea of clear aligners made of SMPs is aiming to reduce the cost and time of the treatment by using a dynamic aligner that can change its shape intentionally over treatment time, and consequently one shape memory aligner could substitute a series of conventional aligners and overcome the stepwise system. Furthermore, it helps to decrease the plastic consumption by decreasing the number of plastic aligners per treatment plan and thus raise concerns about the ethical responsibility toward the environment (Elshazly et al., 2021). Despite many tryouts mentioned before (Choi and Kim, 2005; Jung and Cho, 2010; Lai and Rule, 2020; Elshazly et al., 2021), still there is a great lack of data in the literature about clear aligners made from SMPs. So far, it is difficult, biomechanical-wise and biocompatibility-wise, to favor an appropriate material.

Thermoresponsive SMPs are a subcategory of smart polymers, which have a novel capacity, to recover their original shape after being deformed, upon specific thermal initiation (Zhang et al., 2009; Meng and Li, 2013). At the molecular level, polymer network-based SMPs consist of at least two different segments, hard and soft, with two different glass transition temperatures (Tg) (Lendlein and Langer, 2002). Shape memory mechanism is attributed to the cooperation of the hard and the soft segments. Phase separation is essential in this mechanism. The separation occurs only above a threshold temperature (transition temperature); prior to it, no phase separation occurs. Soft segments act as a switch (matrix phase) responsible for shape changing, and hard segments act as cross-links responsible for preserving the original shape (Lendlein and Kelch, 2002; Behl and Lendlein, 2007; Zhang et al., 2009). Many of SMPs have a Tg near the body temperature; thus, the body temperature could act as an initiator for shape memory change (Gorna and Gogolewski, 2003). Moreover, many SMPs have the advantage of possessing several inherent properties, such as transparency, low density, and reduced cost (Jung and Cho, 2010). In addition, the shape recovery of some SMPs could last up to approximately 3 months, which might be suitable for orthodontic applications (Small et al., 2010). These advantages may qualify them to be introduced in the fabrication of orthodontic appliances for treatment of initial alignment and leveling of aesthetically concerned patients (Nakasima et al., 1991), as well as the correction of malaligned and severely rotated teeth (Mahmood et al., 2019).

On planning of an orthodontic treatment with an aligner system, it is important to make a biomechanical analysis of the used material and the appliance and know the exact distribution of the forces and moments. The flexure modulus is a mechanical property that relates stress to strain in flexural deformation, and it is an indicator of the material's tendency to resist bending. The developed force is directly proportional to the flexure modulus and to the third order of the thickness in bending direction (Zweben et al., 1979). In orthodontic appliances such as aligners, it is an indicator of the effectiveness for tooth movement (Ryu et al., 2018). The 3-PB test is a method used to determine the flexure modulus and the maximum force delivered upon deflection (Kwon et al., 2008; Min et al., 2010). Additionally, to know the exact force systems of the aligner in all three planes of space, an OMSS was used (Drescher et al., 1991; Bourauel et al., 1992). Moreover, based on the force system, the control program of OMSS calculated the developed tooth movement by using a mathematical model, taking into consideration the center of resistance of the measured tooth (Pedersen et al., 1990).

Optimal force delivery is a must for an ideal orthodontic treatment, in order to achieve a maximum rate of tooth movement without causing irreversible damage to the biological tissues (Kwon et al., 2008). A light continuous force is required for ideal tooth movement. In case of excessive force to a target tooth, indirect bone resorption can occur; accordingly, the speed of tooth movement will be slower, or root resorption may occur. On the contrary, if sufficient force is not delivered to a target tooth, tooth movement will not be obtained (Proffit et al., 2000). Consequently, optimal forces are important for ideal tooth movement. For instance, the optimal forces for tipping movement of a single tooth were reported to be from 0.50 to 0.75 N, for rotation control are 1.00–1.50 N, for torque control are 0.75–1.25 N, and for bodily movement are 0.75–1.25 N (Proffit et al., 2000; Kwon et al., 2008). In conventional aligner systems, the force delivery to a target tooth is generated by the tendency of the plastic material through its resiliency to return to its resting state instead of being deformed 0.25–0.33 mm in some systems (Simon et al., 2014a) or 0.50–1.00 mm in other systems (Sheridan et al., 1993). However, in the 4D-printed aligner system, the aligners are made of SMPs, and the force delivery is obtained from the shape recovery of the material upon appropriate stimulations (Elshazly et al., 2021). Additionally, the 3D printing of the material gives advantage of avoiding the significant decrease of mechanical properties after deep drawing of thermoformed material (Ryu et al., 2018).

The technology of 4D printing is based on the 3D printing of SMPs. In our study, a 3D-printable material (ClearX v.1.1), reported by the supplier to possess thermoresponsive shape memory properties, was used in fabrication of orthodontic clear aligners (4D aligner). A typodont model was used in the study as an initial proof of the movement of the tooth, similar to many other reports (Ishida et al., 2020; Elshazly et al., 2021; Ho et al., 2021). A simple orthodontic case was used in the study, where only a bodily movement of one tooth (maxillary upper incisor, tooth 21) was tested, whereas the other teeth remained fixed in the resin and were used to provide retention to the whole aligner. The maximum forces generated on 2-mm deflection at different temperatures were measured. Furthermore, the forces generated from shape recovery, which should be responsible for the tooth movement, were measured by a custom-made biomechanical system (OMSS).

The results show success of the shape memory aligner to achieve a significant movement of tooth 21 on the typodont, and a congruent movement was also measured in OMSS. The targeted alignment movement (3.00 mm) was not reached; only 2.06–2.82 mm was achieved, which could be referred to the resistance of the wax (in typodont test) and the rigidity of the sensor (in OMSS), in front of the low forces generated by the shape recovery. Nevertheless, the results are satisfactory, and the achieved movement by one shape memory aligner equals nearly the movement that could be achieved by 10 conventional aligners.

