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Original article

Finite-element analysis and optimization of the mechanical properties of polyetheretherketone (PEEK) clasps for removable partial dentures

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ABSTRACT

Purpose: Polyetheretherketone (PEEK), a high-strength, aesthetic, and non-allergic thermoplastic polymer, recently became a candidate for replacing metallic components in dental prosthesis. However, as PEEK is flexible, the need for retention presents a key challenge in terms of its clinical application. In this study, clasps prepared using PEEK were optimized and evaluated to provide the mechanical properties required by dentures.

Methods: Seventy-two three-dimensional rod-shape models, based on four thickness/width ratios, three base widths, and six taper ratios were created. These models were analyzed using finite-element methods to determine which modified clasp arm shape provided the most appropriate mechanical properties. Three shape-optimized PEEK specimens and one standard-shape Co–Cr alloy specimen were then fabricated. Constant-displacement fatigue testing was performed to calculate load values and deformations after ten years of clinical use.

Results: Shape optimization indicated a maximum stress concentration that was consistently located at the base of the specimen, a correlation between mean load values and thickness that was greater than that with the width, and a correlation between taper ratio and mean load values. Fatigue testing showed that although PEEK exhibited significantly lower average load values than the Co–Cr alloy, these were sufficient for clinical use. All specimens exhibited significant deformation during the first period of cycling; however, there was no significant difference in the deformation between the two materials after fatigue testing.

Conclusions: PEEK exerts fewer stresses on abutments compared to standard-alloy clasps, provides adequate retention, and satisfy aesthetic demands, indicating that PEEK presents a promising alternative to conventional metal clasps.

1. Introduction

The development of computer technology ensures the indispensability and popularity of computer-aided design and manufacturing in the field of restorative dentistry, while developments in digital processing mean that materials that were difficult to process are now easily available for manufacture. These factors have been the source of tremendous changes in the field of dentistry during the past few decades [1,2].

Metal alloys remain the materials of choice for removable partial denture (RPD) frameworks; however, these materials are not aesthetically pleasing because of their metallic color, they carry a risk of causing allergic reactions, and their processing is both difficult and time consuming. This has led to an increasing trend in which patients request metal-free restorations [3,4]. To achieve completely metal-free restorations, either fiber-reinforced composites or thermoplastic resin retentive elements are used to replace metal components. However, the long-term durability of these alternative materials is controversial [5–7]. Moreover, various types of high-strength zirconia-based ceramics materials,

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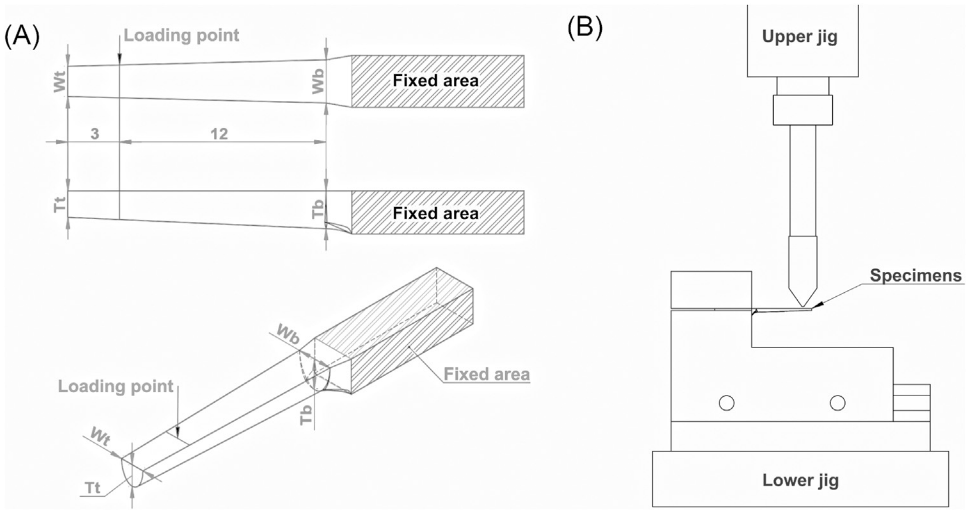

