Dimensional Optimization of Graphene-Modified Polymethyl Methacrylate Material Used as an Aesthetic Removable Partial Denture Clasp Material

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Abstract

Objective Although graphene-modified polymethyl methacrylate material is a good candidate for partial denture clasp material, it lacks adequate strength. Therefore, the study aims to assess the optimal dimension of this nanomodified material required for such an application.

Materials and Methods A parametric finite element analysis study was conducted on 54 clasp 3D models at two displacement levels (0.25–0.5 mm) placed 3 mm from the clasp tip. The clasp models were categorized based on the dimensions into A, B, and C (3 subgroups in each) and six tapers from the tip to the base (0.5–1). Both reaction force in (N) and maximum principal stress in (MPa) were recorded and analyzed. The study was validated using the mechanical tester after digital manufacturing of the clasp specimens that showed satisfactory results.

Statistical Analysis The correlations between width and thickness against reaction force and maximum principal stress were checked by a statistical analysis software package (SPSS version 22; IBM Corp., Armonk, New York, United States). Data of the reaction force demonstrated nonparametric behavior, as tested by the Kolmogorov–Smirnov test. Accordingly, Spearman's rho test for correlation was used. In contrast, the maximum principal stress data showed normal distribution, as tested by the Kolmogorov–Smirnov test. Thus, Pearson's test of correlation was applied.

Results The results demonstrated the best retention force values, considering aesthetics, in subgroups C3 (taper 0.6), C3 (taper 0.8), and B3 (taper 1). The maximum principal stress results showed the highest values in group C followed by group B and then group A. Positive correlations were calculated between thickness and width versus reaction force and maximum principal stress. The correlation coefficient value between thickness and reaction force was 0.699 and that between width and reaction force was 0.621, while the correlation coefficient between thickness and maximum principal force was 0.899 and that between the width and maximum principal force was 0.740.

Conclusion It could be concluded that the studied material might be recommended as a valid aesthetic clasp material. Both clasp thickness and width showed a positive correlation with the clasp retention force with more impact by the thickness.

Keywords
- graphene
- shape optimization
- aesthetic clasp

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Introduction

The ideal removable partial denture (RPD) material should have various mechanical, physical, and biological characteristics. It should have adequate flexural and yield strength to avoid permanent deformation during function and good hardness to resist abrasion and indentation.[1,2] It must grant inertness and biocompatibility in the oral environment. In addition, color matching with the surrounding tissues and aesthetic properties are better maintained.[3] Although these properties might be acquired using metallic alloys such as chrome-cobalt and gold, aesthetic representation on the abutments is unsatisfactory.[4] Certainly, the use of adequate RPD design should consider this issue, but sometimes metal display is unavoidable.[5] Wrought wire clasps are also advised sometimes for better aesthetic and flexibility.[6] Recently, the use of tooth-colored materials have been a good alternative, especially for the clasp components.[7]

Advances in material science revealed different aesthetic biomaterials that suit the oral environment and could be a good alternative to dental alloys. For many years, polymers including acetal resin, polyester, polyamide, and ceria-stabilized zirconia/alumina nanocomposite have been employed in prosthodontics.[3,8,9] Recently, polymers of ketone groups like polyether ether ketone (PEEK), polyaryletherketone (PAEK), and aryl ketone have become frequently used.[10–14] Using these polymers for RPD construction is not only beneficial for aesthetic, but they also have better biological characteristics. They minimize the loading of the abutment periodontium and eliminate the metallic taste of the RPD alloys.[10,11,15]

Graphene is a 2D allotrope with a hexagonal honeycomb crystalline lattice structure. Graphene is characterized by low planar density (0.7 mg/m^2), which makes it a superlight material. Carbon element formed the unit structure of graphene as a hexagonal ring at a surface area of 0.052 nm^2. Derivatives of these materials, like graphene oxide (GO) and its reduced form (GOr), became popular materials in dentistry. They can combine with other materials to improve their qualities. For instance, they could enhance the mechanical properties of several polymers such as epoxy resin, polycarbonate and polymethyl-methacrylate (PMMA).[16–18] Apparently, PMMA is one of the popular polymers used in removable prosthodontics due to its physical properties and ease of processing. However, this material lacks the sufficient mechanical properties that are required for some applications especially in the thin section. Accordingly, studies recommended several additives to enhance its mechanical properties.[18] Graphene proved to be a good additive that could upgrade the strength of the polymers.[17,18]