In the current study, the force delivery upon deflection of the aligner by bodily movement of tooth 21 for 2 mm needed to be simulated; therefore, the span length in the 3-PB test (distance between the two supports) was set at 24 mm, which was equal to the sum of the average widths of the two maxillary central incisors and one lateral incisor, and the specimen was deflected vertically at its center to a maximum of 2 mm (Kwon et al., 2008). The results of our study (**Figure 7**) show that the range of maximum force delivered on a 2-mm deflection at temperatures from 37°C to 55°C (the activation temperature range of the material) with sheet thickness of 1 mm ranged from 1.20 to 0.50 N. This is located within the acceptable range of orthodontic forces, and it is in the same range of forces generated by conventional aligners upon deflections of 0.20–0.50 mm (Proffit et al., 2000; Kwon et al., 2008). The results show also that the maximum forces are decreasing with increasing the temperature, which can be explained by the fact that the heat in such thermoplastic material leads to a type of softening through debonding of the secondary bonds of the cross-links of the material and therefore weakens the material.

The generated forces at different temperatures (37°C, 45°C, 55°C) measured by OMSS (0.30–0.70 N) are also in the range of acceptable physiological orthodontic forces reported by many studies (Hahn et al., 2010; Simon et al., 2014a; Elkholy et al., 2016; Elkholy et al., 2017; Iliadi et al., 2019). Moreover, these findings are supported by a study by Nakasima et al. (1991), in which it was reported that SMPs are able, at properly controlled oral conditions, to produce light long-lasting forces. They used a stretched orthodontic wire of polynorbornene, a type of SMP, and showed that it could reverse gradually to its original shape upon heating at a temperature of 50°C and generate forces in the physiological range, which could be used to move a human tooth.

In our study, the forces generated at 50°C were higher than the forces generated at 37°C, yet in the accepted range. Interestingly, there was a reduction of forces at 45°C in comparison to the forces at 37°C and 55°C. Explanation of such situation, especially in a viscoelastic material such as the tested material, may need further investigation of the material, such as dynamic thermomechanical analysis and differential scanning calorimetry, in order to get a more clear picture of the phase transition at different temperatures.

Contradicting with previous studies (Kwon et al., 2008; Hahn et al., 2009; Min et al., 2010; Ryu et al., 2018), the current study reported that using thicker aligners has no significant effect on the generated force, except at 55°C in the OMSS. That could be due to inaccuracy of the 3D printing in a way that the aligner thickness is not homogenous, thicker in parts and thinner in others. However, the findings are, from other prospective, generally in agreement with Nam and Pei (2020), who revealed that the shape memory effect of 4D-printed parts is mostly influenced by the recovery temperature and the deformation temperature.

This study still has many limitations. We measured forces for an isolated experimental movement of a single tooth, which is a simplified model that cannot reflect the more complex clinical cases, in which several teeth are included in the treatment plan. Also, we did not fully consider the intraoral conditions such as salivation and humidity, especially that some polymers are sensitive to moisture due to presence of hydrogen bonding between the polymeric chains (Yen et al., 1991; McKiernan et al., 2002). Additionally, the OMSS enables both measurements of the forces of the initial situation and the dynamic force progression during tooth movement; however, in the setup of the present study, sensor and tooth were connected rigidly, with the limitation of simulation of some clinical parameters such as periodontal ligament (PDL), mastication, as well as soft-tissue reactions (Bourauel et al., 1992). Besides, OMSS is based on the hypothesis that there is a linear relationship between the speed of tooth movement and the amount of applied force, which could not really simulate the biomechanical behavior of PDL. Moreover, an ideal center of resistance was used for each tooth (Simon et al., 2014a).

Further studies on the mechanical and physical properties of the used SMP materials should be performed. More clinically oriented simulated models for the force delivery by SMP materials should be developed. Moreover, it is still a challenge to introduce a clinically applicable technique to use the shape memory aligners.

CONCLUSION

Initial investigation of a 3D-printed aligner made of SMPs (4D aligner) shows its capability of moving teeth by biocompatible orthodontic forces after a suitable thermal stimulus within the oral temperature range.

DATA AVAILABILITY STATEMENT

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

AUTHOR CONTRIBUTIONS

Conceptualization: TE. Data curation, analysis, investigation, and methodology: TE and YA. Resources: TE, CB, MA, and AG. Software: TE, CB, and LK. Supervision, validation and visualization: CB, AG, MA, WT, and ST. Writing—original draft: TE. Writing—review and editing: TE, YA, and CB. All authors have read and agreed to the published version of the manuscript.

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3.3 Study 3

Computer-aided finite element model for biomechanical analysis of orthodontic aligner

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ORIGINAL ARTICLE

Computer-aided finite element model for biomechanical analysis of orthodontic aligners

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Abstract

Objectives To design a finite element (FE) model that might facilitate understanding of the complex mechanical behavior of orthodontic aligners. The designed model was validated by comparing the generated forces — during 0.2-mm facio-lingual translation of upper left central incisor (Tooth 21) — with the values reported by experimental studies in literature.
Materials and methods A 3D digital model, obtained from scanning of a typodont of upper jaw, was imported into 3-matic software for designing of aligners with different thicknesses: 0.4, 0.5, 0.6, 0.7 mm. The model was exported to Marc/Mentat FE software. Suitable parameters for FE simulation were selected after a series of sensitivity analyses. Different element classes of the model and different rigidity values of the aligner were also investigated.
Results The resultant maximum forces generated on facio-lingual translation of Tooth 21 were within the range of 1.3–18.3 N. The force was direction-dependent, where lingual translation transmitted higher forces than facial translation. The force increases with increasing the thickness of the aligner, but not linearly. We found that the generated forces were almost directly proportional to the rigidity of the aligner. The contact normal stress map showed an uneven but almost repeatable distribution of stresses all over the facial surface and concentration of stresses at specific points.
Conclusions A validated FE model could reveal a lot about mechanical behavior of orthodontic aligners.
Clinical relevance Understanding the force systems of clear aligner by means of FE will facilitate better treatment planning and getting optimal outcomes.

Keywords Biomechanics · Orthodontic force · FEM · Tooth movement · Thermoplastic stent · Removable dental appliances

Highlights
- Experimental biomechanical studies of aligners have many limitations.
- Finite element method might help for better understanding of force transmission by aligners.
- The deformation of the aligner is a combination of bending and stretching.
- The generated forces are almost directly proportional to the rigidity of the aligner.

Introduction

Clear aligners are a series of removable plastic stents, which are customized for each orthodontic patient to effectively move teeth into their desired aligned position. They have a high esthetical appearance because of being transparent

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and almost invisible. Besides, they are more comfortable and easier to keep a good oral hygiene, compared to fixed orthodontic braces [1–3]. In addition, clinically and technical-wise, they are much easier to be handled in every-day practice than fixed appliances. Also, they need shorter dental appointments and seem to be ideal for retreatment cases [4, 5]. As well, they may be used for improvement of some bad parafunctional habits during treatment, such as bruxism, and may also be beneficial for treatment of temporomandibular joint problems [6, 7].

