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Chemical, optical, and morphological properties of TPU and PET-G samples after aging in artificial saliva: an in vitro study

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Abstract

Background Thermoplastic materials, such as glycol-modified polyethylene terephthalate (PET-G) and thermoplastic polyurethane (TPU), undergo alterations due to environmental factors in the oral cavity, which can affect their composition and surface properties over time. While previous studies have explored these changes, a comprehensive characterization of TPU and PET-G properties, particularly after immersion in artificial saliva, remains limited. This study aimed to evaluate the aging process of 24 TPU and 24 PET-G dumbbell-shaped specimens before and after exposure to artificial saliva. The analysis focused on the morphological, chemical, and optical properties of the samples, including thickness, weight, and surface roughness.

Methods The study examined 48 thermoplastic samples, equally divided between PET-G and TPU. The samples were thermoformed into standardized shapes and analyzed at three time points: after thermoforming (T0), after 7 days (T1), and after 14 days (T2) of immersion in artificial saliva at 37 °C. Measurements included weight, thickness, surface roughness, absorbance, and Fourier transform infrared spectroscopy (FTIR). Data were analyzed using one-way ANOVA to identify significant changes over time, with a significance level of $p < 0.01$.

Results Both materials exhibited significant reductions in surface roughness, with TPU showing a decrease in average roughness (Ra) from 99.43 nm at T0 to 76.53 nm at T2 (-23.02%) and PET-G decreasing from 33.25 nm to 20.19 nm (-39.27%). The root mean square roughness (Rq) in TPU declined by 41.67% (from 126.91 nm to 74.02 nm), while PET-G showed a reduction of 28.06% (from 44.98 nm to 32.35 nm). Peak-to-valley roughness (Rt) also decreased by 10.5% in TPU and 27.96% in PET-G. No statistically significant changes were observed in thickness, weight, optical density, or chemical composition ($p > 0.01$). The roughness disparity between TPU and PET-G persisted even after immersion in saliva.

Conclusions Following the simulated intraoral aging process, significant changes in surface roughness were observed in TPU and PET-G specimens. The reduction in roughness, particularly a 39.27% decline in PET-G and 23.02%

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in TPU, has been clinically associated with decreased plaque accumulation and reduced friction between the aligner and the teeth.

Keywords Clear aligners, Thermoplastic materials, Artificial saliva aging, Surface roughness, Morphological properties

Background

In recent years, clear aligners have significantly transformed orthodontic treatment, providing patients with a more aesthetic and comfortable alternative to conventional fixed appliances [1]. However, despite their widespread adoption, the selection of the most effective aligner remains a challenge for orthodontists. The increasing number of manufacturers in the market has led to difficulties in objectively assessing the quality and performance of different aligners before clinical application [2]. This challenge primarily arises from the absence of standardized guidelines defining the material properties and structural characteristics that influence treatment efficacy. Addressing this gap is crucial to enhancing clinical decision-making, as well as ensuring that aligner manufacturers provide comprehensive and transparent data on material composition and mechanical behavior.

Thermoplastic materials are linear or slightly branched polymers characterized by strong intramolecular covalent bonds and weak intramolecular Van der Waals forces. The thermoplastic materials currently used in clear aligner fabrication include glycol-modified polyethylene terephthalate (PET-G), thermoplastic polyurethanes (TPU), polypropylene (PP), polyamides (PA), and polycarbonates (PC) [3]. During the thermoforming process, the bonds in these materials soften, allowing the polymers to be molded at elevated temperatures. Upon cooling, the molecular chains solidify, forming new shapes [4].

These polymers undergo aging due to mechanical stress from physiological oral activities and parafunctional habits (e.g. clenching or grinding). In addition, chemical stress caused by prolonged exposure to saliva, enzymes, bacteria, and their byproducts, along with temperature variations (ranging from 0° and 70° C due to hot orc cold fluid intake) and pH fluctuations, may lead to compositional changes and surface alterations [5–7].

Previous studies have demonstrated that aligners experience a rapid reduction in force over time. Lombardo et al. reported that force release from TPU and PET-G aligners decreases by more than 50% within the first few hours of clinical use. They also found that single-layer materials perform better than double-layer materials [8]. Albertini et al. analyzed aligners stress relaxation over 14 days of use, reporting a force release between 3.9% (PET-G) and 39% (TPU) of the initial value, with stabilization occurring after the first 2–3 days of use. According to the study, the aligners stabilized in a force release between 2 and 8 MPa after the first two to three days of use [9].

These materials may also undergo diminished mechanical strength and transparency, which could impact patient satisfaction [10]. A study by Lira et al. evaluated chemical, physical, mechanical, and morphological properties of 12 SmartTrack (Invisalign®) aligners after intraoral use, revealing a significant decrease in transparency, increased water absorption, and reduced mechanical properties. Although surface roughness increased, the change was not statistically significant [11].

Evidence on surface roughness in the literature is conflicting. Papadopolou et al. found that aligners exhibited reduced roughness after intraoral use due to wear [12]. A recent study by Eslami et al. yielded comparable outcomes; however, it demonstrated how the situation differs when the object in question is a 3D-printed or thermoformed aligner [13]. Conversely, Condò et al. and Gracco et al. observed increased roughness in Invisalign aligners, likely due to microcracks [14, 15]. Bucci et al. focused on the effects of thermoforming and intraoral aging on PET-G aligners, highlighting a statistically significant reduction in thickness after thermoforming and a not statistically significant reduction after intraoral aging [16].

The reduction in thickness after thermoforming and its clinical relevance have been largely confirmed by Palone et al. in a study employing micro-computer tomography evaluation [17].

A comprehensive understanding of the detailed characteristics of these materials is essential for improving the predictability of treatments with aligners. Kravitz et al. demonstrated that the mean predictability of Invisalign treatments increased from 41% in 2009 to 50% in 2020 [18, 19]. Investigating how aligner polymers behave under different conditions can help refine strategies to enhance clinical performance and treatment predictability.

The present study aims to analyze the chemical and physical properties of TPU and PET-G, two widely used aligner materials, by examining and comparing their structural, morphological, and optical characteristics before and after immersion in artificial saliva [20, 21]. A unique aspect of the study is the use of an atomic force microscope for surface roughness analysis, ensuring highly precise measurements [22].

The hypotheses tested were as follows:

- H_0: No significant differences exist in the chemical, optical, or morphological properties of TPU and PET-G samples before and after artificial saliva exposure.

- H_1: Significant differences exist in the chemical, optical, or morphological properties of TPU and PET-G samples after artificial saliva exposure.

Methods

Study design

This preclinical monocentric in vitro study was conducted through a collaboration between the Dental Clinic of the Fondazione Polyclinic Gemelli IRCCS in Rome and the Department of Neuroscience - Institute of Applied Physics - at the Catholic University of the Sacred Heart in Rome.

