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RESEARCH ARTICLE - APPLICATION

Simulation of orthodontic force of archwire applied to full dentition using virtual bracket displacement method

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Abstract

Objective: Orthodontic force simulation of tooth provides important guidance for clinical orthodontic treatment. However, previous studies did not involve the simulation of orthodontic force of archwire applied to full dentition. This study aimed to develop a method to simulate orthodontic force of tooth produced by loading a continuous archwire to full dentition using finite element method.

Method: A three-dimensional tooth-periodontal ligament-bone complex model of mandible was reconstructed from computed tomography images, and models of brackets and archwire were built. The simulation was completed through two steps. First, node displacements of archwire before and after load-ing were estimated through moving virtual brackets to drive archwire deformation. Second, the obtained node displacements were loaded to implement the loading of archwire, and orthodontic force was calculated. An orthodontic force tester (OFT) was used to measure orthodontic force in vitro for the validation.

Results: After the simulation convergence, archwire was successfully loaded to brackets, and orthodontic force of teeth was obtained. Compared with the measured orthodontic force using the OFT, the absolute difference of the simulation results ranged from 0.5 to 22.7 cN for force component and ranged from 2.2 to 80.0 cN•mm for moment component, respectively. The relative difference of the simulation results ranged from 2.5% to 11.0% for force component, and ranged from 0.6% to 14.7% for moment component, respectively.

Conclusions: The developed orthodontic force simulation method based on virtual bracket displacement can be used to simulate orthodontic force provided by the archwire applied to full dentition.

KEYWORDS

appliance loading, continuous archwire, finite element method, full dentition, orthodontic force, virtual bracket

1 | INTRODUCTION

In orthodontic treatment, teeth are moved by orthodontic force provided by appliances installed on the dentition. The orthodontic force would determine the movement pattern and speed of teeth,¹⁻³ thus directly affect the outcome of orthodontic treatment. Therefore, the estimation of orthodontic force after appliance loading is of great importance for treatment planning, appliance design and optimization, and treatment prediction.

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Highlight

Simulation of orthodontic force produced by a continuous archwire applied to full dentition provides an important guidance for clinical orthodontic treatment. However, it is challenging and has not been addressed previously. This study proposed a two-step simulation method to address this issue. Using the method, the orthodontic force produced by the loaded archwire can be estimated.

The clinical orthodontic force applied to teeth is provided by an appliance which is difficult to measure. This study implemented the simulation of clinical cases involving the appliance loading, thus would benefit the clinical orthodontic treatment.

Orthodontic force can be estimated through in vivo experiment,⁴ in vitro experiment,⁵ and theoretical calculation.⁶ There are few works on orthodontic force measurement in vivo. Friedrich et al⁷ used a purpose-developed device to measure the 3D force and torque released by the archwire-bracket system in orthodontic treatment in vivo. Duyck et al⁸ proposed a method to measure three-dimensional (3D) force on oral implant in vitro and in vivo. Monitoring orthodontic force in vivo is attractive; however, it is very difficult to be implemented in clinical cases.

Lots of works on in vitro force measurement have been reported. These works can be categorized into three classes. The first class of measurement systems measured the frictional force between bracket and archwire or the activation force on teeth produced by specific functional appliances. Frank et al⁹ designed an apparatus to measure the frictional force between the bracket and archwire of the canine-retraction case. Fathimani et al¹⁰ developed a computercontrolled friction measuring system and implemented the accurate measurement of 3D frictional force and moment during sliding mechanics. Chen et al¹¹ built an instrument to measure the force and moment on teeth released by an orthodontic T-loop spring. Baccetti et al¹² used an experimental model to measure the forces applied on the canine bracket released by the bracket-archwire system during the alignment period to compare the forces released by the different ligature method. The second-class measurement system involved all teeth of a dentition and could measure the force on one or a few teeth released by general appliance. Montasser et al¹³ developed an orthodontic measurement and simulation system containing a resin dental model and electronics measurement devices to study the effect of the archwire diameter on tooth alignment with a different bracket-archwire combination. Mittala et al¹⁴ proposed a measurement method involving dental models and load cells to measure 3D forces and moments on teeth released by the archwire. Compared with the previous two classes of measurement systems, the third class implemented the simultaneous measurement of force on all teeth. Badawi et al¹⁵ designed a promising system to accurately measure the six degrees of freedom of orthodontic forces applied on all teeth by fixed appliances. The designed system was successfully used to study orthodontic force on full dentition with an archwire in several treatment scenarios.¹⁶⁻²⁰ These in vitro measurement systems provide useful tools for the clinical estimation of orthodontic force. However, it is timeconsuming and costly to physically produce the oral treatment condition in vitro for accurate measurement.