Fortunately, graphene has antimicrobial properties.[19,20] This unique property encouraged researchers to study incorporating graphene into the dental application. Graphene has been used successfully as implant abutment, fixed prosthesis, restorative material, bone regeneration, and an adhesive for orthodontic bracket bonding.[16–18,21]

One method to incorporate graphene into polymers is the doping method.[20] It could manufacture computer-aided design–computer-aided machine (CAD-CAM) disks for digital dentistry applications.[22] The doping method is carried out either directly or as a post-treatment step. In the direct synthesis process, doping occurs at the graphene growth stage while the post-treatment is achieved after synthesizing graphene. Post-treatment doping is more controllable and could be done with wet and dry mechanisms. The wet mechanism may include several techniques such as acid etching and organic material coating. The dry mechanism could be performed by plasma or thermal treatment.[23]

Many polymers were investigated for their performance as an alternative clasp material. Bending and retention force laboratory simulations considering cyclic fatigue have been studied.[10,13,24,25] Virtual analysis by digital mathematical methods as the finite element analysis (FEA) was also considered.[1,26] Because of the marked difference in the elastic modulus of the tested polymers versus the frequently used alloys, less retention force was generated. Based on the previous studies, clasp retention should exceed 1.6 N to be functional.[5,27] As a result, the polymeric clasp should meet the minimum retention value while deforming within the elastic limit.[26] For this purpose, the shape and dimensions of the polymers should be optimized to achieve the mechanical requirements. Some studies focused on testing the best configurations of the polymeric clasps especially for PEEK and aryl ketone polymers.[13,14,26] The retention force of the graphene-modified PMMA versus PEEK clasps was tested on the simulated tooth after cyclic fatigue. The study recommended specifying the criteria for using the graphene-modified PMMA as a valid clasp material. It also encouraged optimization studies for the material before clinical application.[24]

To the best of the author's knowledge, no study has investigated optimizing the dimensions of a clasp made with CAD-CAM technology from graphene-doped PMMA. Thus, the current study aimed to assess the optimal dimensions of aesthetic clasps milled from graphene-doped PMMA CAD-CAM disks by a validated parametric FEA. The study hypothesized that graphene-doped PMMA could be used as a valid aesthetic clasp material after dimensional optimization for undercut areas (0.25 and 0.5 mm).

Materials and Methods

A simulated CAD 3D model was designed in the design modeler of the ANSYS software (ANSYS workbench v 21, ANSYS). The design included the simulated clasp arm and the attachment part. The clasp arm's base side was attached to the fixed part where the arm was grasped. The shape and details of the dimensions can be seen in ►**Fig. 1(A)**.

Fifty-four clasps were designed at a different base and tip dimensions (tapers). These dimensions were set based on the valid dimensions mentioned in the literature for polymeric aesthetic clasps.[26] Specimens were categorized into 3 groups (A, B and C) and 3 subgroups for each considering 6 taper values (0.5, 0.6, 0.7, 0.8, and 0.9, 1; see ►**Table 1**). The values of ►**Table 1** were used for designing different clasps in a parametric finite element study to check the effect of