Sample selection

Eligibility criteria

Samples were selected based on the following requirements:

- Material: glycol-modified polyethylene terephthalate (PET-G) or thermoplastic polyurethane (TPU), supplied as thermoformed sheets;
- Thickness of material sheets before thermoforming: 0.75 mm;
- Material stratification: single layer.

Sample size

The sample size was estimated for a one-way ANOVA between the three timepoints, considering a large effect size of 0.8. To detect a difference with a power of 80% and a Type I error of 0.05, a minimum of 7 samples per group was required. To account for potential failures during the experiment, the sample size was increased to 8 per group.

Study timeline

A total of 24 PET-G samples (Erkodur, Erkodent, Pfalzgrafenweiler, Germany) and 24 TPU samples (F22 Aligner, Sweden & Martina, Due Carrare, Padua, Italy) were selected and divided into the following groups:

- 8 samples per material were analyzed after the thermoforming process, without immersion in artificial saliva (T0);
- 8 thermoformed samples per material were analyzed after 7 days of aging in artificial saliva (T1);
- 8 thermoformed samples per material were analyzed 14 days of aging in artificial saliva (T2).

Samples were analysed at three different time points as shown in Table 1.

The total duration of 14 days was chosen based on the average wearing time recommended by the manufacturers for clinical use of the aligner during orthodontic treatment [23].

Table 1 Study timeline

Timepoints	Operating sequence	Sample size
T0	Analysis of samples subjected to the thermoforming process only.	- 8 TPU samples - 8 PET-G samples
T1	Analysis of samples subjected to the thermoforming process and 7 days of immersion in artificial saliva.	- 8 TPU samples - 8 PET-G samples
T2	Analysis of samples subjected to the thermoforming process and 14 days of immersion in artificial saliva.	- 8 TPU samples - 8 PET-G samples

Sample production

Two commonly used thermoplastic materials were selected: thermoplastic polyurethane (TPU) (F22 Aligner, Sweden & Martina, Due Carrare, Padova, Italy) and glycol-modified polyethylene terephthalate (PET-G) (Erkodur, Erkodent, Pfalzgrafenweiler, Germany).

The materials were provided as circular sheets with a diameter of 125 mm and a thickness of 0.75 mm. The first step involved thermoforming the sheets, followed by the creation of 24 specimens of known morphology ("dumbbell-shaped") per material type, using a laser cutting machine (BCL1309X, Bodor, Jinan, Shandong, China). The specimens were produced according to the size and thickness specifications of EN ISO 527-2 for type 5B specimens.

Thermoforming was performed using a Ministar S machine (Ministar S, Scheu, Iserlohn, Germany) in accordance with the manufacturer's recommendations for pressure, heating time and cooling time; a pressure of 4/4.2 bar, a temperature of $175 \pm 10°$, a heating time of 28" and a cooling time of 30" were applied. The temperature of the disk surface was measured using a laser thermometer (Fluke 62 Max +, Fluke, Everett, Washington, United States). Each sheet was subjected to vacuum thermoforming without the use of any mould to simulate the stress associated with the thermoforming procedure.

Salivary aging

To simulate intraoral aging and replicate the effect of saliva on aligners, 200 ml of artificial saliva (Fusayama/Mayer Artificial Saliva, Alfatech SPA, Genoa, Italy) was used, as shown in Table 2 [24].

Four custom supports (Fig. 1) made of transparent polylactic acid (PLA) material (Ultimaker, Geldermalsen, Netherlands) were 3D printed (Ultimaker S3, Ultimaker, Geldermalsen, Netherlands) for immersing the specimens in artificial saliva. The samples were distributed as follows:

Table 2 Chemical composition of the artificial saliva (ph:6.0) used to recreate the biochemical environment of the human saliva

Chemical compound	Percentage (%)
Distilled water	97–100%
Potassium chloride	< 0.1%
Urea	< 0.5%
Sodium chloride	< 0.1%
Sodium phosphate monobasic dihydrate	< 0.1%
Calcium chloride dihydrate	< 0.1%

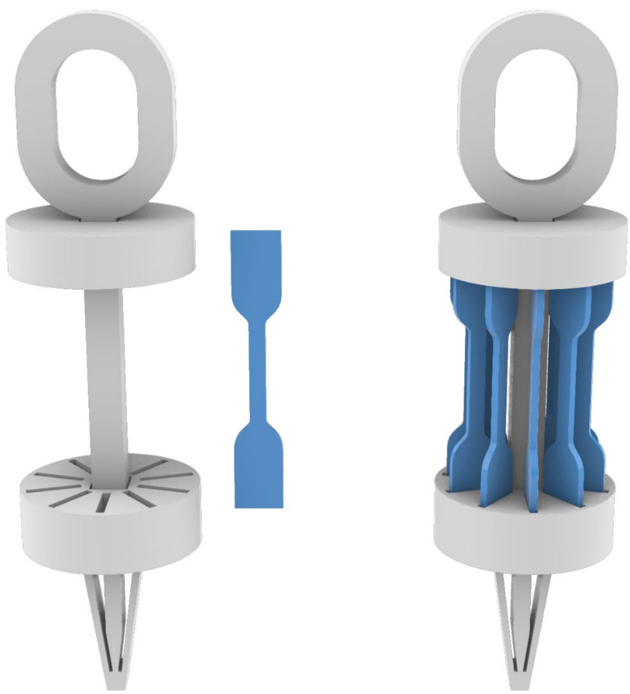

Fig. 1 PLA customized supports

- S1 contained 8 TPU (T1) samples;
- S2 contained 8 PET-G (T1) samples;
- S3 contained 8 TPU (T2) samples;
- S4 contained 8 PET-G (T2) samples.

The supports were immersed in artificial saliva at a constant temperature of 37 °C using an incubator (CAPP Rondo CM-I1, AHN Biotechnologie GmbH, Nordhausen, Germany). After 7 days, supports S1 and S2 were removed for analysis at T1. After an additional 7 days, supports S3 and S4 were removed from for analysis at T2. Once removed, samples were rinsed with distilled water and dried using a stream of air spray and absorbent paper, as described by Cremonini et al. [10].

Sample analysis

The following tests were performed at T0, T1 and T2.

- Weight analysis;
- Thickness analysis;
- Surface roughness analysis;
- Absorbance analysis;
- Fourier-transform infrared spectroscopy (FTIR).

All measurements were performed at a constant temperature of 23 °C.

Weight analysis

Three consecutive weightings were performed for each group of analysed samples using an Entris balance (Entris, Sartorius, Germany). Subsequently, an average of the three measurements was calculated for each study group, and the differences between T0, T1, and T2 were analysed.

Thickness analysis

Three measurements were taken for each sample using a digital electronic caliper (Kroeplin K110, Kroeplin GmbH, Schlüchtern, Germany), which has a reading range of 0.0005 mm. Subsequently, an average of the three measurements was calculated for each study group, and the differences between T0, T1, and T2 were analysed.