Compared with the measurement method in vitro, theoretical calculation represented by finite element method (FEM) with the advantages of controllable experimental conditions, low cost, and short experimental cycle is more and more popular in recent decades.²¹⁻²⁴ Various methods for orthodontic force simulation which applied external force loads to teeth or appliances can be found in literature. Liao et al¹ applied distally directed tipping and bodily forces to human maxillary to investigate optimal orthodontic force. Ammar et al²⁵ loaded forces with various magnitudes and directions to the mandibular left canine to study the stress in PDL and bone. Kamble et al²⁶ applied orthodontic forces in various directions to the tooth axis at the bracket level to investigate stress distribution in the roots of maxillary central incisors. Jeon et al²⁷ applied force at the center of the buccal crown surface of maxillary first molar to study the alveolar bone loss. Because the clinical orthodontic force applied to teeth is provided by an appliance which is difficult to be measured, these studies cannot implement the simulation of clinical cases involving the appliance loading. Methods on the simulation of orthodontic force produced by the activated orthodontic appliance have also been studied. Kojima et al⁶ activated an uprighting spring with a helical loop for the tipping of the left second molar. Kim et al²⁸ applied retraction force to the power arm to study the optimal conditions for parallel translation of maxillary anterior teeth. Kojima et al²⁹ applied constant force to the brackets of canine and first molar to simulate the retraction of a maxillary canine and the movement of the anchor teeth by sliding mechanics.

The above research made it possible to estimate the orthodontic force of a specific clinical case in vitro, thus greatly promoted the progression of evidence-based orthodontics. However, they mainly addressed the simulation of

orthodontic force provided by some specific kinds of functional appliances which were activated by directly loading force or displacements to the appliances. In orthodontic treatment, leveling and aligning are generally the first phase of treatment which is important to the outcome of the treatment. In this phase, the orthodontic force was applied by loading a continuous archwire to full dentition to initially level and align the teeth.³⁰ The simulation of the loading in this phase is challenging due to the following two reasons: (1) it is difficult to analytically calculate the constant displacement loads to move the archwire segment into corresponding bracket slots; (2) the archwire might slide along the bracket slots during the loading procedure, and displacements of archwire within a short segment might be different. Thus, the above methods^{6,28,29} which directly applied force or displacement loads to appliance are inapplicable for the simulation of orthodontic force provided by archwire loading on full dentition during the leveling and aligning phase. In Canales et al's work,³¹ a method was proposed to simulate the procedure of inserting a session of archwire into four brackets. However, the study only implemented the loading of the archwire segment to one bracket and cannot be used to simulate the loading of a continuous archwire to full dentition.

To our best knowledge, no method for the simulation of orthodontic force of full dentition during the leveling and aligning phase has been reported. Therefore, this study developed a method to simulate the loading of a continuous archwire to full dentition and the orthodontic force of tooth after the archwire loading using FEM. Being different from previous studies which implemented archwire loading by directly applying known force or displacement to appliance, the method implements archwire loading through free deformation of archwire, thus can be used to simulate orthodontic force of full dentition during the leveling and aligning phase. An orthodontic force tester (OFT)^{14,32} was applied to measure orthodontic force in vitro to validate the simulation method.