Fig. 1. Schematic illustration of (A) the specimens and (B) the constant displacement fatigue test.
Fixed area = portion for fixation to the machine, loading point = the loading location used by the testing machine, W_b = width of the base, W_t = tip width, T_b = thickness of the base, and T_t = tip thickness (all in mm).

such as yttria-stabilized tetragonal zirconia polycrystal (Y-TZP) and ceria-stabilized zirconia/alumina nanocomposite (Ce-TZP/A), have been recently developed and applied within mainstream restorative dentistry. Although the application of zirconia ceramics to RPD clasps has recently been attempted, their clinical lifespan must still be evaluated [7,8].

Developments in materials science have led to the introduction of polyetheretherketone (PEEK), a high-performance thermoplastic polymer, to restorative dentistry, as a candidate for replacing metallic components in dental prosthesis. The mechanical properties of PEEK do not change during the sterilization process and its elastic modulus is similar to those of human bone, enamel, and dentin, suggesting it to be a suitable restorative material. PEEK features stable chemical properties, and is biocompatible, wear-resistant, stable at high temperatures, insoluble in water. This material also presents low reactivity with other materials, is non-allergic, and has lower plaque affinity than other materials such as metals and resins. Furthermore, PEEK can be processed using computer-aided design and computer-aided manufacturing (CAD/CAM), rendering it easily reproducible in the event of failure, and easily relined in the case of resorption [9–16].

The combination of these unique mechanical and physical properties renders PEEK a promising material for replacing metal frameworks. To date, there have been few clinical studies that discuss the application of PEEK as a framework material for RPDs [17,18]; nevertheless, according to its superior flexible properties, obtaining the necessary retentive force and fatigue resistance will be key challenges in the development of PEEK RPD clasps [19,20]. Therefore, the objective of this study is to optimize PEEK clasp design in order to provide the mechanical properties required by RPDs.

2. Materials and methods

2.1. Generating three-dimensional models

Three-dimensional (3D) models with clasp arms in the form of a rod-shape were designed by SolidWorks 2013 (Dassault Systèmes SolidWorks, Waltham, MA, USA). The 3D models were 15 mm in length and the loading point was set at 3 mm from the tip (Fig. 1). These models were classified into four groups based on thickness/width ratios (T_b/W_b), and each group was then divided into three subgroups according to the base width. In each subgroup, the cross-sectional area was defined using six taper ratios, as shown in Table 1. Overall, a total of 72 differently shaped 3D models were created.

2.2. Shape optimization

Shape optimization was performed using the finite element method (FEM). Load values for various clasp arm shapes at displacements of 0.25 mm and 0.50 mm were measured, and stress distributions were calculated under each loading condition. The material used for optimization in the present study was assumed to be linearly elastic, homogeneous, and isotropic, so as to approximate the real properties of PEEK (VESTAKEEP DC4450 R (Lot No.: 57781699), Evonik Japan Co., Tokyo, Japan). The following data were used, as supplied by manufacturers: tensile strength stress at yield = 110 MPa; modulus of elasticity = 4.8 GPa; specific gravity = 1.52 g/cm^3; linear thermal expansion = 0.45×10^{-4} K^{-1}, and each model was assembled using linear FEM (Autodesk Nastran In-CAD, AutoDesk Inc., San Rafael, CA, USA). A finer mesh was generated at the material interface to ensure the accuracy of force transfer, and all nodes in fixed area were restrained. A concentrated load was applied to the loading points of the models. Clasp arm shapes with tapered uniformly from the tip to the base and thinner in width or thickness exhibited better functionality and lower abnormal sensation [22]. Due to this, the appropriately three shape-optimal 3D models with the required mechanical and aesthetic properties could be extracted and fabricated into test-specimens.