Surface roughness analysis

The surface roughness was assessed using an atomic force microscope (JPK Nanowizard II, Bruker, Germany). The evaluated surface roughness parameters included:

- Ra (average roughness): the arithmetic mean of the absolute values of profile heights over the evaluation length;
- Rq (RMS roughness): the root mean square (RMS) average of the profile heights over the evaluation length;
- Rt (peak-to-valley roughness): the observed distance between the highest and lowest points on the measured surface.

Measurements were conducted randomly at multiple points on the sample, and subsequently, the mean of the obtained values was calculated.

Absorbance analysis

The absorbance was quantified within the visible light spectrum (frequency range: 230–700 nm; step: 5 nm) using a Cytation3 spectrophotometer (Cytation3 Imaging Reader, Biotek, Santa Clara, United States). Each sample was placed within a dedicated plate (*take 3*) of the apparatus. It has been demonstrated in the literature that even slight movements of the sample can lead to significant variations in the detected absorbance [25]. In order to address this issue, a specific support was created using a 3D printer (Creality Ender-3 Longhua Dist., Shenzhen,

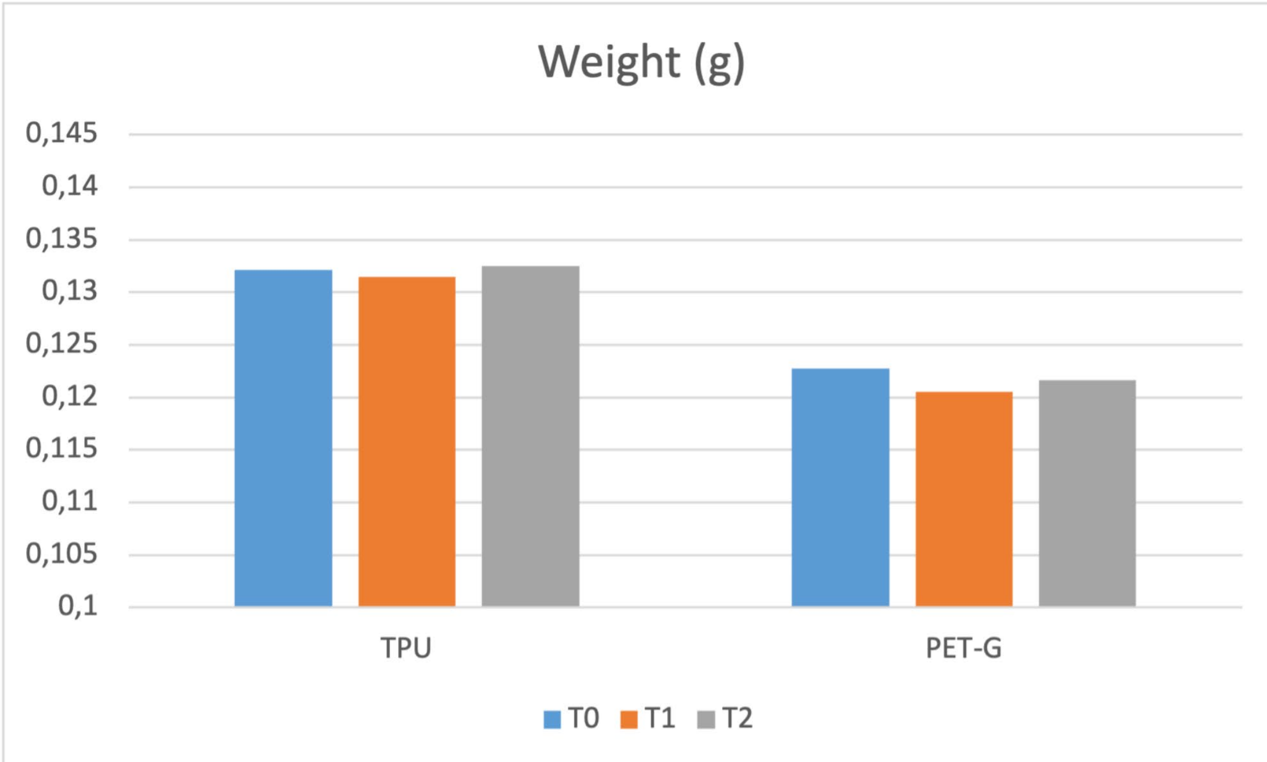

Fig. 2 Average weight of the TPU and PET-G samples at T0, T1, T2

China) in thermoplastic polyurethane material. This support could secure the samples consistently at the same distance and in the same position for each measurement. Subsequently, the data were exported from the machine to a dedicated software program (Gen 5), specifically designed to collect and analyze the data [26].

Table 3 Weight of the samples at T0, T1, and T2; data expressed as mean ± standard deviation

Average weight (g)	TPU	PET-G
T0	0,132 ± 0,002 g	0,122 ± 0,002 g
T1	0,131 ± 0,001 g	0,120 ± 0,001 g
T2	0,132 ± 0,003 g	0,121 ± 0,002 g

FTIR spectroscopy

FTIR analysis was conducted to investigate potential variations in the chemical composition of the two different materials under consideration after immersion in artificial saliva. Measurements were performed using the Alpha II spectrometer (Alpha II, Bruker, Germany), a device capable of detecting the absorbance of samples placed on a dedicated support and comparing the spectrum of results obtained with an internal library in the software containing spectra from a multitude of commercially available materials. Spectral transmittance data were obtained within a frequency range (MIR) of 4000–600 cm^{-1}; the spectral resolution related to the interferometer of the device (ROCKSOLID Interferometer, Bruker, Germany) was 0.001 cm^{-1}; 24 scans were conducted for each measurement [27].

Statistical analysis

All data are expressed as mean ± standard deviation. A Shapiro-Wilk test was first performed to assess whether the data followed a normal distribution. The test yielded a positive result, allowing us to proceed with further analyses using one-way ANOVA.

One-way ANOVA was selected to assess significant differences in the physical properties of the materials at the three time points. To assess the intra-operator reliability, all the procedures were repeated by one senior researcher. The significance level was set at $p < 0.01$. All data were analysed using Systat software (version 8.0, SYSTAT Software Inc. (SSI), San Jose, California, USA).

Results

Weight

As shown in Fig. 2; Table 3, there were no statistically significant variations between the weight of the specimens at baseline and after aging in artificial saliva, neither for TPU nor for PET-G ($p > 0.01$).

