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DIC analysis of mechanical response of tooth aligners under simulated swallowing acts

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Abstract. In this work, the mechanical and deformation behavior of clear Polyethylene Terephthalate-glycol (PET-g) aligners, under cyclic loading was investigated using a full-field optical technique: the Digital Image Correlation. In particular, the PET-g aligners thermoformed from 0.88 mm thick discs, were subjected to cyclic compression tests for 13000 load cycles from 0 to 50 N in the atmospheric environment (~25°C). This number of cycles was chosen because it simulates, on average, the intraoral load associated with the swallowing acts that an aligner is subjected to during the time of use of 1 week. At the same time, the results from the analysis of hysteresis loops obtained by the DIC technique were compared with those obtained by the testing machine. The mechanical response of clear aligners was evaluated in terms of maximum displacement, energy loss and relative stiffness along the load direction to seven different stages of the 13000 load cycles. A comparable trend was found between the measurements obtained by Digital Image Correlation analysis and the analysis of the hysteresis loops obtained from the cyclic compression tests. Furthermore, the morphological features of the PET-g aligner at the end of the tests were analyzed by optical microscopy (OM). The OM analyses showed that the surface of PET-g aligner was affected by morphological variations such as high depressions and cracks.

Keywords: PET-g aligners, mechanical behaviour, digital image correlation technique, DIC technique, compression tests, deformation behavior

1. Introduction

In the last decades, the rising demand among adult patients, for dental misalignment problems or the treatment of malocclusion, of aesthetic devices has led to an exponential growth in the market of clear aligners [1-5]. The orthodontic treatment with these devices consists in the sequential use of clear aligners characterized by appropriate geometry and made with a thermoplastic polymeric material. Based on the specific orthodontic treatment plan, these aligners, through a controlled distribution of forces, allow gradual repositioning and reorientation of the teeth [6].

Since, the forces exerted by clear aligners on the dental arch, depend substantially on their geometry, it is necessary to make orthodontic devices that do not undergo important deformation throughout the treatment period. In addition, among the parameters that influence the quality of the force applied to the teeth, and thus the final outcome of orthodontic treatment, the mechanical properties of the manufacturing material are of fundamental importance. Generally, the desired properties for an aligner material are: biocompatibility, transparency, low rigidity, good formability, environmental stability and resistance to aging [7].

To date, PolyPropylene, PolyCarbonate, Polyethylene Terephthalate glycol, Ethylene Vinyl Acetate and Thermoplastic PolyUrethanes are just some of the thermoplastic materials available on the market for this type of application [1,8-10]. Nonetheless, only some materials among those available exhibits both before and after use of the same chemical characteristics. As a result, the mechanical and especially the optical properties of many aligner materials will be affected differently by factors, such as food colourings, masticatory stress and salivary enzymes, to which they are normally exposed in the oral cavity during the period of use [10]. Several scholars have shown that factors such as temperature, humidity, thickness, characteristics of the forming process, and time elapsed after elastic deformation can influence the deformation of aligner material under load [11,12]. Therefore, knowledge of deformation behavior is of fundamental importance not only for the proper design of aligners made from these materials but also to guarantee correct functionality during their use. Besides, the knowledge of the mechanical and deformation behaviour of the aligner can help the orthodontist to accurately define the most suitable strategy to use, simultaneously improving the patient's comfort and treatment time.

At the present time, thanks to its exceptional formability and its excellent aesthetic characteristics, the polyethylene terephthalate-glycol (PET-g) is forenumber used plastic material for the production of such devices [11,13]. Nowadays, the majority of researchers that have focused on aligners' mechanical behaviour and the effect of the intraoral environment perform tests on rectangular strips of material cut from the discs used to thermoform these devices. However, this way of evaluating the performance of aligners is entirely questionable because it does not capture the complexity of the behavior of a geometrically complex device such as a dental aligner. Therefore, unlike the works in the literature, in this research work, the effect of intraoral loading on PET-g aligners was evaluated by performing tests directly on the thermoformed aligners from 0.88 mm thick discs. Particularly, PET-g aligners were subject to cyclic compression tests for 13000 load cycles in the atmospheric environment (~25°C). Each load cycle was increased from 0 to 50 N. 13000 cycles were chosen because it simulates, on average, the intraoral load associated with the swallowing acts that an aligner is subjected to during the time of use of 1 week. Digital image correlation (DIC) [14,15] was used to investigate the cyclic compression behavior of clear aligners. This is an innovative full-field measurement technique for this type of application. This, being a contactless optical technique, allows to follow the evolution of the aligner behavior, instant by instant, taking into consideration the entire arch-aligner set of teeth.