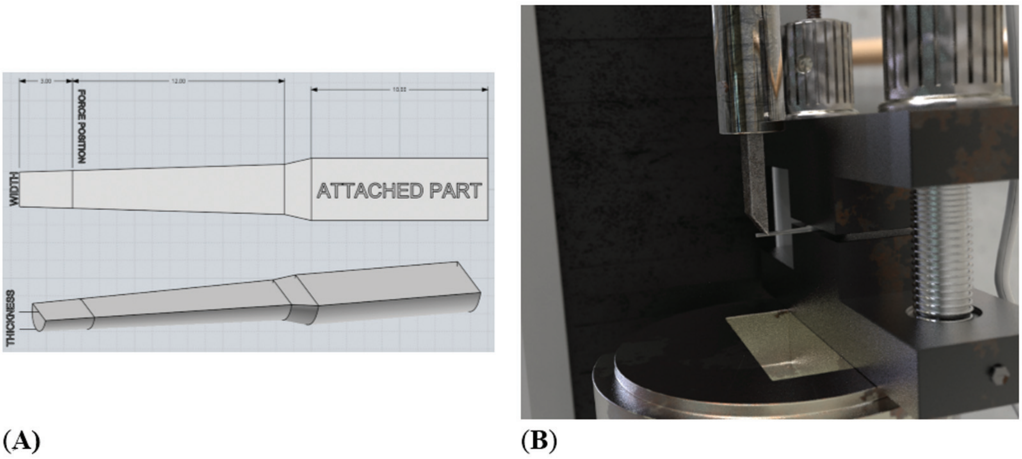

Fig. 1 (A) Designed clasp demonstrating dimensions, line of force application, and extended attachment part. (B) Representative image of the tested clasp specimen attached to the mechanical machine before the application of force.

changing width and thickness. The parameter checkboxes of the thickness and width were activated to assess the output values of the 54 clasp models.

Based on the manufacturer's data, the properties of the material (G-CAM, Graphenano Dental S.L., Valencia, Spain) are the following: bending strength = 140 MPa, yield strength = 92 MPa, surface hardness =88 (shore), water sorption =4 μg/mm^3. The assigned engineering material of the graphene-based material included young's modulus (3,200 MPa) and Poison's ratio (0.3).[28] The finite element meshing step was performed and enhanced after a mesh convergence study, where minimal element required able to converge a valid results. The mesh was also treated to avoid the generated singularities or the stress raiser that could affect the outcome. The model mesh was produced with Tet-10 element type (SOLID187) with 70,556 nodes and 39,789 elements. Some refinement was done in certain areas using an adaptive convergence tool to improve the accuracy of the stress distribution of the studied model.

Two scenarios of the boundary condition were based on the degree of displacement. The first scenario simulated 0.25-mm displacement applied 3 mm from the clasp arm tip, while 0.5 mm was used for the second. The two scenarios represent the engagement of two levels of tooth undercut. All models were constrained at the attachment area of the clasp base. The output values of the reaction force in newtons (N) and maximum principal stress (MPS) in (MPa) were recorded and tabulated. The width and thickness were checked for correlation with the output data, the reaction force and MPS, using a statistical analysis software package (SPSS version 22; IBM Corp., Armonk, New York, United States). Data of the reaction force demonstrated nonparametric behavior, as tested by the Kolmogorov–Smirnov test. Accordingly, Spearman's rho test for correlation was used. In contrast, the MPS data showed normal distribution, as tested by the Kolmogorov–Smirnov test. Thus, Pearson's test of correlation was applied.

Based on the finite element study's results, three clasp designs were selected with a satisfactory retention force and reasonable aesthetic characteristics.[26] The models of the three designs were manufactured by a five-axis CAD-CAM milling machine (DWX-520, Roland, California, United States) from the G-CAM disks to validate the finite element study.

Table 1 Dimensions of the base and tip (in mm) of the designed clasps considering the different taper values

Groups	Subgroups	BW/2	BT	TW/2	TT	TW/2	TT	TW/2	TT	TW/2	TT	TW/2	TT	TW/2	TT
				0.5 taper		0.6 taper		0.7 taper		0.8 taper		0.9 taper		1 taper	
A	A1	1	1.25	0.5	0.63	0.6	0.75	0.7	0.88	0.8	1	0.9	1.13	1	1.25
	A2	1.25	1.56	0.625	0.78	0.75	0.94	0.875	1.09	1	1.25	1.125	1.41	1.25	1.56
	A3	1.5	1.88	0.75	0.94	0.9	1.13	1.05	1.31	1.2	1.5	1.35	1.69	1.5	1.88
B	B1	1	1.5	0.5	0.75	0.6	0.9	0.7	1.05	0.8	1.2	0.9	1.35	1	1.5
	B2	1.25	1.88	0.625	0.94	0.75	1.13	0.875	1.31	1	1.5	1.125	1.69	1.25	1.88
	B3	1.5	2.25	0.75	1.13	0.9	1.35	1.05	1.58	1.2	1.8	1.35	2.03	1.5	2.25
C	C1	1	1.75	0.5	0.88	0.6	1.05	0.7	1.23	0.8	1.4	0.9	1.58	1	1.75
	C2	1.25	2.19	0.625	1.09	0.75	1.31	0.875	1.53	1	1.75	1.125	1.97	1.25	2.19
	C3	1.5	2.63	0.75	1.31	0.9	1.58	1.05	1.84	1.2	2.1	1.35	2.36	1.5	2.63