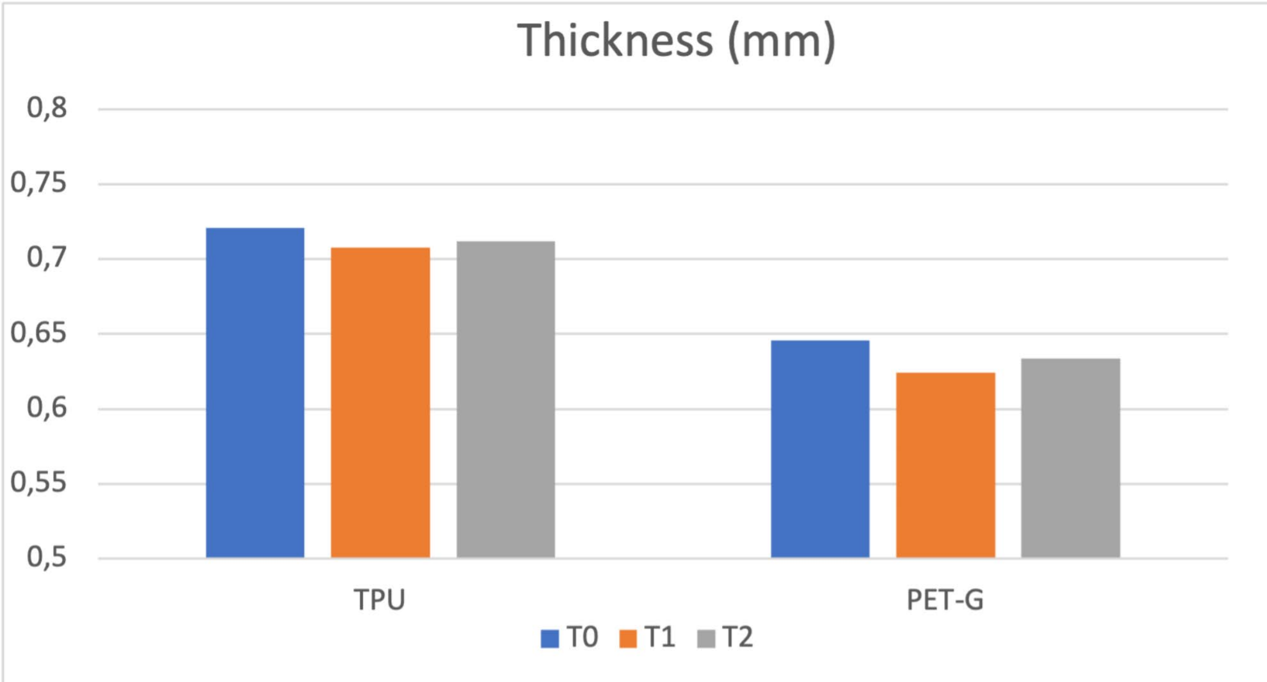

Fig. 3 Average thickness of the TPU and PET-G samples at T0, T1, T2

Table 4 Thickness of the samples at T0, T1, and T2; data expressed as mean ± standard deviation

Average thickness (mm)	TPU	PET-G
T0	0.72 ± 0.01 mm	0.65 ± 0.01 mm
T1	0.70 ± 0.009 mm	0.62 ± 0.009 mm
T2	0.71 ± 0.01 mm	0.63 ± 0.01 mm

Table 5 Mean values and standard deviations of roughness average (Ra), RMS roughness (Rq) and Peak-to-valley roughness (Rt) of TPU and PET-G samples at T0, T1 and T2

TPU	Ra	Rq	Rt
T0	99,43 ± 5,14 nm	126,91 ± 5,72 nm	967,69 ± 201,95 nm
T1	90,61 ± 1,37 nm	93,53 ± 14,88 nm	929,96 ± 218,74 nm
T2	76,53 ± 5,75 nm	74,02 ± 9,37 nm	865,52 ± 236,86 nm
PET-G	**Ra**	**Rq**	**Rt**
T0	33,25 ± 2,14 nm	44,98 ± 4,19 nm	519,76 ± 47,86 nm
T1	29,32 ± 2,86 nm	41,24 ± 5,33 nm	495,25 ± 63,01 nm
T2	20,19 ± 0,9 nm	32,35 ± 3,05 nm	374,39 ± 83,22 nm

Thickness

As shown in Fig. 3; Table 4, there were no statistically significant reductions between the thicknesses of the specimens at baseline and after aging in artificial saliva, neither for TPU nor for PET-G ($p > 0.01$).

Surface roughness

Table 5; Figs. 4 (a-f) and 5 revealed statistically significant reductions for both materials across all analysed parameters from T0 to T2 $p(< 0.01)$. Specifically, after 14 days of simulated intraoral aging:

- concerning TPU samples, Ra, Rq, and Rt reduced of 23.02%, 41.67%, and 10.5%, respectively.
- concerning PET-G samples, Ra, Rq and Rt reduced of about 39.27%, 28.06%, and 27.96%, respectively.

As illustrated in Fig. 6 (a-c), the surface roughness of the materials and its evolution over time exhibited notable differences.

At baseline, TPU was approximately three times more rugged than PET-G in terms of average roughness (Ra) and peak-to-valley roughness (Rt) and almost 2 times in terms of peak-to-valley Roughness (Rt) Rt. At T2, this gap between the two materials seemed to remain consistent. The TPU surface was approximately four times rougher than that of PET-G in terms of the average roughness (Ra), and approximately 2.3 times rougher in terms of the root mean square roughness (RMS) and peak-to-valley roughness.

Upon examination of the graphs, it becomes evident that the reduction in roughness of TPU from T0 to T1 and from T1 to T2 was proportional. Conversely, it appears that PET-G exhibited a greater capacity to maintain its roughness during the initial week, from T0 to T1, and subsequently experienced a significant decline during the second week, from T1 to T2.

Absorbance

As shown by Figs. 7 and 8, there were no statistically significant differences in the optical density of TPU and PET-G samples following 14 days of in vitro intraoral