In this research, the mechanical response of PET-g aligners was evaluated in terms of maximum displacement, energy loss (irreversible work) and relative stiffness along the load direction (y axis). These terms were derived from the analysis of the load-displacement curves obtained by the DIC technique. At the same time, a comparison of these quantities with those obtained from the analysis of the hysteresis loop of the test machine was performed to assess whether this technique is suitable to describe the aligners' behavior. Finally, the morphological features of the aligners surfaces at the end of the loading test were investigated under an optical microscope (OM).

2. Experimental Procedure

2.1. Materials

The clear aligners samples were manufactured from PET-g discs of 0.88 mm nominal thicknesses using an Erkodent® 3D vacuum machine (Figure 1b). Especially, Polyethylene Terephthalate-glycol was an Ace® Plastic produced by GAC International, made of 95% copolyester and 5% trade secret. Before thermoforming, it was necessary to make a digital dental record and then print a resin dental cast of a patient's mouth (Figure 1c). The clear thermoformed aligner is shown in Figure 1a and the overview of the occlusal plane of the 1st molar before performing the cyclic tests is reported in Figure 1d.

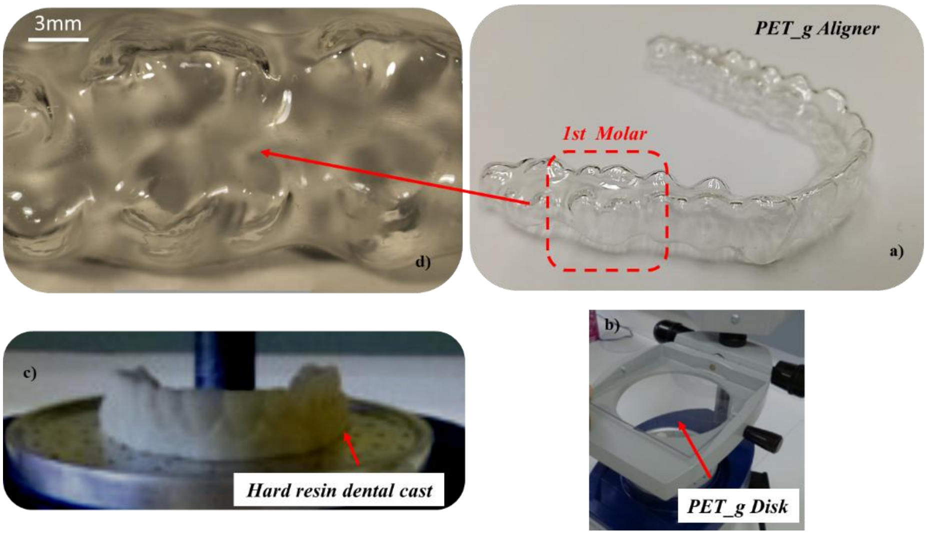

Figure 1. a) PET-g aligner sample after thermoforming, b) PET-g disc of 0,88 mm thick inserted in the support plate of the Erkodent® 3D vacuum machine used for termoformed the clear aligners c) resin dental cast of a patient's mouth and d) view macrographic of 1st molar