Formerly, treatment planning for aligners was accomplished on plaster models at a millimeter scale. Recently, and with the revolution of digital scanning, CAD-CAM technologies, and 3D–printing, digital treatment planning is applied for more accurate outcomes at the scale of hundredths of millimeter [8]. However, for a better treatment planning and to get optimal outcomes, a very good understanding of mechanical behavior of the aligners should be available. To our best knowledge, and despite several investigations of clear aligners in many aspects, still, there is lack of data in the literature about the biomechanical behavior of orthodontic aligners [9, 10].

Tooth movement by aligners is based on a limited programmed deviation between the setup position and the position of the targeted real tooth. The geometry of the aligner's tray defines the amount of movement [11]. In most popular aligner systems, each single aligner of the treatment series is designed to move the targeted tooth by around 0.2 mm for translations and about 3° for rotations in a period of approximately 10–14 days [3, 12, 13].

Many methods were used for biomechanical analysis of aligners, such as strain gauge [14, 15], pressure sensors [16–18], pressure sensitive films [19, 20], and different customized biomechanical systems [3, 21–23]. However, all applied techniques have shortcomings and limitations and showed discrepancies of the reported results [3, 19, 20, 24]. Hence, as a promising alternative approach, using the finite element method (FEM) might lead to a better understanding of the behavior of the orthodontic aligners, through a mechanical numerical stress/strain analysis validated by standardized experimental setups, as well as well-controlled clinical studies [24].

From the time of the 70 s of the last century, FEM has been a widely used tool to evaluate the effectiveness of dental appliances [25]. It is a modern engineering tool for structural analysis that is applicable to bodies of irregular geometries and heterogeneous material properties. The structure is divided into finite number of elements connected by nodes. By choosing a suitable mesh and an appropriate mathematical model for each element, the reactions and interactions of the structure could be yielded [26]. In the literature, many articles are reporting about FE biomechanical analysis of orthodontic fixed braces [27–30]. So far, few studies have been made for biomechanical modeling of orthodontic aligners [31–33], but many of them were much simplified and far from reality.

The aim of the current study was to report about designing a numerical realistic 3D finite element model that can be used to study the mechanical behavior of orthodontic aligners. Additionally, for validation of the model, we designed our model trying to simulate the same experimental setup used in some studies in the literature [13, 21, 34, 35] and then, the resultant forces generated — during facio-lingual translation of upper left central incisor tooth (tooth 21) — were compared with the reported values in these studies. Afterward, in future studies, modifications of the model will be done by adding the periodontal ligament (PDL) and the bone, in order to widely study the forces and the moments generated by the aligners with various teeth and in different directions of movement.

Materials and methods

A custom-made typodont model, already utilized for other experimental studies by our research team, was used in the current study. It was made up from acrylic teeth (Frasaco; Teltnag, Germany) and a resin (Technovit 4004; Kulzer, Wehrheim, Germany). The upper left central incisor (Tooth 21) was embedded malaligned 3 mm palatally in a pink wax, while the other teeth were aligned and fixed by the resin (Fig. 1). The typodont was scanned using a 3D lab-scanner (D2000; 3Shape, Copenhagen, Denmark). The generated digital model was exported as an STL file to a 3D image processing and editing software package (Mimics Innovation Suite, Mimics 24.0/3-matic 16.0; Materialise, Leuven, Belgium) (Fig. 1).

In 3-matic, the STL data were reconstructed to 3D surface models. The upper left central incisor (Tooth 21) was chosen as the treated tooth in the current study and was separated to be individually moveable. The first approach to design the aligner was to scan a thermoformed aligner; however, even with using special opaque sprays, the generated 3D scan was inaccurate, due to the transparency of the aligner. Additionally, many problems were met to establish a correct contact between the aligner and the teeth. So, the modeling tools of the 3-matic software were chosen to model the aligner with homogenous predefined thicknesses.

For aligner modeling, the surface element of the tooth crowns was selected and duplicated, with a clearance offset of 0.02 mm between the aligner and the teeth, and then by applying the solid uniform offset tool in 3-matic, full arch aligners were modeled. Four different thicknesses of the aligner were designed, namely 0.4, 0.5, 0.6, and 0.7 mm. Although thermoplastic sheets are supplied commonly in thickness of 0.75 mm, different thicknesses were modeled, referring to the material thinning resulted from

Fig. 1 Generation of a digital 3D model from a typodont model using a 3D-lab scanner

the deep-drawing process of the aligner sheet on the cast [35, 36]. Moreover, we considered the spacing foil (nearly 0.02 mm) at the internal surface of the aligner opposing to the tooth surface, defined by Elkholy et al. [23] as the primary offset, which is removed after thermoforming, and acting as an acceptable spacer for saliva and to facilitate removing of the aligner, along with delivering acceptable forces [37]. The sharp edges at the trimming line of the aligner were smoothened using the finishing/smoothing tool of 3-matic to get a scalloped design of the aligner margins following the gingival line of the teeth. Different trimming designs [38] are used in the market: scalloped, straight, and straight extended, but the scalloped design was chosen in the current study. In future studies, the effect of the trimming line design on the force transmission is planned to be investigated using the current FE model.

The 3-matic tool of adaptive element meshing was applied for re-meshing of the external aligner surface. By this tool, smaller elements were given at areas of complex geometry and larger elements at areas of less geometric complexity. The root with PDL and bone structures was not designed in the current study, to mimic the experimental conditions reported in earlier studies [23, 34] (Fig. 2).

The whole model was imported as 3-noded triangular surface elements model into an FE analysis pre-processing and post-processing software package (Marc/Mentat 2015; MSC Software, Los Angeles, Calif). In Marc/Mentat software, the triangular surface elements of the model were remeshed and converted to solid elements. A series of sensitivity analyses were performed to select the best parameters for the numerical simulation. For meshing of the aligner, different element classes and types were tried; 4-noded tetrahedral elements (Tetra 4), 10-noded tetrahedral elements (Tetra 10), 8-noded hexahedron (Hex 8), and 20-noded hexahedron (Hex 20), and the resulting values are reported in the current article. However, and based on the outputs, we selected (Tetra 4) for meshing of the cast and the teeth and (Tetra 10) for meshing of the aligner, and with these conditions, the number of elements and nodes of every part of the model are reported in Table 1.