2 | MATERIALS AND METHOD

2.1 | Materials

A 3D mandibular TPBC model of one subject under orthodontic treatment was reconstructed from cone-beam computed tomography (CBCT) images.³³ The treatment of the subject was in the final stage of leveling and aligning with small displacements of tooth movement. In the reconstructed TPBC model, the thickness of PDL is set to be 0.25 mm.²⁸ The model of the archwire with a cross section of 0.016×0.016 inch and models of brackets with slots of 0.022 inch were established. The archwire model was designed based on the shape of the planned dentition. The original dentition and planned dentition are shown in Figure 1, and the planned displacement of each tooth is presented in Table 1 (teeth from the left second molar to the right second molar were numbered according to the FDI dental numbering system for adult teeth). The brackets were modeled from scanned data using ATOS Triple Scan (GOM, Germany). The ligature of brackets was a stainless wire with a diameter of 0.01 inch and was modeled based on previous studies.³⁴⁻³⁶ This study was reviewed and approved by the Institutional Review Board of Shenzhen Institutes of



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TABLE 1 Planned displacement of each tooth

Displacement, mm							
Tooth	x	у	z	Vector sum			
Left second molar (37)	0	-0.10	0	0.10			
Left first molar (36)	0	0	-0.10	0.10			
Left second premolar (35)	0	0.10	0.10	0.14			
Left first premolar (34)	0	0.50	-0.10	0.51			
Left canine (33)	0	0.10	0.10	0.14			
Left lateral incisor (32)	0	0	0.30	0.30			
Left central incisor (31)	0	0	-0.50	0.50			
Right central incisor (41)	0	-0.10	0.05	0.11			
Right lateral incisor (42)	0	-0.05	0.10	0.11			
Right canine (43)	0	0.90	-0.50	1.03			
Right first premolar (44)	0	-0.20	0	0.20			
Right second premolar (45)	0	0	-0.20	0.20			
Right first molar (46)	0	-0.10	0	0.10			
Right second molar (47)	0	-0.10	0	0.10			

Advanced Technology, Chinese Academy of Sciences (approved number: SIAT-IRB-140315-H0050). Written informed consent of the subject was obtained.

The models of archwire-brackets-TPBC were imported into finite element (FE) software ANSYS Workbench15.0 (Ansys, Canonsburg, PA), and the corresponding FE models (see Figure 2) were generated after meshing using 20-node solid element SOLID186 (archwire) and tetrahedral structural solid element SOLID187 (others). A convergence test³⁷ was applied to estimate the effect of various mesh densities on discretization approximation to validate the accuracy of the FE model. The number of node and element of the FE model was presented in Table 2.

Brackets and archwire were assumed as isotropic and homogeneous materials. The PDLs were assumed to be bilinear elastic.^{36,38} As indicated in previous studies,^{6,39,40} the material parameter change in alveolar bone and tooth was unlikely to decisively influence the initial tooth mobility as the elasticity parameters of bone and tooth were much higher than those of PDL. Thus, the teeth and alveolar bone were assumed as isotropic and homogeneous materials



FIGURE 2 Finite element model of archwire, brackets, and tooth-periodontal ligament-bone complex. A, The complete model; B, detailed view of the model

TABLE 2 The material properties used in the finite element model of archwire, brackets, and TPBC

Model	Young's Modulus, MPa	Poisson' Ratio	Number of Node	Number of Element
Teeth	2.00×10^4	0.30	189 690	109 743
PDL	Bilinear ($E_1 = 0.05, E_2 = 0.20, \varepsilon_{12} = 7\%$)	0.30	116 906	57 709
Bone	3.45×10^2	0.30	47 817	27 928
Bracket	2.00×10^5	0.30	519 469	293 894
Archwire	1.89×10^{5}	0.30	941 160	200 556

without discriminating internal tissues (enamel, pulp, and dentin for teeth, and cancellous and for bones). Material properties including Young's modulus and Poisson's ratio were determined based on previous studies^{28,41,42} (Table 2).

2.2 | Method for the simulation of orthodontic force

2.2.1 | Overview

As the archwire was designed based on the shape of the planned dentition, it does not match the brackets on the original dentition. In the clinical loading of the archwire, the archwire is deformed manually to match and be inserted into the bracket slots. The deformation of the archwire is generally irregular, and the displacement of each segment or unit of the archwire induced by the deformation is difficult to be calculated explicitly. In addition, the displacement of each segment or unit of the archwire may change with the sliding between archwire and brackets during the loading of the archwire. As a result, the simulation of the archwire loading is challenging.