2.3. Test-specimen fabrication

Three PEEK (VESTAKEEP DC4450 R (Lot No.: 57781699), Evonik Japan Co) test specimens were fabricated for the shape-optimized 3D models using CORiTEC 250I/DRY (imes-icore, Eiterfeld, Germany). One standard-shape (base thickness/width of 1.00/2.00 mm (Group A1), taper ratio of 0.8) cobalt–chromium (Co–Cr) alloy specimen (Co 63%; Cr 30%; Mo 5%; Wironit Extra-hard, Bego, Bremen, Germany) was also prepared for comparison, and the plastic pattern (SHERAprint-vast, SHERA Werkstoff-Technologie, Lemförde, Germany) for the cast was created using Rapid Shape D30 II (Rapid Shape, Heimsheim, Germany), then invested and cast according to the manufacturer's instructions.

Table 1. 3D models with 72 different shapes (4 groups, 3 subgroups, and 6 taper ratios for each subgroup).

Group[a]	Subgroup[b]	Base (mm)		Tip (mm)											
		W_b	T_b	0.5-taper[c]		0.6-taper[c]		0.7-taper[c]		0.8-taper[c]		0.9-taper[c]		1.0-taper[c]	
				W_t	T_t	W_t	T_t	W_t	T_t	W_t	T_t	W_t	T_t	W_t	T_t
A	Group A1	2.00	1.00	1.00	0.50	1.20	0.60	1.40	0.70	1.60	0.80	1.80	0.90	2.00	1.00
	Group A2	2.50	1.25	1.25	0.63	1.50	0.75	1.75	0.88	2.00	1.00	2.25	1.13	2.50	1.25
	Group A3	3.00	1.50	1.50	0.75	1.80	0.90	2.10	1.05	2.40	1.20	2.70	1.35	3.00	1.50
B	Group B1	2.00	1.25	1.00	0.63	1.20	0.75	1.40	0.88	1.60	1.00	1.80	1.13	2.00	1.25
	Group B2	2.50	1.56	1.25	0.78	1.50	0.94	1.75	1.09	2.00	1.25	2.25	1.41	2.50	1.56
	Group B3	3.00	1.88	1.50	0.94	1.80	1.13	2.10	1.31	2.40	1.50	2.70	1.69	3.00	1.88
C	Group C1	2.00	1.50	1.00	0.75	1.20	0.90	1.40	1.05	1.60	1.20	1.80	1.35	2.00	1.50
	Group C2	2.50	1.88	1.25	0.94	1.50	1.13	1.75	1.31	2.00	1.50	2.25	1.69	2.50	1.88
	Group C3	3.00	2.25	1.50	1.13	1.80	1.35	2.10	1.58	2.40	1.80	2.70	2.03	3.00	2.25
D	Group D1	2.00	1.75	1.00	0.88	1.20	1.05	1.40	1.23	1.60	1.40	1.80	1.58	2.00	1.75
	Group D2	2.50	2.19	1.25	1.09	1.50	1.31	1.75	1.53	2.00	1.75	2.25	1.97	2.50	2.19
	Group D3	3.00	2.63	1.50	1.31	1.80	1.58	2.10	1.84	2.40	2.10	2.70	2.36	3.00	2.63

W_b = width of the base, W_t = tip width, T_b = thickness of the base, T_t = tip thickness (as Fig. 1).
[a] Groups are divided based on the thickness/width (T_b/W_b) ratio (Group A: 0.500; Group B: 0.625; Group C: 0.750; Group D: 0.875). [b] Subgroups are divided based on the width of the base (W_b) (Subgroup 1: 2.00 mm; Subgroup 2: 2.50 mm; Subgroup 3: 3.00 mm). [c] Taper ratios are the ratio of the cross-sectional dimensions at the tip to those of the base [$W_t/W_b = T_t/T_b$].