In any FE simulation, the material model must be correctly specified to each component of the model. In agreement with many studies of hard oral tissues [27, 28, 31, 33], and for simplification of the model, the linear elastic constitutive mode was used. The Poisson's ratio was set at 0.3 for all structures [27, 30, 31, 33]. Young's modulus of teeth was chosen to be similar to enamel, without taking into

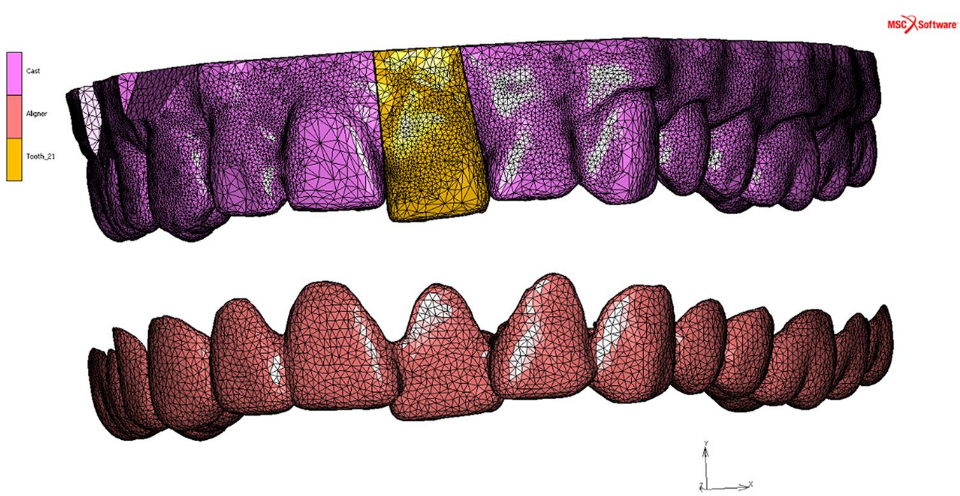


Fig. 2 Digital model of aligner and cast with separated moveable upper left central incisor (Tooth 21) for finite element studying of the orthodontic aligners

Table 1 Number and type of elements and nodes of all objects of the finite element model

Object	Element class/type	No. of elements	No. of nodes
Aligner 0.4 mm	Tetra 10, type 130	123226	245414
Aligner 0.5 mm	Tetra 10, type 130	186298	329915
Aligner 0.6 mm	Tetra 10, type 130	194323	338287
Aligner 0.7 mm	Tetra 10, type 130	380308	622539
Tooth 21	Tetra 4, type 157	13541	3450
Cast	Tetra 4, type 157	252808	62739

consideration the division into dentin, enamel, and pulp [31, 33]. Despite the large variations of the reported Young's modulus of enamel in literature from 18 GPa [27, 31] to 112 GPa [39], the value of 80 GPa was opted as reported in some recent articles [40, 41]. Nevertheless, in the current study, and by a sensitivity analysis, no significant difference was found when Young's modulus of 18 GPa for the teeth material was input. The reported Young's modulus of aligner materials in literature is in the range of 0.5 [33] to 2.2 GPa [42]. Young's modulus of aligner was elected to be 1.5 GPa, similar to a polyethylene terephthalate glycol-modified (PETG) thermoplastic sheets, commonly used for aligner fabrication and reported in some studies [42, 43]. Additionally, one of the aims of this study was to investigate the effect of the aligner's rigidity on the generation of forces; hence, the forces generated by 0.6-mm-thick aligners were calculated after varying Young's moduli: 0.5, 1.0, 1.5, and 2.0 GPa. Material parameters are shown in Table 2.

All components were defined as deformable (meshed) contact bodies. A contact table was created to define the contact interaction between different contact bodies. Contactless interaction was defined between the cast and the moveable teeth, while a touching sliding contact interaction was defined between the aligner and the tooth/cast surfaces, with a frictionless mode and with interference closure of −0.04. At the advanced contact control options of Marc/Mentat software, a node to segment method was used, and an optimized contact constraint equations mode was activated with a double-sided deformable-deformable method.

As the upper jaw model is arch-shaped, using the same coordinate system of the jaw for movement of the moveable teeth will not be correct. In other words, moving in *Z*-direction means a facio-lingual movement in anterior incisors but means mesio-distal movement in posterior molars.

Table 2 Material parameters assigned to aligner, cast, and teeth in the finite element model

Structure	Young's modulus (GPa)	Poisson's ratio
Plastic aligner	1.5	0.3
Cast and teeth	80	0.3

Additionally, the targeted Tooth 21 is following the curve of the arch. Therefore, for an accurate movement, a distinct local coordinate system should be defined for the tested separated Tooth 21 in a way that the *X*-axis pointed to the transverse mesio-distal direction, the *Y*-axis to the vertical intrusion-extrusion direction, and the *Z*-axis to the transverse facio-lingual direction, with the positive direction toward the facial, mesial, and intrusion of the tooth individually.

Boundary conditions were applied on the cast, the aligner, and the moveable tooth, through the structural fixed displacement function of Marc software. The cast was fixed in the 3 directions of translations at its lower surface nodes (a total of 3403 nodes). Moreover, the aligner was required to be preferably fixed during the simulation, which is somehow different from the clinical situation; however, some sort of numerical stability was necessary to be applied. For aligner fixation, a non-rigid indirect fixation was used at first, but many problems were faced in the model, so a rigid fixation was applied at nodes of the most distal ends of the aligner far from the loaded tooth, and the stresses at this fixed part were checked and found to be negligible. The movement boundary condition of Tooth 21 was applied to the surface nodes at the lower apical side (a total of 190 nodes). The Tooth 21 was loaded with a linearly increasing displacement in both facial (+*Z*) and lingual (−*Z*) directions to a maximum displacement of 0.2 mm, while it was fixed in the *X*- and *Y*-directions.

Calculations were performed on a computing cluster (Dell; Round Rock, Texas, USA). The calculation time and the data were somehow large. Therefore, as a trial to develop a more simplified model and for reducing the resultant data and decreasing the analysis time (reached 28 h), the size of the model was reduced, either by using an anterior segment or using half segment of the model, in which the span length of the aligner (distance between the two distal ends) would be shorter. However, there was a significant difference in the resultant forces between the full and the reduced model; hence, we ignored the reduced model, and our results in the current article are based on the full model (Fig. 2).