This study developed a two-step method to address this challenge based on FEM. In the first step, virtual brackets were introduced to estimate the node displacements of the archwire before and after loading. In this step, displacement loads of virtual brackets from the position on the planned dentition to that on the original dentition were applied to drive the archwire deformation (Figure 3A). The corresponding node displacements of the archwire before and after deformation were then calculated (Figure 3B). In the second step, the node displacements of the archwire calculated in the first step were loaded to the archwire (Figure 3C). The archwire would be deformed and inserted into the bracket slots on the original dentition, and the orthodontic force can be obtained (Figure 3D).

2.2.2 | Calculation of the node displacements of archwire before and after loading based on moving virtual brackets

In order to calculate the node displacements of archwire before and after loading, virtual bracket models were introduced to drive archwire deformation. The virtual brackets have the same geometry with the real bracket models shown in Figure 4 (bracket models on the original dentition were named real brackets hereafter), but the corresponding position was located on the planned dentition. The archwire matches well with the slots of the virtual brackets because it was designed based on the shape of the planned dentition.

The simulation of this step involved models of ligature, archwire, and virtual brackets. The contact between ligature and virtual bracket was set to be bonded. The contact between archwire and virtual brackets and the contact between archwire and ligature were set to be frictionless to allow free deformation of the archwire along the bracket slots. Displacement loads were applied to virtual brackets. Let $P_P = (P_{P37}, P_{P36}, ..., P_{P46}, P_{P47})$ denote the position of virtual brackets and $P_O = (P_{O37}, P_{O36}, ..., P_{O46}, P_{O47})$ denote the position of real brackets. Virtual brackets were moved from P_P to P_O (Figure 4) to deform the archwire. The displacement load applied to the nth virtual bracket was $D_n = P_{On} - P_{Pn}$ (n = 37, 36, ..., 46, 47), which meant moving the virtual bracket from the position on the planned dentition to that on the original dentition. The magnitude of the displacement load vector $D = (D_{37}, D_{36}, ..., D_{46}, D_{47})$ was the same with the planned displacement of tooth (presented in Table 1), but the directions were opposite.

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FIGURE 3 Procedure of simulation of the orthodontic force of archwire applied to full dentition using virtual bracket displacement method. A, Displacements were applied to the virtual brackets to deform the archwire; B, archwire before and after deformation (deformation was magnified 2.5 times for display); C, finite element model of archwire-bracket-TPBC before archwire loading (there was a geometrical mismatch between archwire and brackets on the original dentition); and D, simulation results after archwire loading (there was no geometrical mismatch between archwire and brackets on the original dentition)



FIGURE 4 Real brackets, virtual brackets, and archwire

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2.2.3 \parallel Simulation of orthodontic force of teeth by loading the node displacements of archwire

The simulation of this step involved models of ligature, archwire, real brackets, and the TPBC models (see Figure 2). The bone surfaces near temporomandibular joints were set be fixed to constrain all degrees of freedom of these surfaces. The contact between ligature and bracket, contact between bracket and tooth, contact between tooth and PDL, and contact between PDL and bone were set to be bonded, respectively. The contact between the archwire and the brackets was

set to be frictional contact, and the friction coefficient was chosen to be 0.15 based on previous in vitro experimental data. $^{43-45}$

In the simulation of the last step presented in the previous subsection, node displacements of archwire were obtained. In this step, the obtained node displacements were used as displacement loads and applied to archwire to activate archwire deformation and produce force to brackets. The above procedure was implemented by two substeps. First, the contact elements between the archwire and brackets were deactivated using birth and death FE method such that there was no interaction force between the archwire and brackets, and the node displacements of the archwire were loaded to insert the archwire into the bracket slots without model interaction. Second, the contact elements between the archwire would occur, and the springback force would be transmitted to brackets. Hence, the orthodontic force of the tooth can be then obtained. In this study, the orthodontic force was defined as the force system including force and moment applied to teeth by brackets. To calculate the orthodontic force, a local Cartesian coordinate system of axes {*x*, *y*, *z*} was established for each tooth (see Figure 5). The origin of each local coordinate system was located at the center of base plane of the bracket, and the *x*, *y*, and *z* axes corresponded to lingual-buccal, mesial-distal, and extrusion-intrusion directions of the tooth, respectively. The orthodontic force was calculated from the stress acting on the tooth surface contacted with bracket.⁴⁶