2.4. Constant-displacement fatigue testing

Test conditions were maintained at room temperature using a Servopulser testing machine (EHF-FD5KN-4LA, Shimadzu Corp., Kyoto, Japan) and carried out under two conditions: one with a constant displacement of 0.25 mm for both the PEEK and Co–Cr alloy specimens, the other at a constant displacement of 0.50 mm for only the PEEK specimens. These constant displacements were maintained at the loading point of the specimens with a sinusoidal wave frequency of 5 Hz. In this way, the present study may assume that the clasps were inserted and removed from the abutment with an undercut of 0.25 mm or 0.50 mm. The load values were recorded in order to analyze deformation during testing; the deformation of the specimens in the direction of the load was observed using a digital microscope (KH-1300, Hirox Co., Tokyo, Japan) every 3000 cycles. A total of 15,000 cycles were performed, representing the simulated insertion and removal of the RPDs over ten years, with the assumption that the patient would perform four complete cycles per day.

2.5. Statistical analysis

The results of shape optimization were recorded, and the correlation between the cross-sectional dimensions, taper ratio, load values, and maximum stress were obtained via Pearson correlation and linear regression. The mean interval load values and deformations were calculated for the constant displacement fatigue tests, and the normality of the distribution and the homogeneity of variance were primarily analyzed using the Shapiro–Wilk test and Levene's test. Data comparisons were conducted using one-way analysis of variance (ANOVA) with post-hoc Scheffé tests. All statistical analyses were performed using IBM SPSS statistical software (SPSS version 24; IBM Corp., Armonk, NY, USA), and the level of statistical significance was set at 5%.

3. Result

3.1. Shape optimization

When the displacement was set at either 0.25- or 0.50-mm, the mean load values for Group B3 (0.9-taper), Group C3 (0.5- to 0.7-taper), Group D2 (0.7- to 0.8-taper), and Group D3 (0.5- to 0.6-taper) were greater than the lowest acceptable retentive force (1.6 N) of RPDs (Fig. 2), and the maximum stresses were less than the yield stress (110 MPa) of the employed PEEK material (Fig. 3). Among those, Group B3 (0.9-taper), Group C3 (0.5-taper), and Group D2 (0.7-taper) were slender and with uniformly tapered; thus, identified as the appropriately three modified shape-optimal 3D models.

The von Mises stress analyses indicated that maximum stress concentrations were consistently located at the base of each model (Fig. 4). For each group, there was a significant difference between the maximum stress values with varying both cross-sectional dimensions and taper ratios ($P < 0.05$). There was also a strong positive correlation between the thickness ($r > 0.8$) and stress concentration (Table 2). Additionally, there was a significant difference in the mean load values that were obtained for different cross-sectional dimensions ($P < 0.05$), and the correlation between mean load values and thickness ($r > 0.9$) was greater than that between the mean load values and the width ($r > 0.6$) (Table 2). For identical dimensions, a larger taper ratio was associated with increased mean load values (Fig. 2).

3.2. Constant-displacement fatigue tests

Three 3D models (Group B3 (0.9-taper), Group C3 (0.5-taper), and Group D2 (0.7-taper)) were selected via shape optimization and used in the fabrication of PEEK specimens. The Shapiro–Wilk test and the Levene's test run on all variables showed normally distributed and homoscedasticity. Table 3 shows the average load values and deformation in the direction of the loads for PEEK and the Co–Cr alloy. The Co–Cr alloy (mean: 8.26 N) exhibited consistently and significantly higher average load values than PEEK (mean: 2.06–3.67 N) during 15,000 cycles ($P < 0.05$).

The deformations in the direction of the loads in all the interval cycles are presented in Fig. 5. All specimens exhibited significantly greater deformation during the first period of cycling ($P < 0.05$), which then remained unchanged until the end of cyclic testing. The final extent of deformation after 15,000 cycles was small, showing no significant differences between each cycle interval. There were no significant differences between the deformation of the PEEK (mean: 0.011–0.017 mm) and Co–Cr alloy (mean: 0.017 mm) samples after 15,000 cycles ($P = 0.11$) (Table 3).