Results

The resultant forces from different aligner thicknesses on 0.2 mm facio-lingual translation of Tooth 21 were within the range of 1.3–18.3 N. A direction-dependency of force generation was displayed, in which lingual translation induced higher forces than facial translation (Fig. 3). Furthermore, the thickness of the aligner had a significant effect on force generation, where increasing the thickness generated higher forces, but the relation was not perfectly linear (Figs. 3 and 4). The course of the resultant force generation during the facial movement of tooth 21 by different aligner thicknesses

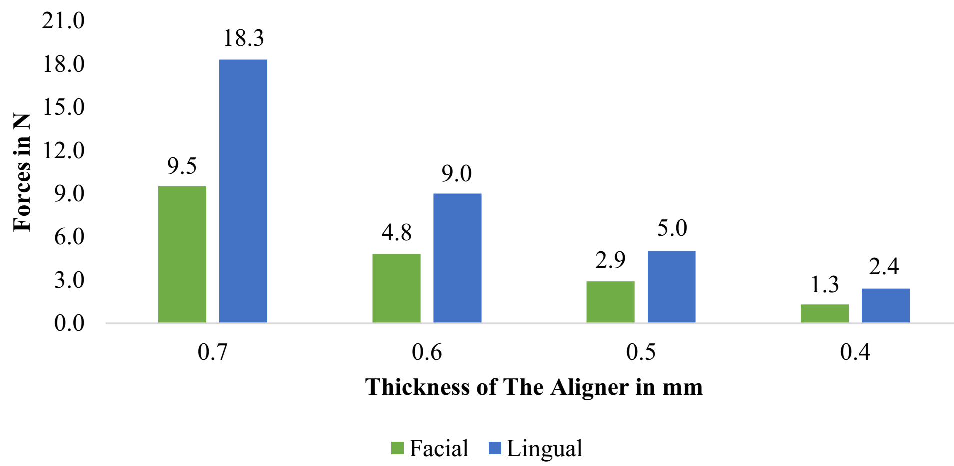


Fig. 3 Maximum resultant forces on 0.2-mm facio-lingual translation of upper left central incisor (Tooth 21) by aligner with different thicknesses

up to 0.2 mm is shown in Fig. 4, where an initial plateau of zero forces up to 0.02 mm can be noticed, corresponding to the initial gap between the teeth and the aligner, followed by a gradual increase of the forces reliant on both amount of displacement of the tooth and thickness of the aligner.

During the finite element model designing stage, selection of element classes and types was investigated in a sensitivity analysis. Using 20-noded hexahedron (Hex 20) or 8-noded hexahedral elements (Hex 8) for the aligner resulted in highest forces as well as high calculation times, while 10-noded tetrahedrons (Tetra 10) showed the lowest forces (Fig. 5) with moderate calculation time. Additionally, the rigidity of aligner material had a remarkable influence on the generated forces, where increasing the rigidity of the aligner generated higher forces, in the range of 500–2000 MPa of Young's modulus (Fig. 6).

The vector plot of Tooth 21 and aligner showed an extrusion tendency of the aligner during the displacement of Tooth 21 (Fig. 7). Moreover, a map of contact normal stresses showed an uneven distribution of contact normal stresses all over the surface, but a concentration of stresses at specific almost repeatable points at the mesial and the distal ridge of the facial surface, where the maximum contact normal stresses were 4.6, 32.9, 11.9, and 15.9 MPa with aligner 0.4, 0.5, 0.6, and 0.7 mm, respectively (Fig. 8).

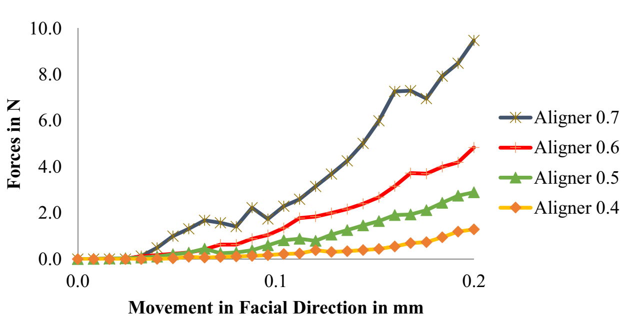


Fig. 4 Resultant forces during the course of 0.2-mm facial translation of upper left central incisor tooth (Tooth 21) by different thicknesses of aligner: 0.4, 0.5, 0.6, and 0.7 mm

Discussion

Biomechanical behavior of clear aligners is more complex compared to traditional fixed braces/wire orthodontic systems; many parameters are involved in determining the outcome of aligner treatment, and the force transferring interface is represented by the overall surface of the tooth crown, without a specific known point of force application [9]. Experimental and clinical methods have usually limitations in understanding these complex force systems. However, the combined efforts of having accurate mathematical modeling [44] and validated FE simulations [10] along with standardized experimental and clinical studies may reveal a lot about the biomechanics of orthodontic aligners [24].

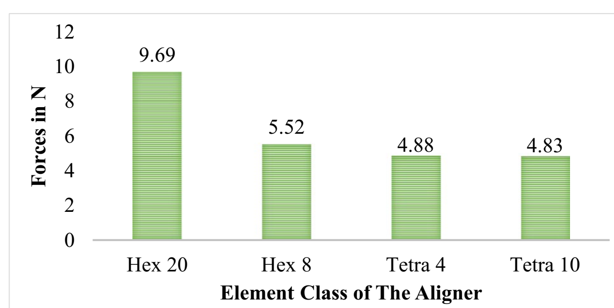


Fig. 5 Maximum resultant force on 0.2-mm facial translation of upper left central incisor (Tooth 21) with aligner of 0.6 mm thickness on using different element classes for finite element meshing; 10-noded tetrahedral elements (Tetra 10), 4-noded tetrahedral elements (Tetra 4), 8-noded hexahedron (Hex 8), and 20-noded hexahedron (Hex 20)

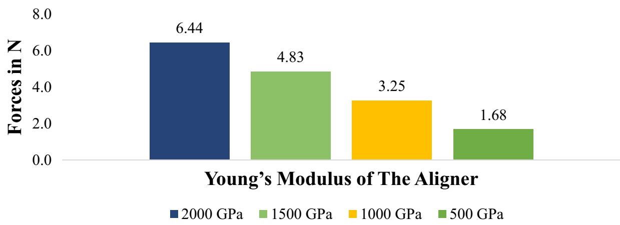


Fig. 6 Maximum resultant force on 0.2-mm facial translation of upper left central incisor (Tooth 21) with aligner of 0.6 mm thickness on using different aligner materials with different Young's modulus values

Therefore, we are aiming in the current article to report about designing a validated FE model, in order to better understand the mechanics of orthodontic aligners.

