Original Article

Expansion rebound deformation of clear aligners and its biomechanical influence: a three-dimensional morphologic analysis and finite element analysis study

Bochun Mao[a]; Yajing Tian[a]; Jing Li[b]; Yanheng Zhou[c]

ABSTRACT
Objectives: To determine the expansion rebound deformation (ERD) of clear aligners (CAs) and its biomechanical influence.
Materials and Methods: A four-premolar extraction treatment plan was carried out for a patient with 2 CA companies. Thirty-six digitally scanned clear aligners with the corresponding 36 virtually constructed "ideal" aligners were constructed. The arch width and length between pairs of reference landmarks of the scanned CAs and corresponding dentition models were measured. Cone-beam computed tomography data and digital dental models were used for three-dimensional (3D) finite element analysis (FEA) modeling. Thirty-six scanned CA models with the corresponding 36 ideal CA models were constructed. One-way analysis of variance was used to determine the differences among deviation values at tooth level, and paired *t*-test was used to compare the displacements of teeth between the two group of CAs.
Results: All CAs were wider and shorter than the digital model from which they were constructed. In the scanned CA model group, significant stress was observed in the buccolingual area of the periodontal ligament on posterior teeth, and the corresponding displacements of teeth were also noted. Significantly larger coronal displacements were noted for the lateral incisor, the canine, the second premolar, and the first molar in the scanned CA group ($P < .05$).
Conclusions: The general trend of ERD of thermoformed CAs was shown. This deformation may cause unforeseen tooth movements and negatively affect treatment outcomes. (*Angle Orthod.* 2023;93:572–579.)

KEY WORDS: Clear aligner; Biomechanics; Finite element analysis; Expansion rebound deformation

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INTRODUCTION

The unsatisfactory predictability and accuracy of clear aligner (CA) treatments, 30%–50% compared with the initial design, have been a long-debated issue for decades.[1,2] Currently, reasons for the low realization rate of orthodontic tooth movement of CA include inadequate mechanical properties of thermoplastic material, unsatisfying attachment efficiency, manufacturing inaccuracy, and ambiguity of the biomechanical features of the appliance.[2,3] The morphology and fit of CAs are also crucial factors for aligner retention, the generated forces and moments, and even accuracy to reach the prescribed movement.[4]

During clinical treatment, some patients complained that their CAs were wider than their dentition. It was explained by the manufacturer that this "expansion rebound deformation (ERD)" is a common problem for thermoformed CA, which may be due to residual stress and permanent deformation during the initial removal.[5,6] Recent studies focused mainly on the inconsistency of the thickness of the CA and the fit between the dental crown and the CA;[3,7,8] however, none of the published studies have investigated the ERD of CAs.

Finite element analysis (FEA) is a numerical method used to study the stress distribution and distortion of a given geometry when loaded, and has been widely used in the study of biomechanical behavior of CA.[9] However, previous studies mostly used ideal CA geometries for the FEA simulation,[9,10] which were built by thickening crowns with equivalent value. The biomechanical features of CAs with real morphology were unclear.

Thus, this study focused on the ERD of thermoformed CAs, and the potential biomechanical influence was also investigated.

MATERIALS AND METHODS

Sample Selection

This research was approved by the Institutional Review Board of Peking University School and Hospital of Stomatology (PKUSSIRB-202059154). Dental model and cone-beam computed tomography (CBCT) data of a 24-year-old female patient with skeletal Class I, mild crowding, and bimaxillary protrusion were obtained. The digital dental model, scanned with a desktop scanner (3shape R900 model scanner, 3shape, Copenhagen, Denmark), together with the patient's clinical records, were uploaded to two CA companies: Invisalign (Align Technology, Inc.) and Angel Align (Wuxi Angel Align Biotechnology Co, Wuxi, China). The clinician (JL) prescribed the same treatment plan for the patient: anterior tooth retraction with maximum anchorage after the extraction of four first premolars. The same V-pattern staging processes (ie, retrusion of canines and incisors successively) and the same tooth movement amount (0.2 mm) with each step was required for the two treatment plans, which ensured the same digital dental models at each step of the two companies were used to fabricate corresponding CAs. Nine stages were selected for analysis, which were obtained from three stages of three types of movement (Figure 1): (1) distal movement of the canines; (2) distal movement of the canines and lateral incisors; and (3) distal movement of the canines and all incisors. The same vertical rectangular attachments were prescribed. The corresponding aligners were scanned with a micro-CT scanner (Inveon MM gantry, Siemens, Germany). In total, 36 scanned CAs were included: 9 (nine staging steps) $\times$ 2 (maxillary and mandibular dentitions) $\times$ 2 (two companies).