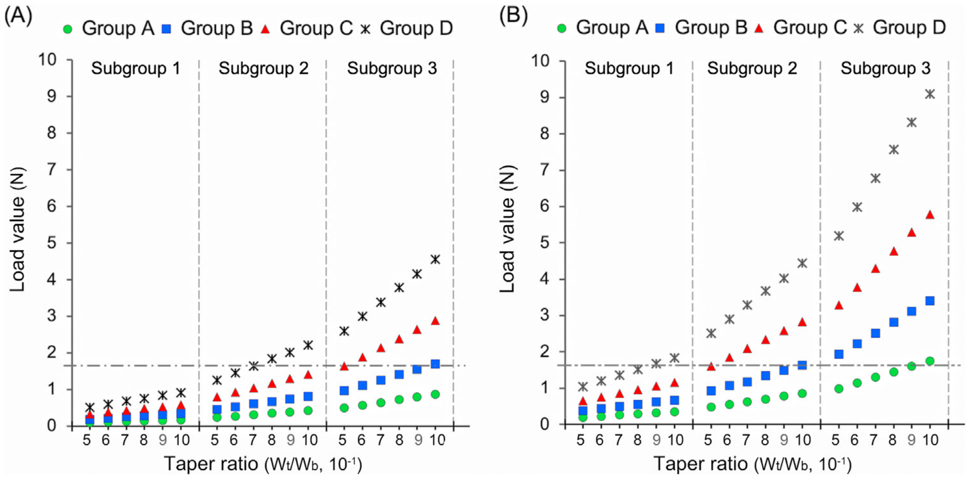

Fig. 2. Load values when constant displacements of (A) 0.25 mm and (B) 0.50 mm were applied to the 3D models.
The horizontal dashed line represented the lowest acceptable retentive force (1.6 N) of RPDs.

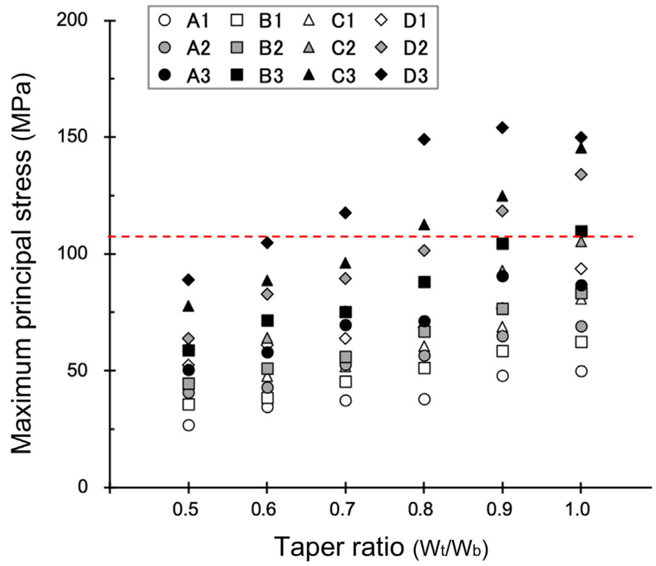

Fig. 3. Maximum principal stress of each 3D model when load measured at constant displacement of 0.50 mm.
When maximum principal stress larger than yield stress (110 MPa, the red dashed line) means that models prone to plastic deformation; yet, when constant displacement of 0.25 mm, the stress values of all models were less than 110 MPa.

4. Discussion

In terms of long-term RPD use, clasp arm design should minimize stress concentration; however, it has been recognized that three factors, clasp material, clasp form, and the amount of undercut, affect the design of a clasp arm [21]. Materials used in RPD construction should exhibit flexibility for use as clasps, but rigidity for the other components [22]. Due to its low elastic modulus, PEEK exhibits superior flexibility but relatively low rigidity compared to conventional Co–Cr alloys (elastic modulus = 3.0–5.5 GPa for PEEK, compared to >200 GPa for Co–Cr alloys) [13,23]; therefore, PEEK clasps should be thicker and with a deeper undercut than Co–Cr alloy clasps in order to provide clinically acceptable functionality.