Abbreviations: BT, base thickness; BW/2, half of the base width; TT, tip thickness; TW/2, half of the tip width.

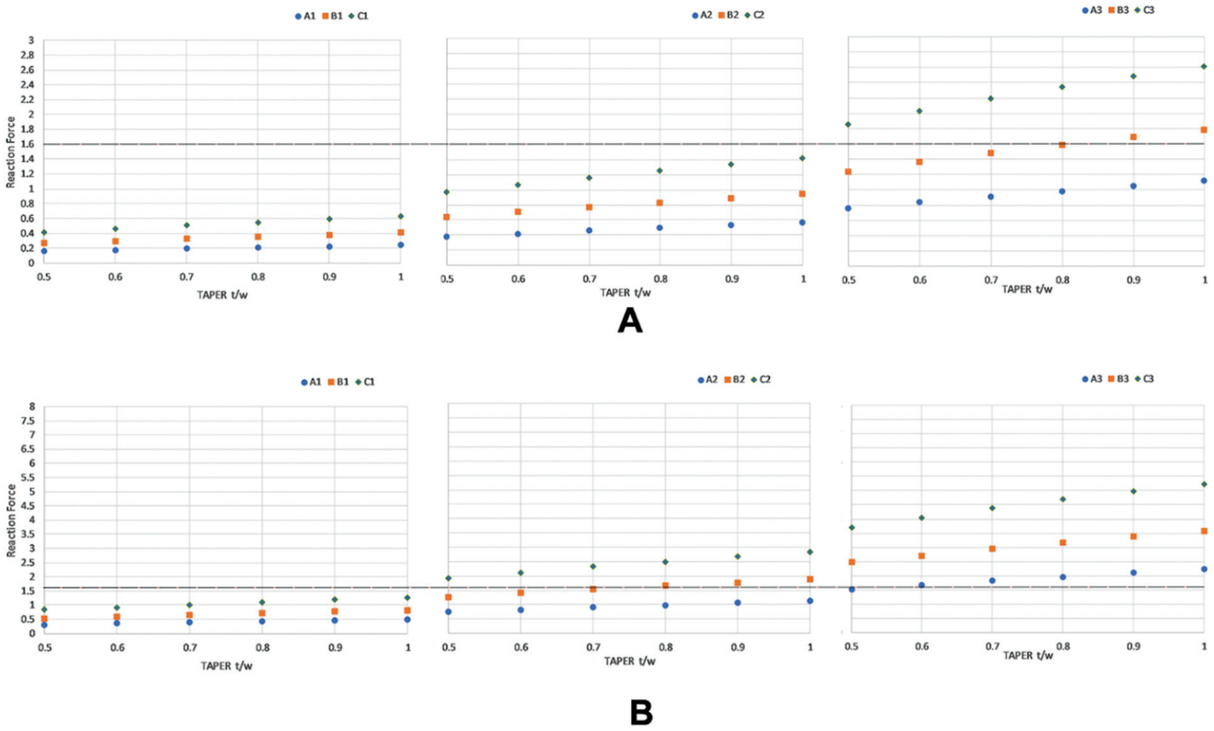

Fig. 2 (**A**) Values of the reaction force for each subgroup at different taper ratios after applying 0.25-mm displacement. (**B**) Values of the same subgroups after applying 0.5-mm displacement.