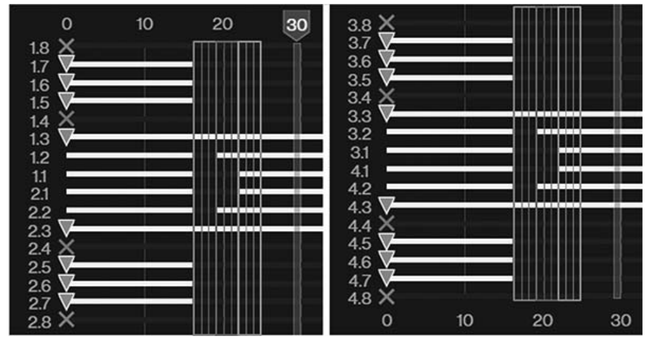

Figure 1. Clear aligner selection for dimensional measurement: nine consecutive steps were selected while the canines started to move distally, covering the V-pattern design of anterior tooth retraction. The V-pattern tooth movement design in three staging processes (marked with vertical rectangles). Each staging process contained three steps. All tooth movements designed in the nine steps were 0.2 mm distal bodily movements of target teeth.

3D Morphological Analysis

Three-dimensional (3D) morphological analysis was carried out in Geomagic Studio (Geomagic Studio 15.0, 3D Systems, Rock Hill, SC). Landmarks at each dental crown were marked, and the width of the dental arch at each tooth level was measured as the segment length between homologous teeth, while the length was measured as the segment length between the mesial point of the central incisor (M1) and each horizontal line. The corresponding measurements of the 36 scanned CAs were carried out with a landmark-transfer method (Figure 2), which can minimize measurement errors theoretically. First, in Geomagic Studio, the CAs were segmented at each tooth level, and each segment was aligned with the corresponding dental crown by the best fit alignment method.[11] Landmarks were transferred from the crown to the