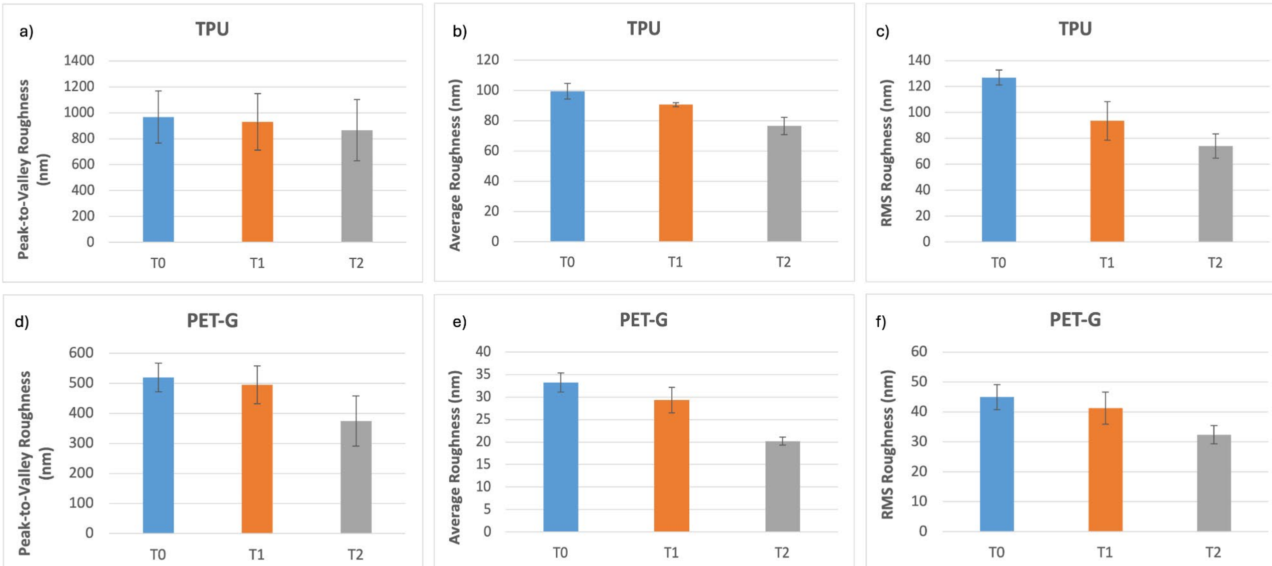

Fig. 4 (**a**) Peak-to-valley roughness TPU charts at T0, T1, T2; (**b**) Average roughness TPU charts at T0, T1, T2; (**c**) RMS roughness TPU charts at T0, T1, T2; (**d**) Peak-to-valley roughness PET-G charts at T0, T1, T2; (**e**) Average roughness PET-G charts at T0, T1, T2; c) RMS roughness PET-g charts at T0, T1, T2

aging: the absorbance spectra are almost entirely overlapping ($p > 0.01$).

FTIR spectroscopy

As shown by Figs. 9 and 10, there were no statistically significant variations in the chemical composition of the two materials following two weeks of simulated salivary aging: the spectra recorded by the equipment at the three time points are almost completely overlapping for both TPU and PET-G ($p > 0.01$).

Discussion

Surface roughness

The present study analyzed the changes in the morphological, optical and chemical properties of TPU and PET-G - two commonly used materials for clear aligners - after aging in artificial saliva. Based on the present findings, we reject the null hypothesis that no statistically significant differences exist between the two materials before and after simulated salivary aging. Both materials exhibit a substantial change in surface roughness, warranting further investigation into its clinical implications.

A statistically significant reduction in surface roughness ($P < 0.01$) was observed for both materials across all analyzed parameters (Ra, Rq, Rt). These findings are consistent with those of Papadopoulos et al., who used an optical profilometer to compare TPU aligners before and after 14 days of intraoral use and found a significant reduction in surface roughness [12]. A reduction in surface roughness may decrease the friction of aligners, potentially leading to a decrease in micromechanical retention with attachments and enamel [12, 28]. This phenomenon may partially explain the decline in aligner engagement over time, resulting in reduced force application to teeth.

The roughness gap observed at baseline remained relatively stable for all three parameters in both materials. TPU was significantly rougher than PET-G at both baseline and after two weeks of salivary aging.

The analysis of material morphological properties is crucial not only for device engagement but also.

because it influences bacterial biofilm formation on the inner and outer surfaces of aligners [29].

A study by Staderini et al. examined the morphological changes in 1-mm-thick PET-G samples following the thermoforming process [22]. Their results showed a significant increase in roughness due to the thermal shock associated with aligner production (approximately 1233% increase in Ra and 1129% increase in Rq). This suggests that materials experience a substantial rise in surface roughness during thermoforming, followed by a significant reduction after intraoral exposure.

In a recent study, Machoy et al. also used atomic force microscopy to assess differences in surface roughness of Invisalign aligners before and after use [27].

At T0, aligners showed an irregular surface with alternating peaks and valleys. With use, the decrease in surface roughness made the surface more homogeneous. Specifically, the average peak height and peak layer volume decreased in worn aligners. This finding is consistent with the results of our study.

Machoy et al. also conducted mechanical tests, showing that the Young's modulus decreases after use. The authors suggest that this reduction may result either from friction between the aligner and the teeth or from chemical alteration due to saliva or food exposure.

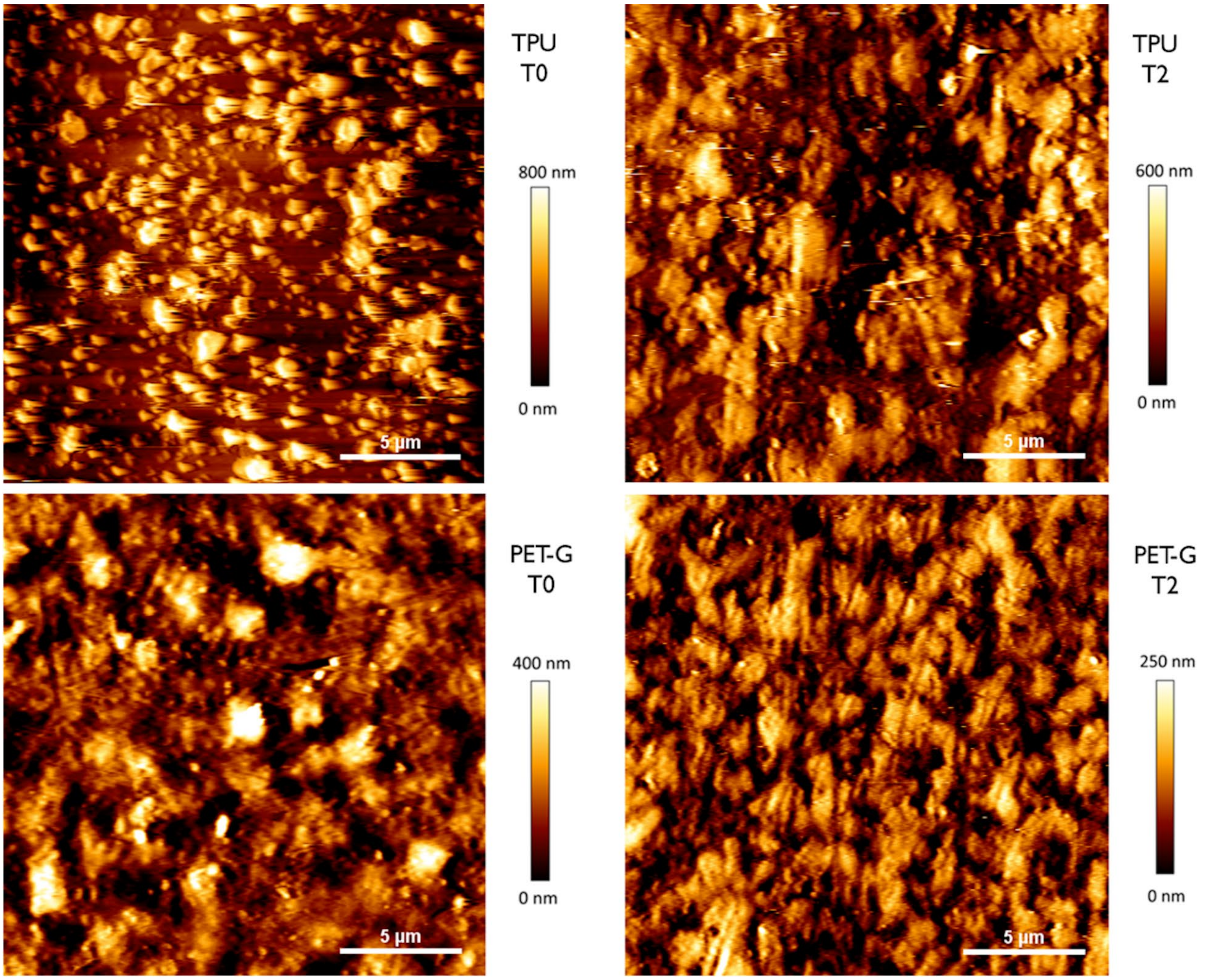

Fig. 5 Representative surface of the TPU and PET-G samples at T0 and T2 made with the atomic force microscope