The attachment area of the specimen was fixed between the clamps of the mechanical testing machine (Instron Industrial Products, Norwood, Massachusetts, United States). At the same time, the load applicator was directed toward the line 3 mm from the specimen tip (see ►**Fig. 1B**). The load was gradually applied, leading to 0.25-mm displacement and then removed in cycles at 5 Hz. The exact process was repeated for the second patch of the specimens at 0.5-mm displacement. The generated force was recorded throughout 10,000 cycles of load application, representing frequent clasp insertion and removal. All data from the three specimens were collected to be compared with the FEA study.

Results

Reaction Force Results

Values of the reaction force in newtons (N) were organized following each subgroup number in each taper and plotted in a chart of reaction force versus the taper level. A horizontal line was drawn to clarify clasps' subgroups that exceed the minimum acceptable retention force (1.6 N) for the RPD clasp.[2,26]

Upon applying a 0.25-mm displacement, the subgroup (C3) demonstrated values ranging from 1.85 to 2.61 N, which is higher than the minimum acceptable value in all taper values. Subgroup B3 demonstrated values exceeding the minimum acceptable value only in taper 0.9 (1.69 N) and taper 1 (1.78 N;, see ►**Fig. 2A**).

As a result of 0.5-mm displacement, subgroups C2, B3, and C3 showed values higher than the acceptable value in all tapers, with values ranging from 1.93 to 2.83 N for C2, 2.47 to 3.57 N for B3, and 3.7 to 5.23 N for C3. In subgroup A3, 0.6 to 1 tapers' values were higher than the minimum value in the range 1.68 to 2.23 N. Only tapers from 0.8 to 1 in the subgroup (B2) exceeded the minimum value in the range from 1.66 to 1.89 N (see ►**Fig. 2B**).

The correlation between thickness and width versus reaction force at (0.25 and 0.5 mm) displacement revealed a significant correlation at the 0.01 level. The correlation coefficient value between thickness and reaction force was 0.699 and that between the width and reaction force was 0.621 (see ►**Fig. 3**).

Maximum Principal Stress Values

The values of the MPS, generated from 0.25-mm displacement, showed the highest values in group C, followed by group B and then group A. Subgroup C3 (range: 20.4–29.3 MPa) was higher than other subgroups in all taper values and subgroup C2 (21.8–23.4 MPa) in higher taper values (0.9, 1 taper). Generally, as the taper increased in all groups, the MPS value increased (►**Fig. 4A**).

Similarly, upon applying 0.5-mm displacement, the (MPS) of group C showed higher values followed by group B and then group A. Subgroup C3 (range: 45–58.6 MPa) demonstrated higher values, especially in tapers 0.6 to 1. In contrast, subgroup B3 and B2 showed high values in taper 1 (42.5 and 40 MPa, respectively; ►**Fig. 4B**).

The results demonstrated a significant correlation at a level (0.01) between the specimens' thickness and the MPS with a correlation coefficient value equals 0.899. Similarly, a

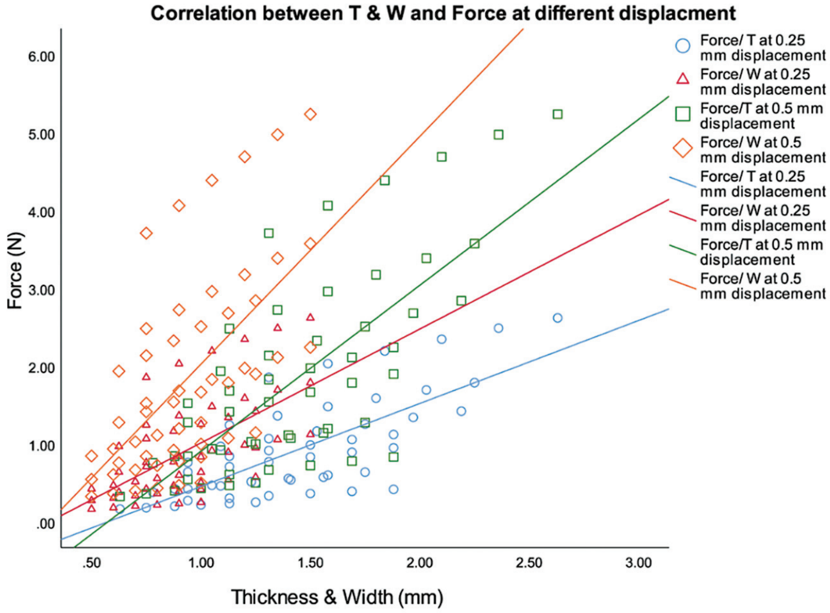

Fig. 3 Chart showing spread of force values in different displacement groups with correlation of changing thickness and width of the specimens and the force values.