2.2. Setup of Cyclic Compression Test and Full-field displacement measurement

Cyclic compression test was performed at room temperature (~25°C) using an Instron 3344 (Norwood, MA, United States) electro-mechanic machine with a single column, shown in Figure 2a, equipped with the software Bluehill 2.15 and a 1 kN loading cell. The aligner was fitted on a proper hard resin dental cast which reproduces the upper dental arc and then the system was put in occlusion with the corresponding lower dental cast, as shown in Figure 2b. The cyclic load, under load control conditions, includes four stages each one lasting 1 s, visible in Figure 2c. The total number of cyclic load was calculated considering the average number of daily dental contacts during the swallowing act (1500 swallowing acts) and the time of swallowing act (1 s). So, one load cycle comprises four stages: the first in which the load increases from 0 to 50 N; the second in which the maximum load is held for 1 s; the third in which a descending ramp brings the load to 0 N; the fourth in which the sample is kept at 0 N for 1 s. The clear aligner was subjected to 14250 load cycles consecutively for 16 hours. This load history corresponds to a one-week usage of a clear aligner, considering that at certain times of the day is not worn for eating or hygiene operations. Measures were taken using a contactless full-field optical technique: Digital Image Correlation (DIC). The measurement setup, comprised the DIC system Dantec Dynamics Q400 (Dantec Dynamics A/S, Skovlunde, Denmark), the INSTRA 4D software (Dantec Dynamics A/S, Skovlunde, Denmark), the Timebox, one GigE CCD Manta cameras of 1628 x 1436 pixels (Allied Vision Technologies GmbH, Stadtroda, Germany) equipped with a high-resolution lens Xenoplan 2.8/50-0902 (Schneider) and the LED light, is represented in Figure 2a. The speckle pattern of black random dots on a white background was realised on the half of dental arc of the clear aligner as is shown in Figure 2d. Before the test the quality of the pattern was evaluated through a Matlab code, so a black/white ratio of 31% was obtained. During the test four acquisitions were taken: the first at the beginning of the test and the others respectively after 1000, 5000 and 13000 load cycles. Thanks to the full-field measurements, local displacements values were extrapolated by placing a virtual strain gauge (small area A) on the 1st molar as shown in Figure 2e. The 1st molar was chosen as the most stressed tooth because of the specific clinical conditions of the patient who has a regular dentition. DIC measurements are based on the differences between the area selected on the reference image, taken at zero load, and the subsequently images captured during the test. The INSTRA software provides the average of the displacements, $\overline{D_F}$, given by the displacement $D_{P_{i,F}}$ of each single pixel, i, contained in area A, for each F image recorded during the test:

$$\overline{D_F} = \frac{\sum_{i=0}^{n} D_{P_{i,F}}}{n} \qquad 0 \le F \le N . \tag{1}$$

Where $P_{i,F}$ is referred to the point P associated with the pixel i of the image F, n indicates the number of pixels contained in the area A and N is the number of frames recorded by the camera. Before the test, the DIC system was calibrated to reduce measurement errors as much as possible. Displacement noise-floor of 0.785 ± 0.734 µm and 0.193 ± 1.518 µm were recorded respectively along the y and the x direction using a subset size of 17 px, a step size of 13 px and ad SSD matching criterion. All the DIC hardware parameters and the DIC analysis parameters used for this experiment are well schematized in [16].

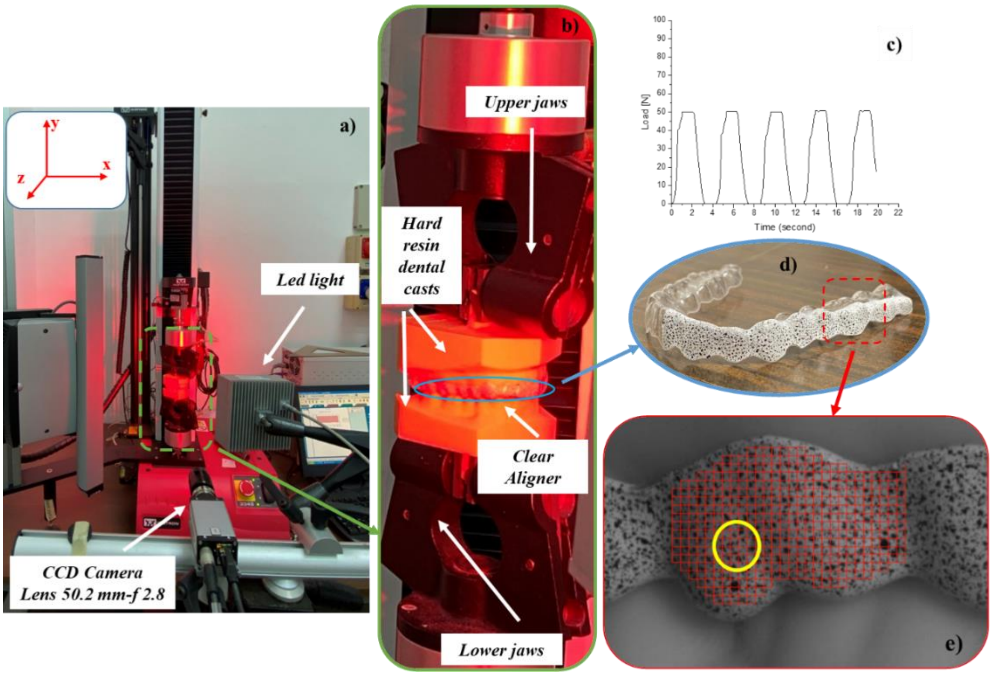

Figure 2. a) Setup of Cyclic Compression Test, b) enlargement of the green box of figure a showing the entire resin dental cast-aligner assembly, c) representation of load as a function of time during cyclic loading, d) image of aligner with speckle pattern of black random dots on a white background and e) enlargement of 1st molar showing the data analysis circular area.