Clasp shape parameters such as thickness, cross-sectional dimension, and taper affect the retention of RPDs; however, a combined variation of these parameters leads to a variety of complex results [21,24,25]. Optimization and simulation are suitable and time-saving methods for predicting optimal shapes before fabricating specimens for mechanical testing; and FEM was selected in the present study as an efficient and flexible method [26–28]. Fitton et al. [29], suggested that resin clasps need to have a greater cross-sectional area than a metallic clasp in order to provide adequate retention, due their relatively high proportional limit and low flexural modulus. The present study used FEM to determine the optimized shape of a modified PEEK clasp arm by adding to the width or thickness of a standard clasp arm (Table 1). Moreover, tooth shape influences retention by determining the depth and steepness of undercut available for clasping [24]. Turner et al. [30] stated that resin clasps require relatively engaged, deeper undercuts to allow adequate retention, thus the present study compared the functional differences of clasps with two undercuts (0.25 and 0.50 mm) by constant-displacement fatigue testing.

According to the shape optimization results and considering both comfort and aesthetic aspects, Group B3 (0.9-taper), Group C3 (0.5-taper), and Group D2 (0.7-taper) were provided sufficient retention (Fig. 2) and not prone to plastic deformation (Fig. 3). Thus, these three designs were selected for the fabrication of PEEK testing specimens. Urano et al. [8], tested the maximum principal stress of Ce-TZP/A clasps using FEM, showing that stresses were consistently observed at the base of each model, and that stress values decreased with decreasing taper ratio. In the present study, the maximum principal stress of the PEEK clasps was also consistently observed at the base (Fig. 4); although in comparison to Ce-TZP/A clasps, PEEK clasps exhibited lower stress concentrations. This difference was due to the fact that ceramic materials exhibit lower elasticity and ductility, but higher brittleness. These results imply that the PEEK clasps are less prone to fracture and deformation.

After repeated loading of the polymer materials, low-cycle fatigue caused cyclic softening and continuously reduced deformation resistance, leading to a gradual increase in the strain [31]. These material performance results indicate that although the shape optimization (FEM) suggested that the specimens selected in the present study were not prone to plastic deformation (Fig. 3), plastic deformation did occur after the fatigue experiments. However, both PEEK clasps (mean = 0.011–0.017 mm) and the conventional Co–Cr alloy clasp (mean = 0.017 mm) exhibited only slight deformation, and there was no significant difference between the two materials after fatigue testing ($P < 0.05$) (Table 3 and Fig. 5).