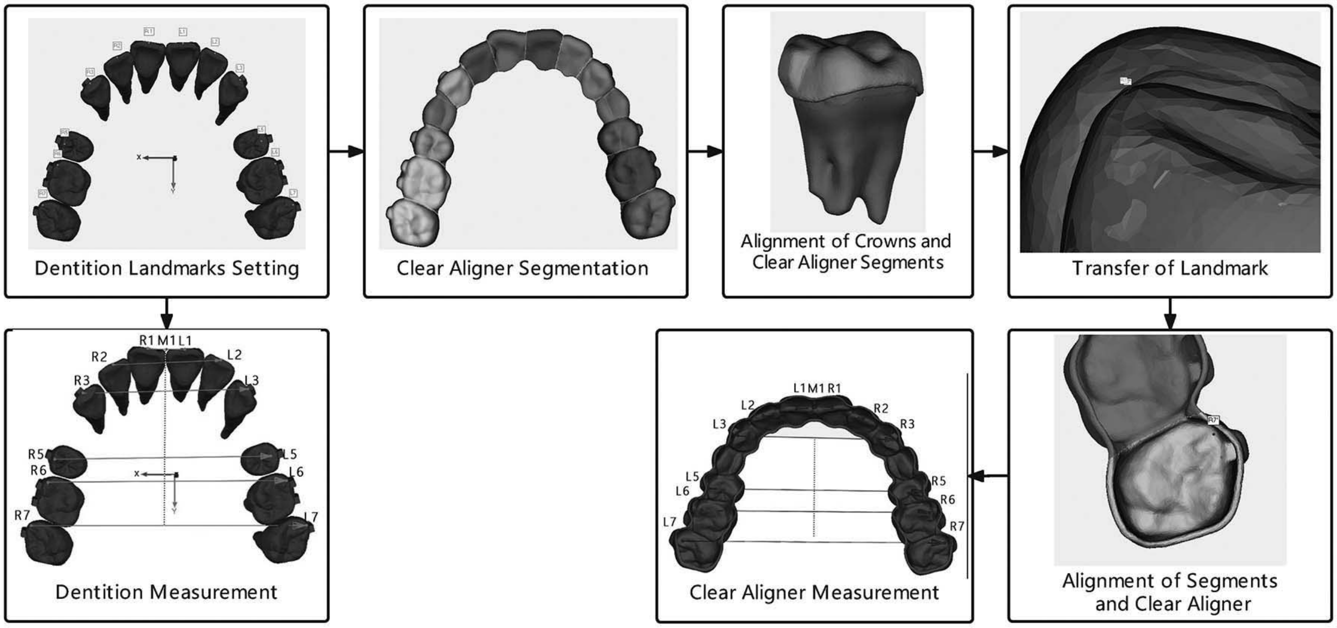

Figure 2. The landmark-transfer method used and the measurement of the width and length of the dentition and clear aligner at each tooth position (M1 indicates midpoint of the R1-L1 line; R/L1, midpoint of the incisal edge of the central incisor; R/L2, midpoint of the incisal edge of the lateral incisor; R/L3, cusp of the canine; R/L5, buccal cusp of the second premolar; R/L6, mesial buccal cusp of the first molar; R/L7, mesial buccal cusp of the second molar).

inner surface of CA segments. Segments were then aligned with the CAs, and the CA measurements of width and length at each tooth level were carried out. All measurements were repeated by another operator, and the reliability was high (intraclass correlation coefficient 0.87 with mean error of 0.04 $\pm$ 0.19 mm).

3D Finite Element Analysis

CBCT data were imported into Mimics (Materialise, Leuven, Belgium) to obtain the bimaxillary bone and dentition model. To obtain the eventual tooth models, the reconstructed dentition model from CBCT was aligned with scanned digital cast data in Geomagic Studio by best fit alignment. The periodontal ligament (PDL) was simulated with a 0.25 mm thick shell.[10] The ideal CA of step "n" was virtually constructed with a uniform thickness of 0.7 mm from the designed dentition of step "n." The ideal CA of step "n" was then put on to the designed dentition of step "n-1" to simulate the ideal CA treatment. Thirty-six ideal CAs were generated corresponding to the scanned CAs. Vertical rectangular attachment models ($3 \times 2 \times 1$ mm) were obtained. All materials except the PDL were assumed to be linearly elastic, homogenous, and isotropic (Table 1).[10,12,13] For the PDL, when the dependent variable of PDL was $\varepsilon < 7.5\%$, E1 $=$ 0.05 MPa; and when $\varepsilon > 7.5\%$, E2 $=$ 0.22 MPa,[14] and the bilinear parameter of PDL was implemented with custom-developed subroutines with Python for ABAQUS. Each tooth was simplified as one material according to previous studies to simplify the calculation.[9,10,12] All models were assembled in Hypermesh (Altair, Troy, Mich), and then processed by Abaqus/CAE (2016, SIMULIA Co, USA) for FEA (Figure 3). The models were meshed to 10-node tetrahedron elements. Bonded contacts were set between the internal surface of the PDL and teeth and between the external surface of the PDL and alveolar bone. The relationship between aligners and crowns was designated as small-sliding surface to surface, and the friction coefficient was set to 0.2.[10] The upper part of the maxilla and the bottom surface of the mandible were set as fixed supports in all directions. The simulation of putting on aligners for ideal CAs was carried out by setting the anterior part of the aligner and teeth in close contact (ie, the incisors and canines), and the posterior part of CA was set up with an interference fit with other teeth. As for scanned CAs, before putting on, a pair of

Table 1. Material Properties of Finite Element Models

Material	Elastic Modulus (MPa)	Poisson's Ratio
Cancellous bone	1370	0.30
Cortical bone	13,700	0.30
PDL	$\varepsilon < 7.5\%$, E1 $=$ 0.05 MPa; and when $\varepsilon > 7.5\%$, E2 $=$ 0.22 MPa	0.45
Tooth	20,000	0.30
Attachment	20,000	0.30
Aligner	1500	0.3