2.3 Optical Microscopy (OM) Analysis

Surface morphology analysis was performed on the occlusal plane of the 1st molar by ZEISS - Axio Vert A1 optical microscopy (OM) under transmitted light. The surface' morphology of the aligners was imaged at the end of the cyclic compression test.

3. Results and Discussions

3.1. Comparison of the load–displacement hysteresis loops

Figure 3a and b show the evolution of the load–displacement hysteresis loops in the y direction (along load axis) obtained from the crosshead displacement of the testing machine and from the full-field (DIC) analysis, respectively. Specifically, seven curves describing load-displacement behaviour, are shown for each analysis technique: 2, 6, 10, 20, 1000, 5000 and 13000 loading cycles. For clarity data reported for DIC analysis, cycles from 2 to 20 were acquired in the 1st acquisition, the 1000th cycle was acquired during the 2nd acquisition, the 5000th cycle was acquired during the 3rd acquisition and the 13000th cycle was acquired during the 4th and least acquisition. Observing Figure 3a, it can be seen that as the number of cycles *n* increases, the hysteresis loops tend to shift to the left toward lower displacements. Especially is interesting to note that the amount of displacement reduction is very small during the very first few cycles. After of 20th cycle, the amount of displacement reduction tends to grow progressively up to 1000 cycles and then decrease significantly again until it stabilizes toward the last cycles. Additionally, the curves remain highly nonlinear until the end of the test and become more narrow (reduction of area of the hysteresis loops) at high cycle numbers [16-18]. With reference to the load–displacement hysteresis loops obtained from DIC technique (Figure 3b), trends comparable to those obtained from the test machine are found up to 1000 cycles. After which the curves tend to return back towards greater displacements (right shift), indicating that after the 1000th cycle the contact point of the dental crown gradually moves upwards. This is due to the fact that as cycles progress, the areas of the dental crown do not always touch in the same way but vary continuously. Therefore, the aligner undergoes the same rigid movement of the dental arches [19]. Also, unlike the loops obtained by the test machine, those obtained by the DIC technique are more linear throughout the test and tend to become narrower as the test progresses.

Therefore, it is clear that the local analysis performed with the DIC allows us to highlight phenomena that cannot be observed from the analysis of the data provided by the test machine.

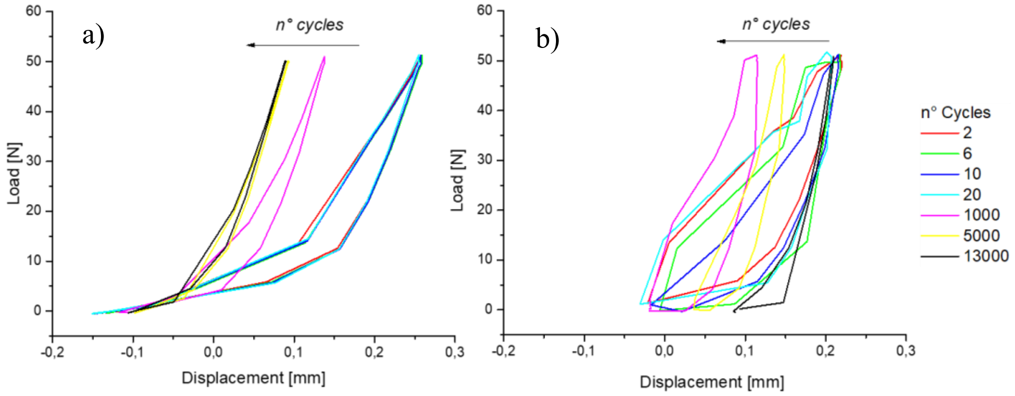

Figure 3. Comparison of the load-displacement hysteresis loops for the PET-g aligner (y direction) obtained from: a) analysis of the displacement of the crossheadand and b) the local analysis carried out with the DIC technique