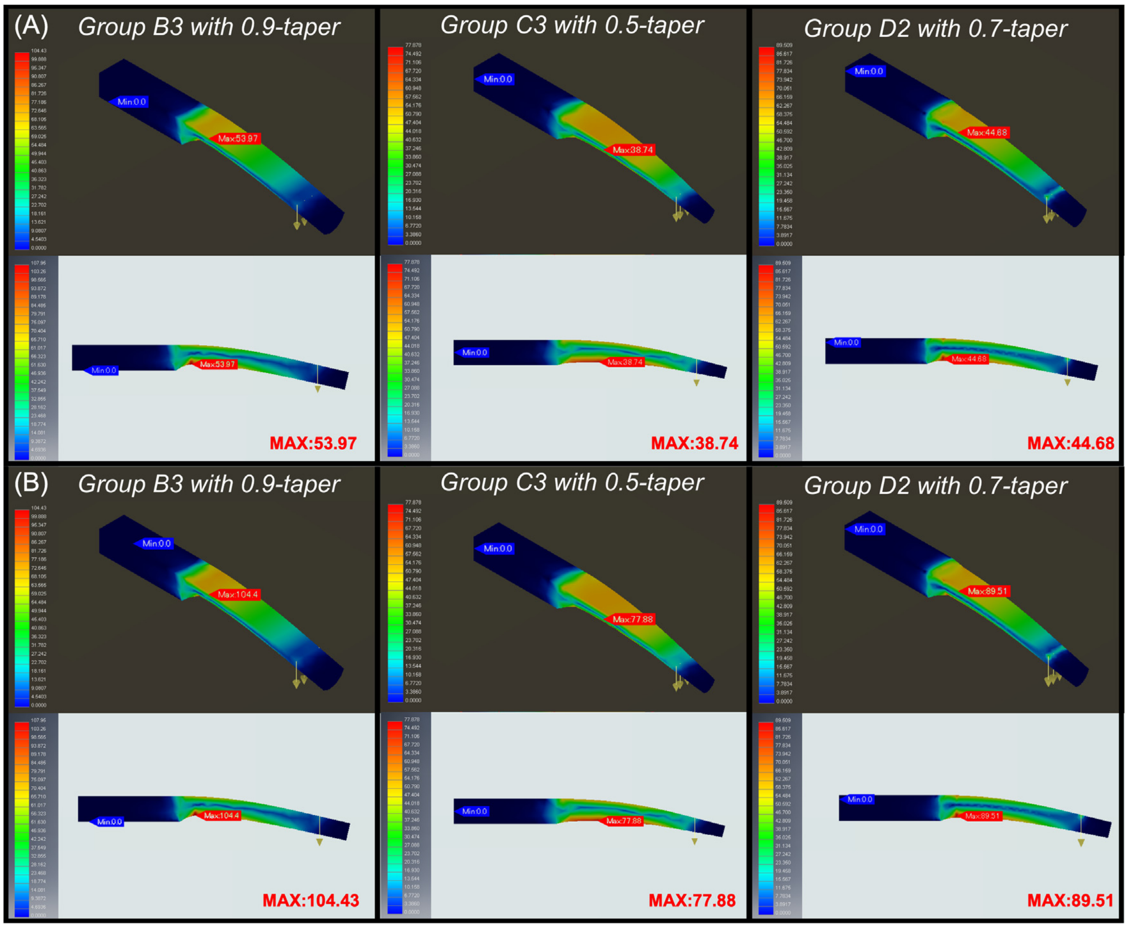

Fig. 4. Representative von Mises stresses (MPa) and distributions, obtained when constant displacements of (A) 0.25 mm and (B) 0.50 mm were applied to the 3D models.

Table 2. Pearson's correlations between variables: width, thickness, and taper ratio.

	Von Mises stress values			Load values		
	Width	Thickness	Taper ratio	Width	Thickness	Taper ratio
Pearson r value	0.61*	0.82*	0.51*	0.64*	0.91*	0.21
P value	>0.001	>0.001	>0.001	>0.001	>0.001	0.080

* Correlation is significant at the 0.01 level (2-tailed).

Table 3. Pairwise comparison of the load value and deformation of specimens (n = 7).

	Displacement	Average load value during 15,000 cycles	Deformation after 15,000 cycles
		Mean ± SD (N)	Mean ± SD (mm)
Co–Cr alloy	0.25 mm	8.26 ± 0.55 ^{a}	0.017 ± 0.004 ^{d}
PEEK Group B3 (0.9-taper)	0.25 mm	2.15 ± 0.08 ^{b}	0.012 ± 0.005 ^{d}
	0.50 mm	3.20 ± 0.32 ^{c}	0.015 ± 0.005 ^{d}
PEEK Group C3 (0.5-taper)	0.25 mm	2.14 ± 0.14 ^{b}	0.011 ± 0.003 ^{d}
	0.50 mm	3.67 ± 0.17 ^{c}	0.017 ± 0.010 ^{d}
PEEK Group D2 (0.7-taper)	0.25 mm	2.06 ± 0.09 ^{b}	0.014 ± 0.006 ^{d}
	0.50 mm	3.54 ± 0.29 ^{c}	0.015 ± 0.005 ^{d}

SD: Standard deviation. Within the same column, different letters indicate groups that are statistically different ($P < 0.05$).