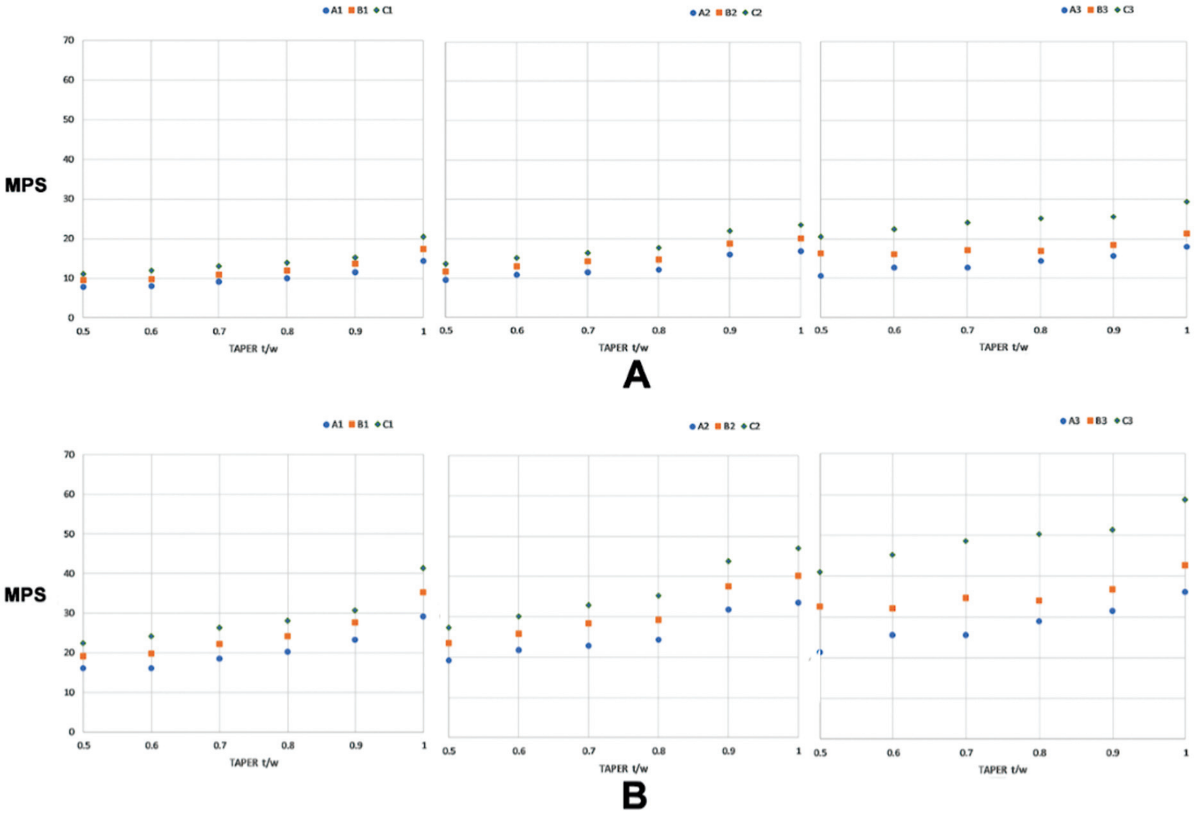

Fig. 4 Values of the maximum principal stress (MPS) in different subgroups. (**A**) Values at 0.25-mm displacement and (**B**) values at 0.5-mm displacement.

significant correlation was found between the width and the MPS, with a correlation coefficient value of 0.740 (see ►**Fig. 5**).