2.3 | Validation

In order to validate the developed simulation method, an OFT^{14,32} was used to measure orthodontic force in vitro. Compared with the system designed by Badawi et al,¹⁵ the applied OFT can only simultaneously measure the six degrees of freedom of orthodontic forces on two teeth and needs multiple identical dentoforms to complete the force measurement of all teeth of a dentition. The experimental setup for the orthodontic force estimation using the OFT was shown in Figure 6. The OFT applies two force sensors (Multiaxis force/torque Nano17; ATI Industrial Automation, Apex, NC)





FIGURE 6 Experimental setup for the orthodontic force estimation. A, The orthodontic force tester; B, detailed view of the sensors and dentoform

to measure the three force and three moment components applied to two target teeth simultaneously. The maximum force range of the sensors was 20 N with a 0.025 N resolution, and the maximum moment range was 100 N•mm with a 0.003 N•mm resolution.

To estimate the orthodontic force of all the 14 teeth, seven identical custom-made dentoforms were printed using a 3D printer, and the orthodontic force on two teeth was simultaneously measured in one dentoform. The following settings were conducted to keep the test condition being consistent with the FE model: (1) the dentoforms were printed from the 3D model used in the simulation (the alveolar bone base of the dentoforms was fabricated to be flat for easy fixing); (2) brackets of the same type and manufacturer with the ones used in the scanning and modeling of the FE model were used; (3) attachments restricting the position of brackets were created on each crown of the dentoforms to accurately locate the bracket at the position of the FE model; and (4) an automatically bended archwire by a robot^{47,48} based on the designed archwire model was used to minimize bending variation.

During the estimation of the orthodontic force of each pair teeth using the OFT, brackets were attached to the crowns of the dentoform. A local coordinate system was established for each target tooth according to the definition in the FE model (see Figure 5). The dentoform was fixed to a platform. After aligning axes of each sensor of the OFT to the local coordinate system of the target tooth, the target tooth was attached to the corresponding sensor with an epoxy adhesive to hold their positions and orientations. Then, target teeth were separated from the dentoform. The sensors were calibrated to obtain force and moment on the target teeth. Finally, the archwire was secured to brackets with a 0.01-inch stainless steel ligature wire, and force and moments on the teeth produced by archwire loading can be read from the sensors. To account for variability, the wire was removed after testing of each pair of teeth and was re-secured and ligated. Then, the force and moments on the teeth were retested. This procedure was performed seven times for the test of each pair teeth.

3 | RESULTS

3.1 | Simulation results of archwire deformation

The simulation results of the archwire deformation in the first step are shown in Figure 7. The node displacements of the archwire are presented by a color map. The maximum node displacement of the archwire was 1.1006 mm which occurred near the bracket on the right canine (the displacement of the corresponding virtual bracket was 1.03 mm). The deformation and corresponding node displacements of the archwire changed continuously. The results showed that, even for the segment within each bracket's slot, the node displacements were different.





3.2 | Simulation results of orthodontic force

The orthodontic force of the 14 teeth provided by archwire loading was calculated and is shown in Figure 8 (direction and amplitude). The maximum force on teeth was 362.4 cN and occurred at the right central incisor. The force applied on anterior teeth was larger than that on posterior teeth. The tooth with a larger displacement of the planned movement did not always obtain a larger orthodontic force.

The stress of the TPBC was obtained and was shown in Figure 9. The stress in the anterior teeth was larger than that in the posterior teeth. The stress in the PDLs near the alveolar ridge was larger than that in other regions. Figure 10 presents the comparison of orthodontic force obtained using the simulation method and OFT. Compared with the orthodontic force obtained by OFT, the absolute difference of the simulation results ranged from 0.5 to 22.7 cN for force component and ranged from 2.2 to 80.0 cN•mm for moment component, respectively. The relative difference of the simulation results ranged from 2.5% to 11.0% for force component and ranged from 0.6% to 14.7% for moment component, respectively.