In FE simulations, the form of meshing has a significant impact on the outcomes [45], and choosing the appropriate element class play a crucial role in the simulation and affect the quality and accuracy of the numerical analysis [46]. Therefore, 4-noded tetrahedral elements (Tetra 4) were used for meshing of the cast and the movable tooth, suitable for their rigidity, while 10-noded tetrahedrons (Tetra 10) were selected for the aligner, coping with its flexibility. Tetra 10 were opted for the structures that might show large displacements/large strains or nonlinear behavior, like aligner. Also, Dumont et al. [45] reported that the mathematical model behind Tetra 10 element keeps a linear relationship between stress and strain over the element volume, while in Tetra 4 element, the stress and strain stay almost constant. The mathematics behind tetrahedron element type is as robust as for a hexahedron. However, after a sensitivity analysis, the result of the hexahedral model has been excluded due to the extreme calculation times and higher generated forces, while the results with Tetra 10 were more accepted, as shown in the results.

Determination of the contact parameters between the aligner and the teeth is tricky, due to the high irregular and customized shape of the aligner which made the exact formulation of load distribution more difficult [10, 31]. Significantly higher resultant forces were found in load cases considering friction. Hence, friction was neglected between the aligner and the teeth, as chosen by Cai et al.

Fig. 7 Vector plot of facial (left) and lingual (right) 0.2-mm translation of upper left central incisor (Tooth 21) showing direction of aligner displacement

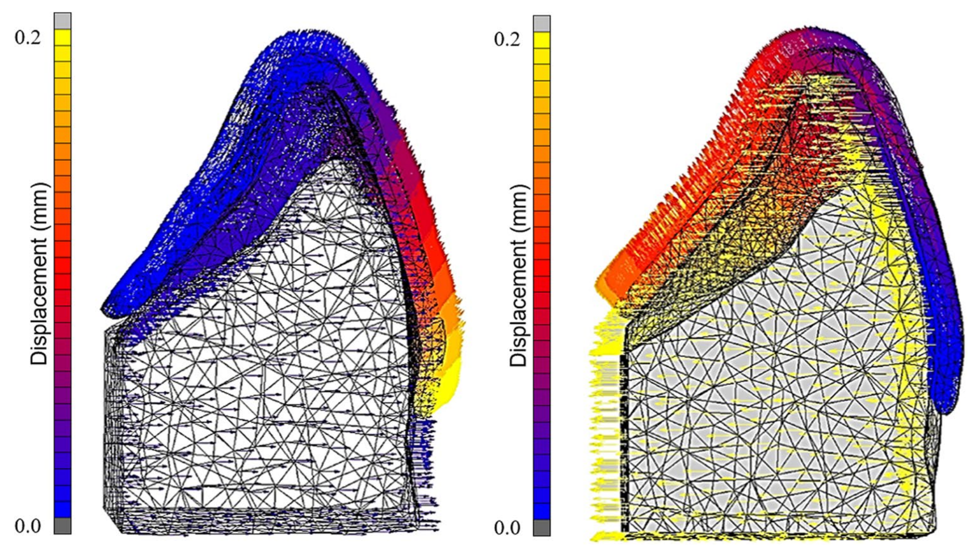
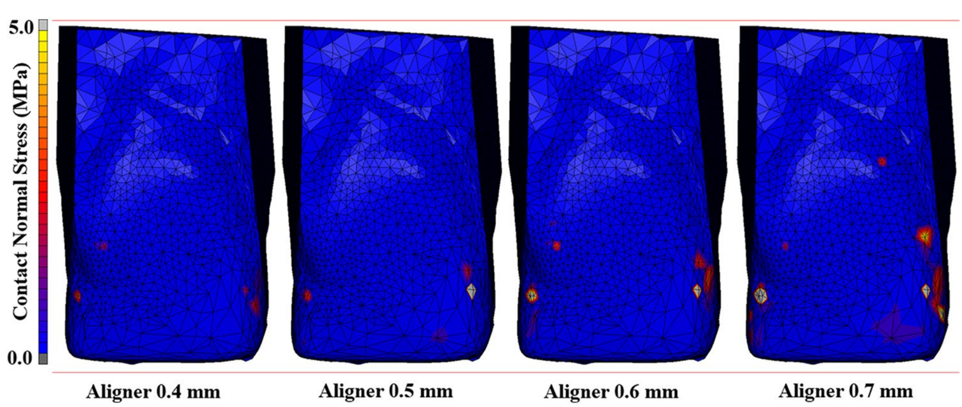


Fig. 8 Visual representation of the areas of contact normal stress (MPa) generated on 0.2-mm facial translation of upper left central incisor (Tooth 21) with different aligner thicknesses



[32] and Barone et al. [31], referring to the existence of dissimilarity between the aligner material and the tooth tissue, and taking into consideration the in-between presence of saliva acting as a lubricant. On the opposite, Gomez et al. [33] defined a friction coefficient of 0.2 in their simple model.

In the current FE model, the movement was applied on the tooth, while the clinical condition is totally the opposite, where the aligner is thermoformed onto a prototyped model with the target tooth already moved. Nevertheless, the resulting loading condition is the same, following Newton's third law, with the advantage that the aligner must be modeled only one time, and afterwards, different types of orthodontic tooth movements can be simulated and analyzed in the FE software [31].

In order to reduce the big resultant data, and for decreasing the analysis time, the size of the model was reduced. However, opposite to a report by Barone et al. [31], the shorter model showed a significant difference in the resulting forces; hence, we depended on the full model in the current study. That is actually in harmony with the concept reported by Hahn et al. [37] and Elshazly et al. [3] that the aligner is retained in the molar region and the whole aligner becomes deformed by the moveable tooth like a bow; the moveable tooth makes a deflection, in which the maximum deflection force increases with decreasing the length of the aligner and vice versa [47, 48].