Frank et al. [32], suggested that a retention of 2.94–7.35 N was necessary in the case of a distal extension RPD to protect against removal during the chewing of food, and Ahmad et al. [33] asserted that the guiding planes would also provide some retentive force (mean retention = 2.41 N). Various studies have discussed the necessary retentive force for RPD clasps, showing that the suitable retentive force for a clasp will actually decide on the type and number of clasps in the RPD; however, the lowest acceptable retentive force for one clasp was determined to be approximately 1.6 N [34,35]. The retentive force required for each component, will differ considerably with varying RPD design. The obtained constant-displacement fatigue test data (Table 3) indicated that

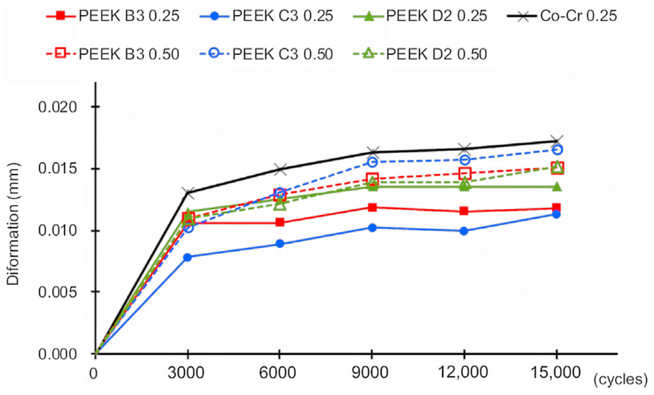

Fig. 5. Deformation of the specimens for every 3000 cycles, in the direction of loading.

the average load values of the PEEK clasp (mean: 2.06–3.67 N) were smaller than those of the Co–Cr alloy (mean: 8.26 N); although, considering all the factors mentioned above, PEEK clasps may provide a sufficient retentive force for clinical use.

Metal materials with larger rigidity are unsuitable for large undercuts, due to the fact that the clasps would place a large stress on the abutments [36,37]. However the lower elastic modulus of PEEK renders this material suitable for use with a larger undercut, which may be advantageous in clinical situations in which more aesthetically pleasing results or improved periodontal health are required [19,20,38]. Moreover, when reinforced by plaque control and regular denture maintenance, there is no evidence suggesting that a deeper undercut will result in microbiological risks related to periodontitis in the abutment teeth of RPD wearers [39,40].

Within the limitations of this in vitro study, it was possible to assert that PEEK specimens with a width of 3.00 mm, a thickness of 2.25 mm at the base (Group C3), a taper of 0.5, and with an undercut of 0.50 mm exhibit the best mechanical properties. However, the curved clasp-arm shape was not considered in the present study; and the various paths of insertion required by actual clinical usage may produce greater loads on the abutment teeth, resulting in permanent deformation of the clasp over a short period of time. The effects of these factors should be confirmed by further research in order to determine the optimal design and clinical efficacy of PEEK clasps. However, the superior flexibility and lower elastic modulus of PEEK, which engages a deeper undercut than the Co–Cr alloy but also exerts lower stresses on the abutments, suggest that this material is appropriate for use in RPDs. Removable partial dentures with PEEK clasps are recommended in clinical cases with sufficient residual tooth, aesthetic concerns, or even predominant concerns about periodontal health. Its benefits range from the maintenance of periodontal health, satisfying aesthetic demands, and the improvement of patient quality of life.

5. Conclusion

A comprehensive consideration of the results of the present in vitro study prompts the following conclusions:

1. The differences between the mean load values provided by clasps with various cross-sectional dimensions were significant, and the effect of thickness was greater than that of width. For clasps of the same dimension, a higher taper ratio was associated with higher mean load values.
2. The load values required for deflecting the Co–Cr alloy (mean $\pm$ SD: 8.26 ± 0.55) were significantly higher ($P < 0.05$) than those of PEEK (mean $\pm$ SD: 2.06 ± 0.09–3.67 ± 0.17), although the PEEK clasps did provide sufficient retentive force for clinical use.
3. Tests on the Co–Cr alloy and PEEK to simulate a ten-year clinical use lifespan (15,000 cycles), showed significantly greater deformation in the earlier cycles than in the later cycles ($P < 0.05$), but there was no significant difference in the long-term deformation of the two materials ($P = 0.11$).

Conflict of interest

The authors declare no conflict of interest.

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