Three specimens were selected based on their performance in the parametric finite element study and aesthetic preference. Specimens were from subgroups C3 (taper 0.6), C3 (taper 0.8), and B3 (taper 1). The calculated average load values of subgroups C3 (taper 0.6), C3, taper 0.8, and B3 (taper 1) at 0.25-mm displacement were 1.93, 2.41, and 1.71 N), respectively. Higher average load values were

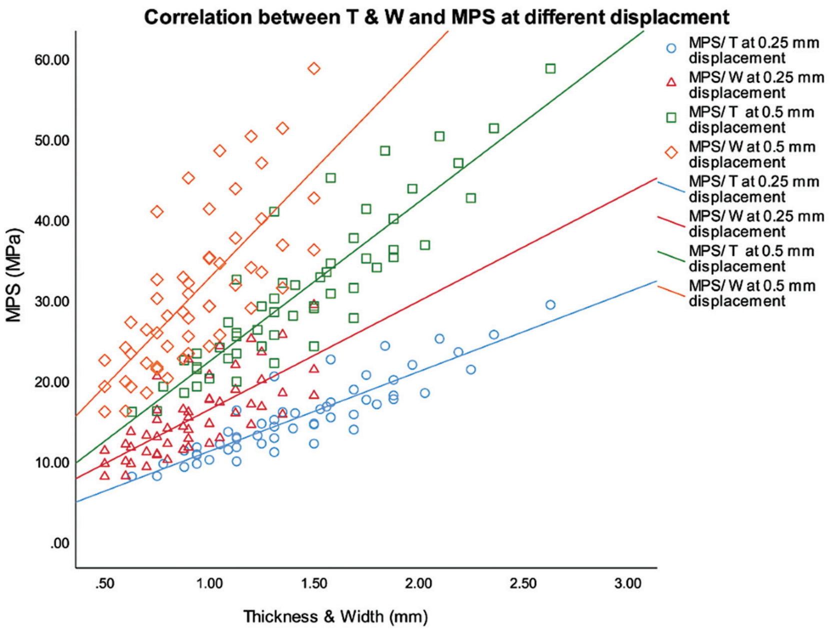

Fig. 5 Chart showing distribution of the maximum principal stress (MPS) data and their correlation with thickness and width of the specimens at different displacement values.

recorded for subgroups C3 (taper 0.6; 4.2 N), C3 (taper 0.8; 4.35 N) and B3 (taper 1; 3.3 N) at 0.5-mm displacement.

Discussion

The current study assessed, by parametric FEA, the optimal dimensions of an aesthetic clasp fabricated from graphene-doped PMMA using CAD-CAM technology. Using the mechanical tester, the suitable clasps were validated. Within the dimensions of the tested specimens, some clasps passed the required criteria. Therefore, the hypothesis of the study could be accepted.

The displacement values (0.25 and 0.5 mm) were selected to represent the undercut areas of the most popular clasps used in RPD designs.[25,29] Different dimensions were applied based on tapers from 0.5 to 1 where the width should not exceed the thickness of the clasp.[26,30] The length was a fixed value to keep tracking the influence of the diameters of the clasp tip and base. The load application area was kept in a line of 3 mm from the clasp tip to standardize the load application. Three clasp dimensions were selected in the validation study to compromise mechanical validity and aesthetics. The acceptable mechanical criteria considered the data in the literature about the minimum acceptable clasp retention (1.6 N).[2,26] In contrast, the clasps should have enough strength to avoid permanent (plastic) deformation beyond the yield strength. Fortunately, all the maximum principal stress recorded values were below the yield strength of the tested material (92 MPa). All selected manufactured clasps could validate the FEA study by recording values close to the virtual values, confirming the validity of using the selected dimensions for aesthetic and mechanical preference. Validation mechanical study proved the suitability of the FEA boundary conditions.