From a biomechanical point of view, clinically during tooth movement, the tooth could move in six degrees of freedom. The type of tooth movement is determined by the relationship between a direction of force vector and the location of its center of resistance. When the force vector passes through the center of resistance, it causes bodily tooth movement [49]. The center of resistance of a single rooted tooth was described at roughly 42% of the height of the alveolar bone, from the alveolar bone crest to the tooth root apex, irrespective of root length and direction of loading [50]. Vollmer et al. [51] reported a significant difference between the movement generated in the idealized models and the realistic model, due to the continuous change of the center of resistance, and hence, it is almost very difficult to simulate the clinical translation movement with idealized models. Also, the orthodontic movement is based on geometrical considerations of both, the crown and the root, as well as their surroundings. Hence, neglecting root geometry, PDL, and bone, as well as applying the boundary conditions as a pure translation movement in 1D, is one of the major limitations of current study, and such simplification would bring somehow to inaccurate outcomes [31]. However, for validation, similar experimental conditions should be simulated, as the PDL is excluded in the experimental studies.

The obtained force values on 0.2-mm facio-lingual translation of Tooth 21 are in the range of 1.3–18.3 N, consistent with experimental reports by Hahn et al. (3.9–5.4 N) [22, 37] and Elkholy et al. (2.3–10.2 N) [13, 23], in which they used customized biomechanical measuring systems. Also, Li et al. [18] used a micro-stress sensor system and reported force levels at 7.7 N. Moreover, Xiang et al. [17] reported instant force values around 8.0 N by conventional PETG aligners measured by a thin-film pressure sensor. The slight dissimilarity could be referred to the variation in the experimental set-up. On the contrary, Simon et al. [21] reported lower force levels at 0.2–1.5 N. This difference could be due to the flexibility in their experimental set up and use of an ideal center of resistance for measured teeth. In harmony with previous reports by Hahn et al. [52] and Elkholy et al. [35], it was clear that the higher the Young's modulus of aligner material, the higher was the generated forces (Fig. 6).

Indeed, a lot of consideration should be put in mind while comparing the experimental condition with the idealized finite simulations. In the experiment, there are a lot of factors which could affect the results. For example, in the FE model, a homogenous thickness of aligner with a pre-defined values (0.4, 0.5, 0.6, and 0.7 mm) was modeled; however, in the experimental situation, there is a great thickness variations of the aligner all over the surface of the teeth referred to the thermoforming over the uneven surfaces of the cast. This local thinning of aligner material (which would not be simulated in the current model) would affect the experimental results significantly. Additionally, for simplification, a linear model of material was applied, but in reality, the material reaction with the experimental model may be somehow different. Moreover, although the experimental set-ups are rigid, there is still some sort of flexibility of the devices which is not considered in the mathematical FE model. All of this mentioned points, and more, could make differences on the order of some Newton but that is still accepted for validation.

Nonetheless, the resulting forces are still higher than the ideal orthodontic forces for bodily movement (0.75–1.25 N) [47, 48]. The absence of PDL is most probably the reason behind this. In addition, some studies [13, 14, 22, 52, 53] reported that the initial forces by aligners may exceed six times the recommended values for orthodontic movement, followed by a dramatic decrease of the forces. Also, alterations in the properties of the aligner material by the effect of the intraoral conditions may indorse force decay to a possible limit similar to, or even lower than, bracket system despite the high initial forces [54].

In agreement with some experimental studies [37, 53, 55, 56], increasing the thickness of the aligner leads to increasing of the generated forces, which is also in harmony with the clinical findings [35] that the risk of root resorption is lower with aligners of reduced thickness. However, indeed, the direct proportionality is apparently not perfect. That could be understandable in a way that the deformation of the aligner is a combination of bending (influence of the thickness with a power of 3) and stretching (direct proportionality). Checking this behavior by comparing with Figs. 3

and 4 shows that force increases stronger than linear. Also, the direction-dependent pattern of the force–displacement curves is likely due to the different facial and lingual morphologies of an upper central incisor [13, 23, 37].

In Fig. 4, the forces do not increase monotonically with displacement and there are unexpected decrease in forces at some intervals of the force/displacement graph. That could be referred to the nature of the idealized surface of the FE model, where there are many triangles and nodes, at which slipping may occur during the simulation, and especially with neglecting the friction, this slipping is reflected as decrease in the forces at some intervals.

From the vector plot of the displacement (Fig. 7), and in agreement with others [13, 22, 23, 52], the facio-lingual displacement of Tooth 21 is clearly accompanied with an intrusive force applied to the tooth referred to the morphology of the tooth that affects the force distribution over the surface and leads to analysis of the force vectors into horizontal and vertical components.

Despite that the orthodontic aligner move teeth by pushing rather than pulling, which should lead to an intimate contact between the aligner and the tooth surface, however, the uneven topography of the tooth surface affects significantly the stress distribution. In harmony with a study by Cervinara et al. [19], there is an uneven distribution of contact normal stress all over the surface of the tooth 21; where there are areas of relief and others with intimate contact, therefore, the force level differs from point to point all over the surface. However, there are an almost repeatable pattern of stress concentration areas/points which could be considered as the point of application of the force (Fig. 8). Excluding the aligner of 0.5 mm thickness, we saw that the stress at these points increased by increasing of the aligner thickness. The very high abnormal stress concentration in case of 0.5-mm aligner could be ignored and referred to a node to node early interference. Nevertheless, the total resultant force/deflection values with 0.5-mm aligner are in raw with the values of other aligners (Fig. 4). Also, the stress concentration mostly at the inciso-mesial and inciso-distal parts could create some sort of lingual-torque moment, owing to eccentric force application at the incisal crown level, in one line with a previous study [13]. Cervinara et al. [19] reported mean stress values at the active areas up to 5.0 MPa and a total pressure value of 15 MPa with 0.7-mm-thick aligner. In Fig. 8, we used the same color scale for the different thicknesses which might lead to absence of some stress points, due to being below the stress limit of the presentation color scale; however, with a more meticulous checking of the stress pattern generated by each thickness individually, we could confirm the repeatability of the stress distribution pattern. Additionally, we should put in mind that the increase of the aligner thickness would affect its bending ability and mobility, hence a slight shift of the stress points between the different thicknesses would be expected.