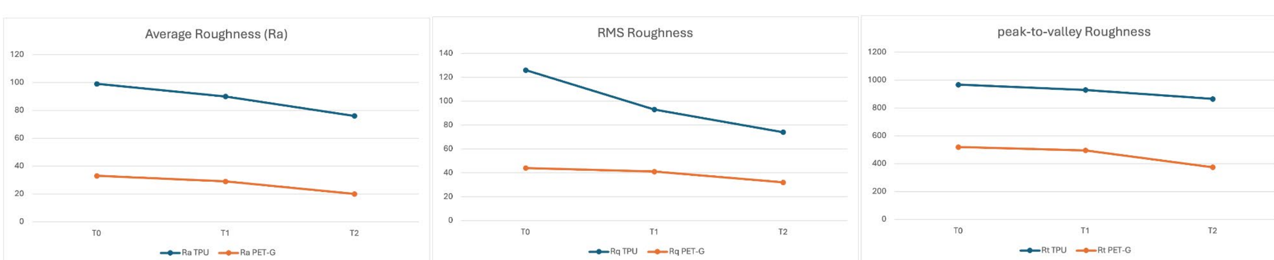

Fig. 6 (**a**) Average Roughness TPU and PET-G Cartesian graph; (**b**) RMS roughness TPU and PET-G Cartesian graph; (**c**) Peak-to-valley TPU and PET-G Cartesian graph

Water absorption

Few studies in the literature have assessed whether intraoral aging can alter the thickness and weight of polymeric materials [30–32]. Tamburrino et al. found that simulated salivary aging led to water absorption, affecting the mechanical properties of the aligners. The authors suggested that the plasticizing effect of water may decrease the glass transition temperature, thereby altering properties such as the elastic modulus. These properties have a directly proportional relationship with the material's glass transition temperature of the material [33].

In the present experimental study, no statistically significant differences were found in the weight of either material at any of the three time points ($P > 0.01$), suggesting limited water absorption and, consequently, a minimal plasticizing effect.