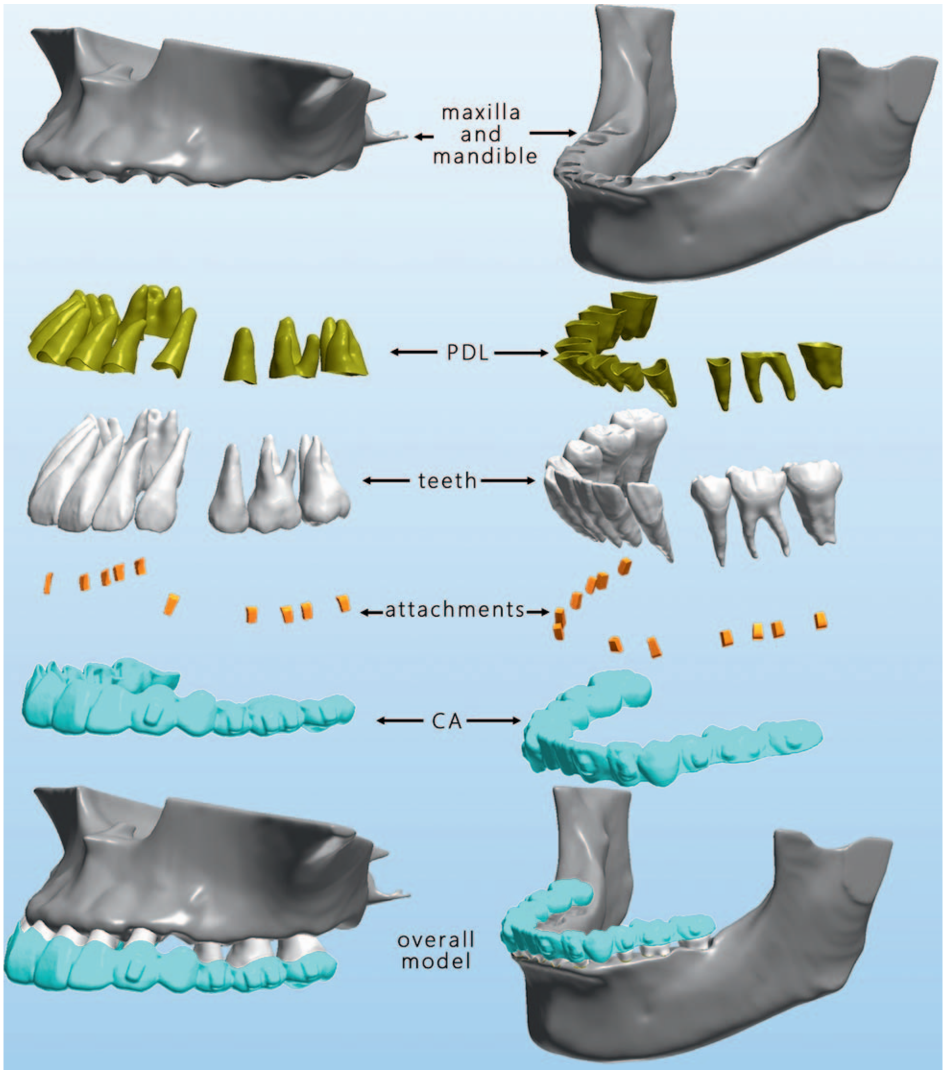

Figure 3. Final components of the model (CA indicates clear aligner; PDL, periodontal ligament).

forces was exerted to the posterior part of CAs at both ends of the dentition to narrow down the width of CAs to gain the same dentition width at the second molars and, after putting them on, the forces were removed. A convergence study was carried out to determine the maximum size of elements to be 0.2 mm.

Tooth displacement and von Mises equivalent stress in the PDL were analyzed. The mesiodistal and buccolingual displacements of landmarks of each tooth marked for previous morphological analysis were recorded.

Data were exported to SPSS 19.0 (IBM, Chicago, Ill) for statistical analysis. One-way analysis of variance and Student-Newman–Keuls q tests were used to determine the differences among deviation values at tooth level, and paired *t*-test was used to compare the displacements of teeth between the two group of CAs. For all comparisons, $P < .05$ indicated statistical significance.

RESULTS

3D Morphological Analysis

As shown in Figure 4, all CAs were wider and shorter than the corresponding digital dental model, and the discrepancies increased posteriorly. CAs were significantly wider at the first and second molars (1.48 $\pm$ 0.57 mm, 1.17 $\pm$ 0.57 mm) compared to other areas ($P < .05$). On average, less than 0.8 mm shortening at each tooth level was also noted. Minimum deviation within 0.35 mm in both dimensions was revealed for incisors and canines. Although the deviations of width in the maxillary dentition (0.92 $\pm$ 0.78 mm) were larger than those in the mandibular dentition (0.81 $\pm$ 0.58 mm), no significant difference was detected ($P = .08$). No significant difference was found between the CAs of the two manufacturers (Invisalign and Angle Align) in either width ($P = .82$) or length ($P = .28$).