Upon applying 0.25-mm displacement, the study's results demonstrated higher values in the subgroup (C3) where the specimens' width and thickness started by 3 × 2.63 mm and 0.5 taper at the tip of the clasp. These dimensions were enough to generate force (1.85 N) higher than the minimal recommended clasp retention. However, at a higher taper (0.8), the retention force was remarkable and became close to the range of the PEEK material in the same application (2.06–3.67 N).[26] The results were as expected and could be attributed to the nature of the tested material. It is a PMMA polymer enhanced by graphene nanomaterial with an elastic modulus (3.2 GPa).[17,24] This value is close to polymers used for a such application as PEEK (3.0–5.5 GPa) and far beyond alloys such as Cr-Co (200 GPa), which allows reduced clasp thickness and width.[1,26,31–33] However, the material has the required flexibility to act as clasp material but is not rigid enough to be shaped in small and thin sections. This finding coincides with other studies that tested the polymeric materials used in RPD manufacturing.[8,12,26,27,30,34]

Similarly, when the displacement was doubled (0.5 mm), subgroups A3, B3, and C3 exceeded the limit. In addition, all tapers in group C2 were higher than the limit. Apparently, this level of displacement expands the possibilities and allows more freedom for aesthetic preference although the material will be limited to certain types of clasps and undercut levels.[1,35] Mostly, engaging deeper undercuts with metallic clasps requires more flexible clasps such as gingivally approaching clasps to avoid harmful effects on the abutment periodontium. In contrast, this shortcoming in metallic clasps is the advantage of using polymeric material. This with studies of Turner et al,[8] Urano et al,[3] and Marie et al[13] that confirmed the preferred undercut extension when polymer materials are used as RPD clasps.

Various studies were conducted to clarify the required retention for each clasp, which ranged from 1.6 N for back-action clasp to 17.5 N for Aker clasps. Any value beyond this range will lead to a nonfunctional clasp, whether there is insufficient retention or is harmful to the periodontium.[2,5,36] The location of the edentulous span affects the RPD retention as estimated by Frank and Nicholls,[6] which was found to be 2.94–7.35 N. Undoubtedly, the guiding planes could play a role in RPD retention.[37] RPD retention is a complex quality and should be planned carefully during RPD design. Planning of RPD retention using the current material required optimization of the clasp dimensions to be a valid RPD clasp option.[38,39] Previous studies showed higher stress values at the connection between the retentive clasp arm and the guiding plane, rendering it more prone to fracture.[1,24,26,38] Thus, keeping larger dimensions in that area is wise to endure stress concentrations. Although adequate tapering of the clasp tips is mandatory for metallic clasps because of their high rigidity, higher flexibility renders polymer clasps acceptable in less tapering values.[3,13] The current study showed higher retentive forces in subgroups with larger dimensions and tapers. In addition, the results showed positive correlations between thickness and width of the clasps versus retention force at 0.25- and 0.5-mm displacement (0.699 and 0.621, respectively; see ►**Fig. 3**). For better retention, less clasp taper is advised but within the acceptable aesthetics. This finding matched the previous studies conducted by Peng et al[26] and Sćepanović et al.[38]

The current study may have some limitations. For example, not all clasps' dimensions were tested mechanically. Only those having good characteristics were tested mechanically. In addition, testing different materials at the corresponding tooth surfaces was another limitation. Accordingly, a virtual study was considered and used as a base for the mechanical study. Testing the retention force in the clinical environment, considering the influence of salivary fluid and masticatory forces, could be beneficial. The influence of temperature and friction against enamel and different restorative materials could be studied. In addition, the number and distribution of direct retainers within the RPD design may be considered. A controlled randomized study will be a good chance to test this application in oral environment, especially in temperature fluctuations expected in the oral cavity. A material fatigue study in these conditions and thin section application may resolve the issue of longevity of the clasp retention particularly after dimensional optimization.

Conclusion

This study proposed using graphene-modified polymethyl methacrylate material as an aesthetic clasp material. Within the limit, the optimized clasp's dimensions demonstrated sufficient mechanical properties and aesthetic characteristics and met the criteria for a successful clasp. Some combinations of different lengths and diameters, such as 0.6 and 0.8 tapers in larger diameters, were more valid and showed sufficient retention beyond the material yield point. When utilizing the tested material, engaging a more undercut depth is preferred for more retention. This encourages using the studied material in teeth with sufficiently undercut areas or in a previously prepared wide depression. Positive correlations were revealed between the retention force and the clasp thickness and width, with more thickness having a greater impact.

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Conflict of Interest
None declared.

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