The current study has some limitations mentioned through the whole article. However, modifications of the model, to approach the realization, will be done in further publications. A more detailed demonstration of the generated forces and moments is to be reported after adding the PDL and bone in future studies. In addition, different trimming line levels of the aligner and different movements of several teeth will be reported.

Conclusions

1. FEM is a promising alternative approach that might lead to a better understanding of the mechanical behavior of orthodontic aligners. The current model has limitations; however, further studies and modifications of the model, to approach the realization, are going on.
2. The deformation of the aligner is a combination of bending (influence of the thickness with a power of 3) and stretching (direct proportionality).
3. The biomechanical concept of the aligner/tooth interaction could be represented as an arrow within a bow, in which increasing the deformation range and/or the span length will generate higher force.
4. Aligner material parameters must be carefully considered in order to deliver the optimal forces for orthodontic tooth movement.
5. In FE simulation, the mesh element class and type should be carefully opted as they significantly affect the results of the model. Based on our simulations, 4-noded tetrahedral elements (Tetra 4) are recommended for meshing of the teeth, and 10-noded tetrahedral elements (Tetra 10) for meshing of the aligner.

Author contribution Conceptualization: TE. Data curation and analysis, investigation, and methodology: TE and LK. Resources: TE, CB, MA, and AG. Software: TE, CB, MA, and LK. Supervision, validation, and visualization: TE, LK, MA, CB, AG, MA, WT, and ST. Writing—original draft: TE. Writing—review and editing: TE, MA, CB, AG, MA, WT, and ST. All authors have read and agreed to the published version of the manuscript.

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Declarations

This article does not contain any studies with human or animal subjects.

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Conflict of interest The authors declare no competing interests.

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4. Discussion with References

4.1 Discussion

ClearX system material from Kline Europe company is claimed to be a thermo-responsive shape memory polyurethane-based material. The material has the ability to recover to its original thermoformed shape after a so-called “reforming step”, by a thermal activation at specific temperature for a certain period of time. Owing to the stepwise shape changing property, this material was introduced to be used for the fabrication of aligners, since it may overcome the rate-limiting staging of conventional aligners, in a way that one SMP aligner may replace three subsequent conventional aligners. Therefore, the number of aligners per treatment could be reduced, saving money and time.

The shape recovery behavior of the material is influenced by the chemical structure and composition of the polymer molecules, as well as the processing conditions. Controlling of these conditions is important for controlling of the properties of the material in practical applications [1]. Hence, the first step of our study was performing a series of sensitivity tests to determine the suitable changeable parameters that could control the result and the success of shape recovery. Temperature, moisture, and time were the main governing parameters of each step. All steps have showed high sensitivity. All selected parameters were input in a software of a custom-made device (ClearX Booster). The activation of the shape memory property was done by this booster in 2 cycles, the first activation cycle can initiate an average of 65 % shape memory recovery in the aligner and the second cycle can initiate an average of 35 % shape memory recovery.

The essential mechanism of shape memory effect of SMPs is the presence of two (or more) domains with different glass transition/melting temperatures. At an ambient temperature, one domain is being hard/elastic, while the other domain is soft/ductile [2]. Hence, the shape memory mechanism in thermal-responsive SMPs is a reversible activation/inactivation process of the polymer-chain motion above and below certain temperature called transition temperature (T_{Trans}). T_{Trans} could be either glass transition temperature (T_g), or melting temperature (T_m) [3, 4]. Once the T_{Trans} is reached, the deformed SMP displays an elastic property and returns to its original shape. This shape recovery generates forces that can move a tooth [5]. Therefore, we have measured the forces delivered by the material using a standardized 3PB test at different temperatures and using a biomechanical test machine (OMSS) device. Maximum forces generated on a 2-mm deflection at temperatures from 37 °C to 55 °C with sheet thickness of 1 mm ranged from (1.2 - 0.5) N [6]. This is located within the acceptable range of orthodontic forces. Also, the generated forces at different temperatures (37 °C, 45 °C, 55 °C) measured by OMSS were (0.3 - 0.7) N, compatible with other studies [7, 8].

Biomechanical behavior of aligners is more complex compared to fixed braces/wire orthodontic systems; since many parameters are involved in determining the outcome of aligner treatment, besides the force transferring interface is represented by the overall surface of the tooth crown [9]. Usually, experimental and clinical methods have limitations in understanding these complex force systems. However, the combined efforts of having precise mathematical modeling [10] and validated FE simulations together with standardized experimental and clinical studies may reveal a lot about the biomechanical behavior of orthodontic aligners. Therefore, in the current article we reported about designing a validated FE model.

In FE simulations, the meshing pattern has a significant impact on the outcome [11], and choosing the appropriate element class/type plays a crucial role in the simulation and affects the quality and accuracy of the numerical analysis [12]. Therefore, 4-noded tetrahedral elements (Tetra 4) were used for meshing of the cast and the tooth, suitable for their rigidity, while 10-noded tetrahedrons (Tetra 10) were designated for the aligner, coping with its flexibility. Additionally, determination of the contact parameters between the aligner and the teeth is tricky, due to the high irregular shape of the aligner which made the exact formulation of load distribution more difficult [13]. In the current model, friction was neglected between the aligner and the teeth, as chosen by Barone et al. [9], speaking of the existence of dissimilarity between the aligner material and the tooth, and considering the in-between presence of saliva acting as a lubricant.

In the current model, the movement was applied on the tooth, opposite to the clinical condition. Still, the resulting loading condition is the same, according to Newton’s third law, with the advantage that the aligner would be modelled only one time, and afterwards different types of tooth movements can be simulated and analyzed in the FE software [9].

As well, orthodontic movement is based on considerations of both, the crown and the root, as well as their surroundings. Therefore, neglecting root, PDL, and bone, as well as applying the boundary conditions as a pure 1D translation movement, is one of the major limitations of our study, and such simplification would lead somehow to inaccurate results [9]. However, the PDL is excluded in the experimental studies, hence, for validation, similar experimental conditions should be simulated. Nevertheless, the obtained force values on a 0.2 mm facio-lingual translation of Tooth 21 were in the range of 1.3 - 18.3 N, consistent with several experimental reports [14–17].

4.2 Conclusions

Aligners made of SMPs showed their ability to move a tooth by biocompatible orthodontic forces, after a suitable thermal stimulus within the oral temperature range. Additionally, a validated FE model could facilitate understanding the force systems of clear aligners and performing better treatment planning.

4.3 References

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