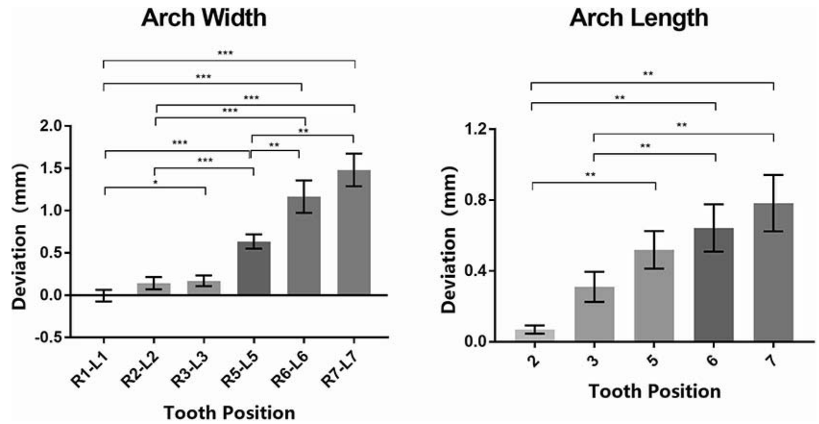

Figure 4. The deviations in arch width and arch length between digital dental models and corresponding clear aligners at different tooth positions (tooth numbering according to the FDI tooth numbering system; * $P < .05$, ** $P < .01$, *** $P < .001$).

FEA Results

Typical FEA results of each staging process were chosen for illustration. Mesiodistal stress was observed in the PDL of teeth with designed movement in the PDLs of both groups (Figure 5). However, for the scanned CA group, larger buccolingual stress was noted for the PDL of posterior teeth, particularly in the second premolars and first molars. Figure 6 depicts the displacement of teeth in each group, and quantified results are shown in Table 2. Since tooth 42 was crowded and protruding out of the mandibular dentition, in the steps that designed its movement, larger displacements were noted. For the scanned CA group, all posterior teeth moved anteriorly and buccally, while all the anterior teeth moved posteriorly and lingually, which may have been due to the "wider" and "shorter" CAs. Without statistical significance, larger displacements were noted in the maxillary dentition than in the mandibular dentition ($P = .891$ for mesiodistal displacement; $P = .106$ for buccolingual displacement). Significant differences were found for the central incisor ($P = .002$), the canine ($P = .008$), the second premolar ($P = .001$), and the first molar ($P = .021$) in the coronal dimension between the ideal and scanned CA. No significant difference in tooth displacement was observed between the two companies ($P > .05$).

DISCUSSION

It was well acknowledged that significant material properties changed after the thermoforming process of the aligner material, and ERD was detected.[1] However, no previously published study revealed the extent and potential clinical impact of ERD. It is believed that this deformation should be taken seriously during treatment design because the study results showed its potential negative clinical influence.

For the ERD of CA, Fang et al.[5] studied the residual stress of five common thermoplastic materials in a simulated oral environment and showed that the residual stress within all five materials decreased with time. Because of the residual stress, the material tends to transform to its initial shape which, in the case of CA, becomes wider in the transverse direction and shorter in the longitudinal direction. Also, it was revealed that deformation of thermoformed CAs beyond 10% to 15% strain is irreversible because of their yielding characteristics.[13] Therefore, permanent deformation may occur during the initial removal of CAs off the cast with relatively large forces.

The fit of CAs has been investigated often in recent years.[3,7,15] Palone et al.[7] scanned CAs with micro-CT after they were being mounted on the cast to evaluate the gap width. Results showed a significantly larger gap width in the posterior area; these results were in agreement with the current study. However, that study ignored the ERD of CAs before wearing. According to the current study, statistical results indicated that the discrepancies increased as the target area moved posteriorly, which refers to buccal movement-derived deformation of CAs. No significant difference was observed either in deviation in width or length between the two brands of CAs. Another study used micro-CT to investigate the thickness of six brands of aligners,[8] and larger thicknesses and greater gaps were also observed in the posterior teeth. Likewise, a recent study suggested that the largest discrepancies of CAs were found at the buccal side of molars.[16] During space closure, the decrease in arch length due to ERD could be considered a kind of anchorage loss, which potentially affected anchorage design. According to the results, although without statistical significance, larger buccal inclination of posterior teeth was noticed in D3 of scanned CA groups with larger posterior anchorage requirements compared with D1 (Figure 6).