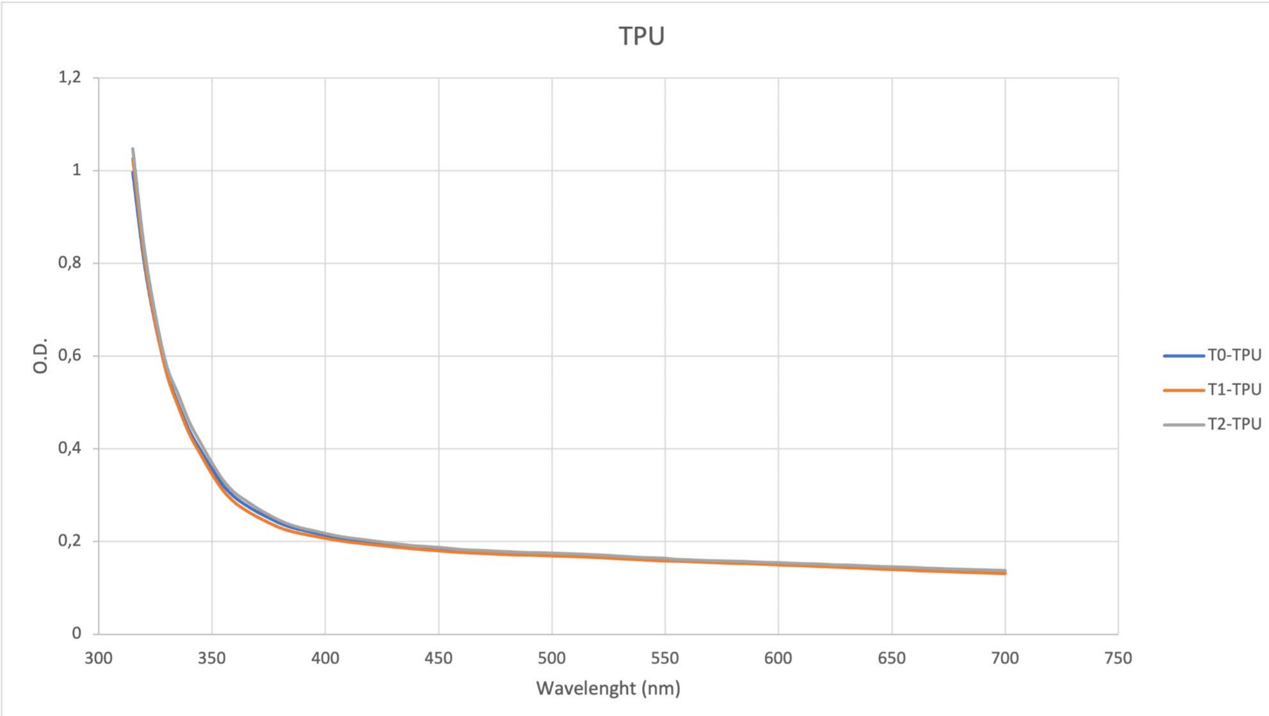

Fig. 7 Absorbance spectra of the TPU samples at T0, T1 and T2

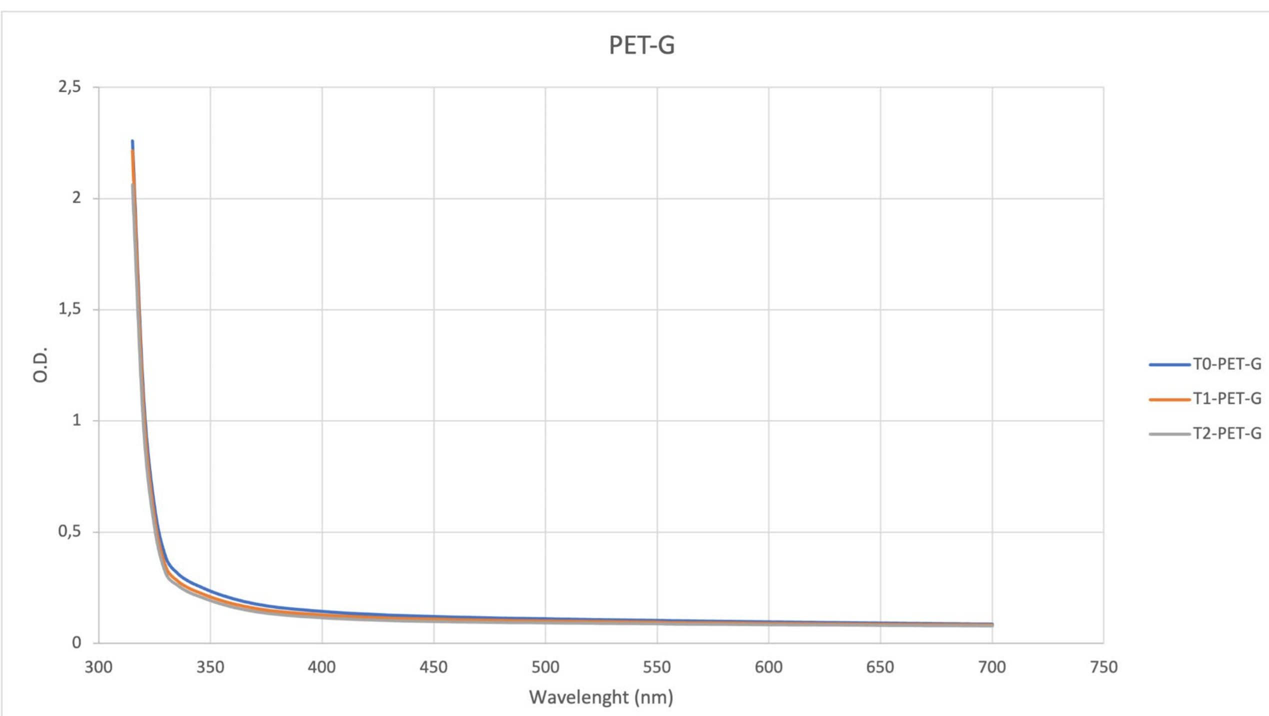

Fig. 8 Absorbance spectra of the PET-G samples at T0, T1 and T2

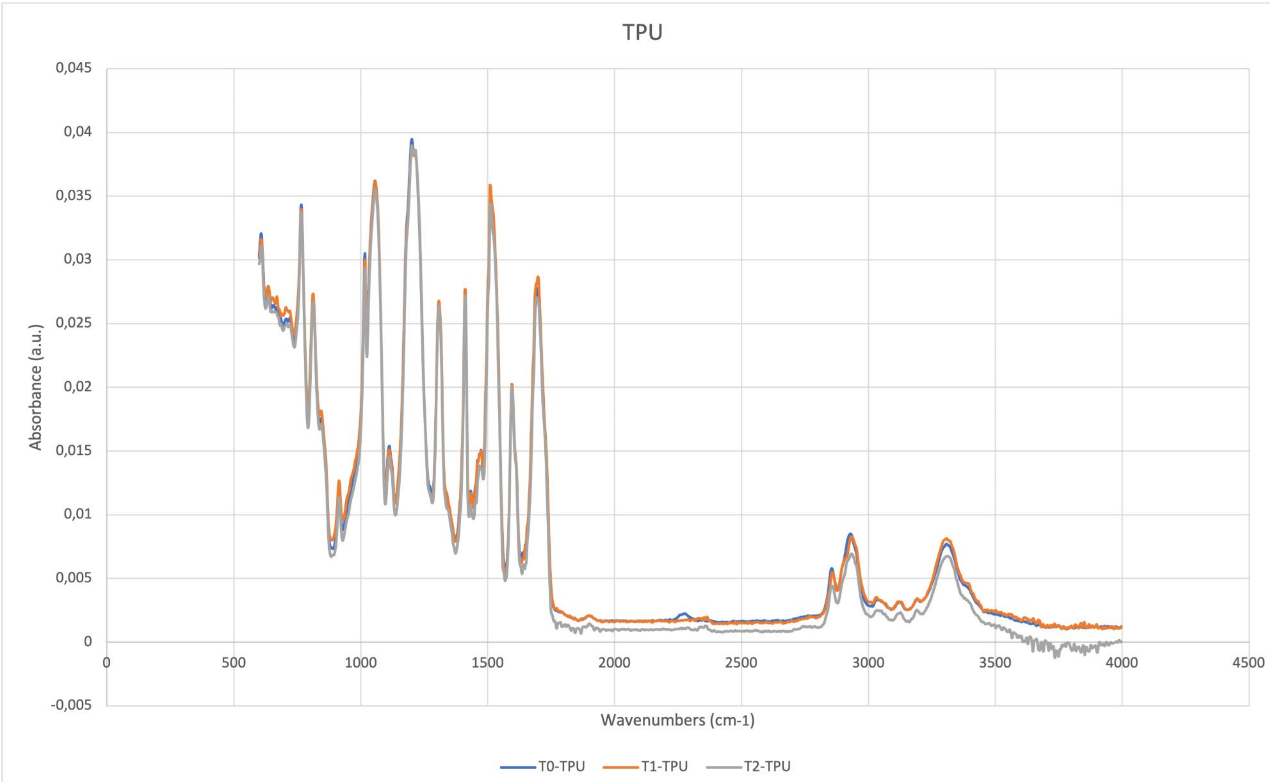

Fig. 9 Average FTIR spectroscopy spectrum of the TPU samples at T0, T1 and T2

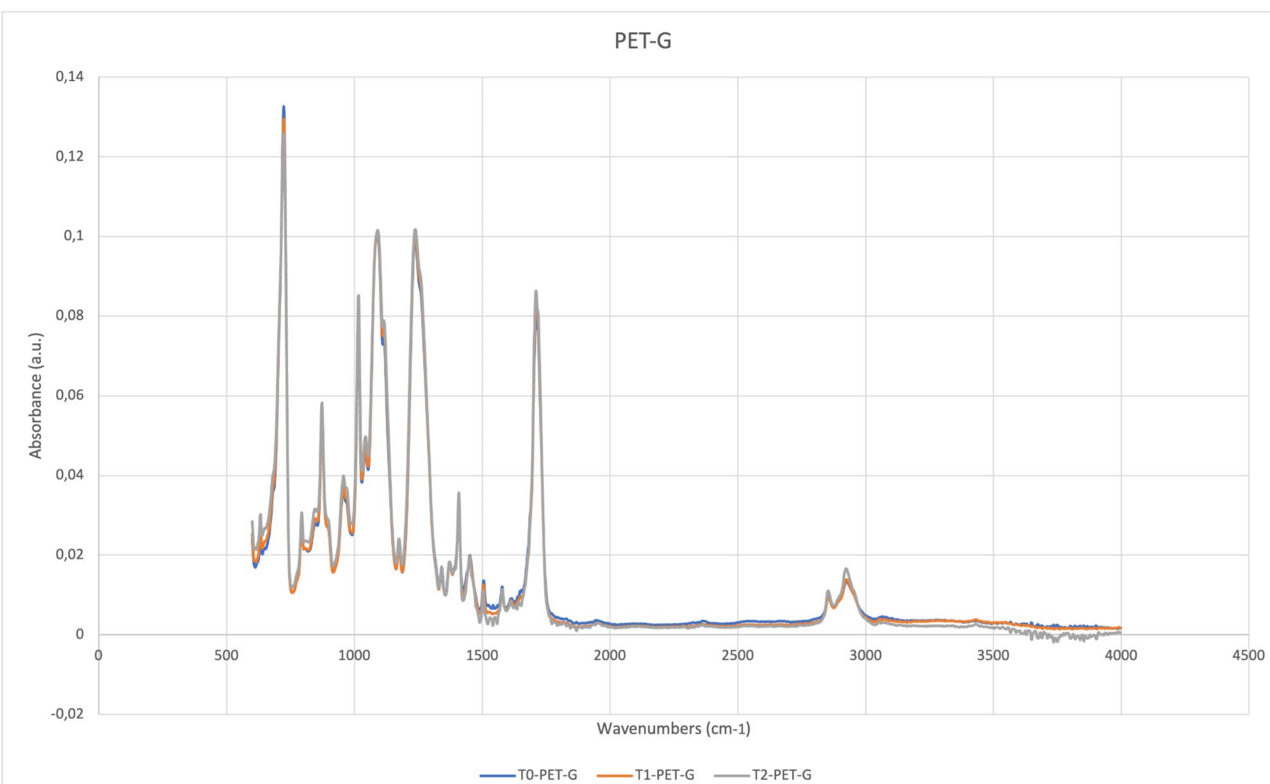

Fig. 10 Average FTIR spectroscopy spectrum of the PET-G samples at T0, T1 and T2

Our results indicate that, following immersion in artificial saliva, both TPU and PET-G specimens initially experienced a slight reduction in thickness and weight (T1). After a two-week immersion period (T2), both thickness and weight showed a minimal, non-significant increase. These results agree with Bucci et al., which observed that PET-G samples exhibited a reduction in thickness after 10 days of intraoral exposure [16].

Chemical properties

However, regarding chemical properties, studies by Jaggy et al. and Lira et al. demonstrated that polymer chains remain stable despite thermal shock from the thermoforming process or simulated salivary aging [11, 34]. The results of the present study agree with the current evidence, since the FTIR spectra remained nearly identical across all time points, indicating the preservation of chemical bonds within the polymers [22]. This spectral consistency indicates that saliva exposure does not trigger chemical alterations that could be responsible for the deterioration of the aligners' mechanical properties [20].

Mechanical properties

Maintaining the structural properties of the aligners during use is crucial for achieving planned movements in orthodontic treatment [35]. These findings are in agreement with data from a pilot study by the same research group, which showed a reduction in the elastic modulus of both materials after immersion in artificial saliva (data not shown).

This suggests that the reduction in mechanical properties could be related to changes in tribological characteristics rather than chemical modifications.

Further investigation into the correlation between surface roughness changes and mechanical properties could provide deeper insight into this topic.

Optical properties

As for optical properties, no statistically significant differences were observed when measured using a spectrophotometer after simulated intraoral use. However, PET-G exhibited approximately twice the optical dentistry of TPU at baseline, indicating that TPU is more transparent. These results align with the findings of Cremonini et al. and Lombardo et al. [31, 36], although the difference is not clinically significant.

Nonetheless, the optical properties of aligners can be affected by extrinsic chromophores from food and beverages, leading to reduced transparency [31, 37]. The dyes in substances such as coffee, tea, and red wine are primarily responsible for altering the absorbance and transmittance values of materials, rather than the saliva itself [37].

Strengths of the study

The present study adhered to European ISO guidelines for thermoplastic materials, ensuring conformity in sample selection. Furthermore, the sample size was increased by approximately 100% from previous studies conducted by Dalaie et al., resulting in a total of 8 samples [38, 39]. This increase aimed to enhance the statistical power of the study. Another strength lies in the use of an atomic force microscope for surface roughness measurements. Compared to the optical profilometer employed in previous research, atomic force microscopy offers superior resolution and sensitivity [12, 29]. Additionally, a digital electronic caliper with a resolution of 0.0005 mm was used to to ensure precise data acquisition.