4 | DISCUSSION

In previous studies, several methods^{6,28,29} for the simulation of orthodontic force provided by appliance loading have been reported. These methods implemented the simulation of appliance loading by applying constant force or displacement loads to the appliance to activate the appliance and were mainly employed to simulate orthodontic force induced



FIGURE 8 Orthodontic force of teeth obtained using the simulation method. A, The direction of the orthodontic force; B, the amplitude of the orthodontic force







by specific functional appliances including uprighting spring, power arm, and appliance in sliding mechanics and so on. There was also work trying to simulate the orthodontic force provided by the general archwire.³¹ However, this work only involved the loading of the archwire section on partial teeth, and the loading of the archwire section was also implemented by applying constant displacement loads to a segment of the archwire.

The major contribution of this study was the development of a new method for the simulation of orthodontic force provided by continuous archwire free deformation. In orthodontic treatment, the leveling and aligning are generally completed by loading continuous archwire to full dentition. The simulation of the archwire loading to full dentition is challenging. First, the archwire deformation before and after loading is irregular and cannot be described explicitly. It is difficult to analytically calculate the constant displacement loads to move the archwire segment into corresponding bracket slots. Secondly, the archwire might slide along the bracket slots during the loading procedure, and the node displacements of archwire within a short segment might be different (as shown in the results of Subsection 3.1). Thus, previous methods which directly applied loads to appliance are inapplicable for the simulation of orthodontic force



FIGURE 10 The comparison of orthodontic force obtained using the simulation method and orthodontic force tester. A, Force component; B, moment component

provided by archwire loading on full dentition. This study developed a new method to address this challenge. Instead of directly applying constant displacement loads to archwire segments, it first calculates the node displacements of archwire before and after loading by simulating the archwire free deformation procedure using virtual brackets, then loads the node displacements to the archwire to simulate the orthodontic force of teeth.

The simulation results using the developed method provided both amplitude and direction reference of the force that the archwire would apply to teeth after loading. Based on the reference, orthodontists could optimize the design of the archwire according to a specific case such that the designed archwire would supply proper orthodontic force to teeth after loading. In clinical orthodontics, a medium force was regraded to fall within the range of 6 to 10 ounces (170 to 283 cN).⁴⁹ According to the simulation results, the force applied to the left central incisor, right central incisor, right lateral incisor, right canine, and right second premolar exceeded the range of the medium force. The orthodontists might need to optimize the archwire to reduce this force magnitude. Figure 11 shows the comparison of simulated initial teeth movement and planned tooth movement direction. Most of the teeth would move as planned after the archwire loading. However, the movement direction of planned. The left second premolar, right second molar, and left canine were expected to have a buccal or labial movement, but these teeth would have a lingual crown tipping movement after the appliance loading. Thus, the archwire designed based on the shape of the planned dentition needs to be optimized to supply a proper force driving teeth move toward the planned direction.

The limitations of the presented FE model mainly include the material property setting of bone and PDL, the friction coefficient of archwire, and the ligation of bracket. The heterogeneous and anisotropic material property of PDL and bone should be considered. The frictional coefficient between the bracket and the archwire directly affects sliding friction mechanical properties, thus is an important factor in the simulation of orthodontic force.^{42,50,51} A frictional coefficient of 0.15 was chosen in this study according to previous in vitro experimental data. The effect of a different frictional coefficient on the orthodontic force should be further studied in future. What is more, the simulation for the ligating of



FIGURE 11 The direction comparison of planned tooth movement and simulated initial tooth movement (the planned tooth movement direction was presented by yellow arrows with bigger size, the simulated initial tooth movement was presented by color arrows with smaller size, different colors from blue to red denote initial movement amplitudes from small to large)

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brackets is also an important factor to affect the results of orthodontic force.⁵² In this study, a stainless steel cylinder with a diameter of 0.01 in is fixed on the bracket to simply simulate the ligation which ignores a possible gap between the archwire and the bracket in buccal-lingual direction. More flexible methods of ligation should be investigated in the future.

5 | CONCLUSION

Simulation of orthodontic force provided by loading continuous archwire to full dentition is of great importance for clinical orthodontic treatment. However, no proper method has been developed to address this issue. This study proposed a two-step method to simulate the loading procedure of a continuous archwire to full dentition and the orthodontic force of teeth applying the FEM. Using the proposed method, a continuous archwire designed according to the planned dentition was loaded to the original dentition successfully. The orthodontic force of the teeth was calculated, and the stress of the TPBC was also obtained.

CONFLICT OF INTEREST STATEMENT

We declare that there is no conflict of interest related to this paper.

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