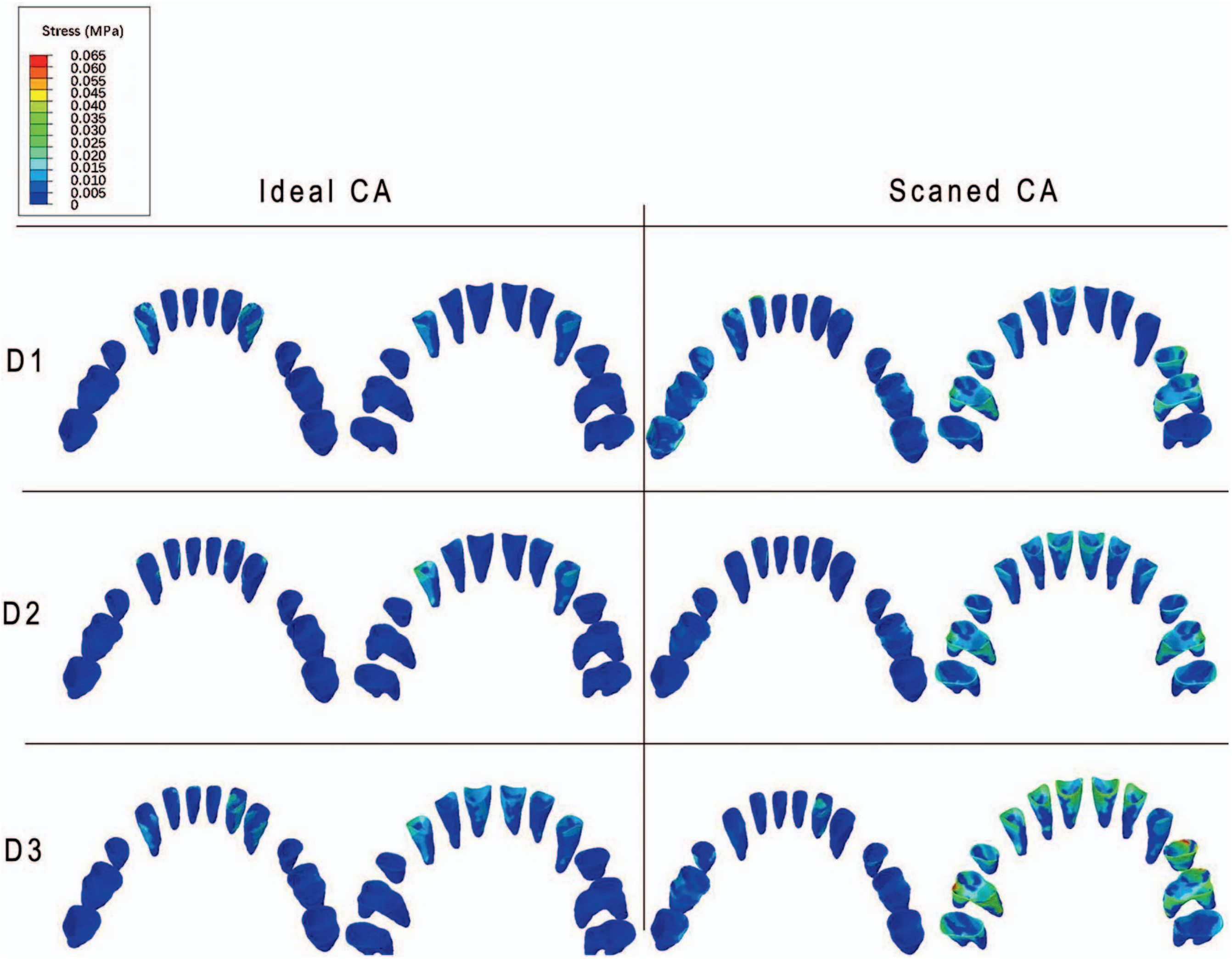

Figure 5. Equivalent stress in the periodontal ligament of one model in each group. CA indicates clear aligner; D1-3, dentition from the 3 staging processes (unit: Pa).