Limitations of the study

A limitation of this study is the exclusive use of dumbbell-shaped specimens instead of actual aligners. Since aligner shapes vary due to differences in patients' arch morphology, achieving reproducible data would be challenging. Furthermore, the simulated salivary aging process did not include the organic components of saliva or account for the impact of chewing forces experienced during clinical use. Another limitation could be the sample size, which may affect the generalizability of the findings.

Implications for further research

The findings of the present study highlight the importance of understanding aligner material properties under intraoral conditions to optimize the predictability of clear aligners. Currently, TPU is more expensive for manufacturers than PET-G. As for surface roughness, a statistically significant difference between PET-G and TPU was found. However, further investigation is needed to determine whether surface roughness can represent a determinant factor in the clinician's decision-making process for the choice for clear aligners' manufacturing. Additional studies should also assess aligner surfaces in vivo to evaluate bacterial colonization and aligner engagement over time. Moreover, further research is needed to evaluate the cost-effectiveness of different aligner materials, ensuring an optimal balance between performance and affordability in clinical practice.

Conclusions

Upon simulated intraoral aging, the following alterations were observed in dumbbell-shaped TPU and PET-G specimens:

a) Morphological Properties: The thickness and weight of both TPU and PET-G specimens did not exhibit statistically significant changes after exposure to artificial saliva aging. Conversely, significant reductions in surface roughness were noted across all analysed parameters for both types of specimens. TPU is initially rougher than PET-G, and this disparity in roughness persists even after two weeks of intraoral aging.

b) Optical Properties: The optical density of both TPU and PET-G samples remained unchanged following artificial saliva aging.
c) Chemical Properties: No statistically significant variations were observed in the chemical composition of either material under analysis.

Take home message

The main finding of the present study is related to the statistically significant reduction of surface roughness, which affected both types of material. Furthermore, a significantly greater roughness of TPU compared to PET-G was evident in all three time points. While greater roughness may facilitate plaque accumulation, it also appears to play an important role in the retention of the aligners, a factor that is crucial for their ability to exert force on the teeth.

Abbreviations

PET-G	glycol-modified polyethylene terephthalate
TPU	thermoplastic polyurethane
PLA	polylattic acid

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Author contributions

Conceptualisation, E.S. and G.C.; methodology, E.S., G.C. and M.Pap.; software, M.Pal.; validation, L.L. and M.C.; formal analysis, M.P.; investigation, E.S., G.C. and M.Pap.; resources, M.Pal.; data curation, G.C.; writing—original draft preparation, E.S. and G.C.; writing—review and editing, G.C.; supervision, L.L and M.C. All authors have read and agreed to the published version of the manuscript.

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Data availability

The datasets used and/or analysed during the current study are available from the corresponding author on reasonable request.

Declarations

Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Competing interests

The authors declare no competing interests.

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