The results indicated that ERD may increase anchorage loss of posterior teeth. Prashant et al.[3] indicated dimensional differences in dental crown height of 3D printed (1.94%) and thermoformed (4.52%) aligners with respect to the reference digital casts. In that study, although only differences in crown height were measured, it could be deduced that approximately 2 mm differences in dentition width at the second molar level for thermoformed CAs might exist with the same deformation ratio, which supported the results of the current study.

The "straightening" tendency of CAs caused the appliances to be shortened and wider with a more flattened dental arch curve, which caused posterior teeth to move anteriorly and buccally and anterior teeth to move posteriorly and lingually as shown by the FEA results. Edelmann et al. pointed out that a discrepancy in aligner fit may lead to the poor fulfillment ratio of planned tooth movement up to 57% in some cases.[15] Previous FEA studies of CAs mostly used the ideal CA model for the simulation, ie, models built with extraction crowns, which ignored the dimensional deviation of the actual CAs.

The limitations of this research should be stated. First, this research aimed to reveal the ERD of CAs and its potential biomechanical impact with instantaneous results. The limitations of currently used PDL material parameters are obvious, and only qualitative results could be obtained. Therefore, only qualitative conclusions were made instead of quantitative ones. Nevertheless, in the long term, tooth movements are affected by many other factors including bone density distribution, viscoelastic behavior of aligner material in the oral environment, biological factors, etc. More samples with different treatment designs from various companies may increase the accuracy of the results. In

Table 2. Displacement of Different Teeth in the Ideal and Scanned Clear Aligner Groups With Paired *t*-Test Results[a,b]

	Sagittal Displacement (X)							
Group	Ideal CA (Mean ± SD)	Scanned CA (C1+C2) (Mean ± SD)	Ideal-(C1+C2) *P*	Scanned CA (C1) (Mean ± SD)	Ideal-C1 *P*	Scanned CA (C2) (Mean ± SD)	Ideal-C2 *P*	C1-C2 *P*
Tooth								
1	0.004 ± 0.028	0.019 ± 0.115	.515	0.006 ± 0.017	.793	0.012 ± 0.036	.533	.285
2	0.016 ± 0.085	0.001 ± 0.106	.608	0.007 ± 0.062	.889	0.025 ± 0.108	.651	.733
3	0.019 ± 0.076	0.005 ± 0.105	.574	0.004 ± 0.059	.979	0.034 ± 0.094	.580	.524
5	0.009 ± 0.006	0.016 ± 0.112	.467	0.009 ± 0.002	.595	0.008 ± 0.008	.469	.808
6	0.003 ± 0.006	0.039 ± 0.134	.291	0.004 ± 0.006	.297	0.002 ± 0.006	.310	.756
7	0.004 ± 0.011	0.033 ± 0.099	.215	0.001 ± 0.012	.281	0.008 ± 0.010	.186	.248

[a] CA indicates clear aligner; C1, the first company (Invisalign); C2, the second company (Angel Align).
[b] Tooth numbering according to the FDI tooth numbering system.
* $P < .05$.

addition, for the FEA simulation, including various factors such as temperature and hygroscopic expansion, could further enhance simulation accuracy, which should be a focus of future research.

CONCLUSIONS

- In conclusion, this study showed the general trend of ERD of CAs, ie, wider in the transverse direction and

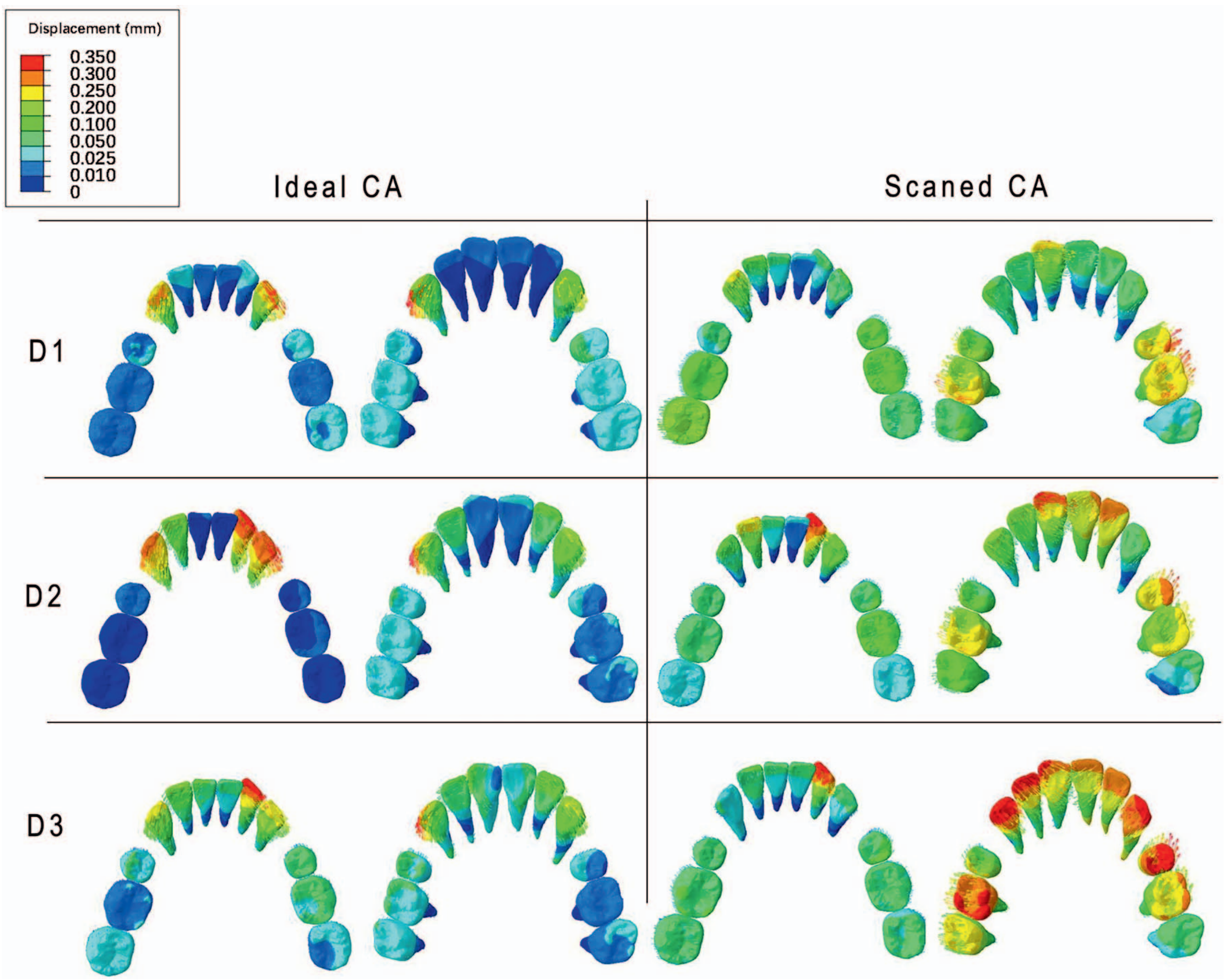

Figure 6. The displacement of teeth in each group. CA indicates clear aligner; D1-3, dentition from the 3 staging processes (unit: m).

Table 2. Extended

Coronal Displacement (Y)							
Ideal CA (Mean ± SD)	Scanned CA (C1+C2) (Mean ± SD)	Ideal-(C1+C2) *P*	Scanned CA (C1) (Mean ± SD)	Ideal-C1 *P*	Scanned CA (C2) (Mean ± SD)	Ideal-C2 *P*	C1-C2 *P*
0.015 ± 0.028	0.078 ± 0.055	.002*	0.012 ± 0.031	.015*	0.019 ± 0.026	.023*	.703
0.092 ± 0.088	0.122 ± 0.079	.106	0.055 ± 0.043	.073	0.130 ± 0.108	.856	.146
0.169 ± 0.042	0.105 ± 0.051	.008*	0.148 ± 0.017	.065	0.189 ± 0.050	.004*	.085
0.024 ± 0.032	0.128 ± 0.090	.001*	0.023 ± 0.034	.014*	0.026 ± 0.034	.017*	.875
0.034 ± 0.017	0.087 ± 0.075	.021*	0.038 ± 0.013	.046*	0.030 ± 0.021	.027*	.459
0.026 ± 0.025	0.014 ± 0.026	.208	0.038 ± 0.009	.013*	0.014 ± 0.030	.974	.109

shorter in the longitudinal direction, which may negatively affect treatment outcomes.
- Significantly larger coronal displacements of the central incisor, canine, second premolar, and first molar were noted for the scanned CA group compared to the ideal.

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