3.2. PET_g mechanical behavior

The mechanical behavior of the PET_g aligner can be detailed better by determining the maximum displacement reached, the relative stiffness and the energy loss per cycle (Figure 4a-c). Furthermore, this last parameter also allows evaluating the viscoelastic nature of the thermoplastic material. In particular, the energy (N*mm) was determined by integrating the load-displacement hysteresis loops while the stiffness (N/mm) was determined as the slope of a linear regression fitting of the hysteresis loops. It can be observed from Figure 4a-c that the measurements derived from the analysis of the load-displacement loops (Figure 3) show similar trends. In particular, both curves show substantial changes from the 20th cycle up to the achievement of the 5000th cycle, after which these values tend to remain almost constant. More specifically, it can be seen that the maximum displacement decreases as n° increases (Figure 4a); while the rigidity of the aligners tends to increase significantly with increasing cycles (Figure 4b) and the energy loss (irreversible work) decreases (Figure 4c). Therefore, the reduction in max. displacement is associated with a significant increase in aligner stiffness as it is fatigued. In other words, the orthodontic thermoplastic material becomes stiffer and less viscoelastic as cycles increase. The observed stiffening effects may be due to several factors. First of all, the stiffening can be attributed to the entanglement of the polymer chain that occurs as an effect of the application of the load, and secondly to the stress generated during the mechanical compression cycle. It is known that the stresses are generated in orthodontic device by the initial deformation and they tend to cumulate with increasing the loading cycles [19]. Other hypotheses that could explain the increase in stiffness are related to the absorption of water molecules from the air (environmental humidity) during the cyclic compression test [16,20,21]. In addition, comparing the stiffness curves shown in Figure 4b, it can be seen that the stiffening values obtained by the DIC technique are greater than those provided by the testing machine. Particularly, with reference to the DIC technique, a maximum stiffness of 451 N/mm was found, while the maximum stiffness value obtained from the cyclic tests is 256 N/mm. However, the increase in stiffness measured with the DIC is 131.4% compared to that measured by the test machine which is 107.4%. On the other hand, this is completely normal as the DIC technique, based on local analysis, provides us with information regarding the actual behavior of the aligner. While the results obtained from the crosshead displacement analysis of the testing machine represent only an average behavior of the aligner, thus not grasping in detail, the behavior of the aligner that is characterized by a rather complex geometry.

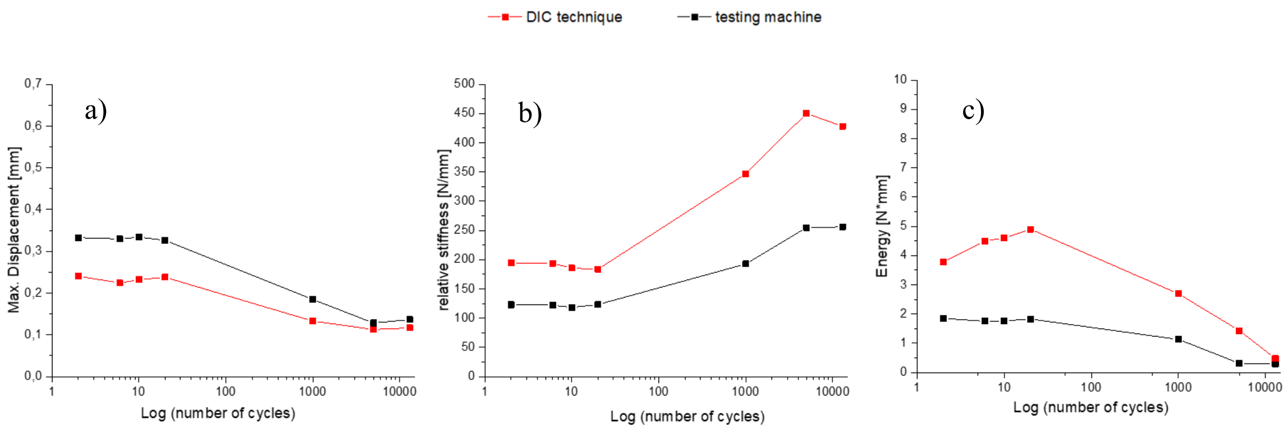

Figure 4. Comparison of the maximum displacement (a), energy loss (b) and relative stiffness (c) as a function of the log of number of cycles obtained by the two different techniques

If the displacement data recorded by the testing machine give information only along the y direction, the DIC technique allows us to obtain full-field measurements, and therefore also to know the total displacement component (which is directly related to the direction of the load distribution) and the principal compression strains. Figures 5 and 6 show the results deriving from the analysis of the total displacement component and the deformation chromatic maps (i.e. compressive strain), respectively. By analyzing Figure 5, it can be observed that the first 20 cycles are characterized by a constant total displacement component developing in the same verse and direction. In accordance with what was seen above (Figure 3), during the very first cycles, the aligner has a displacement component of about 300 µm. This value tends to decrease to about 100 µm at 1000 cycles. Interestingly, at 1000 load cycles the total displacement component is mirrored along the vertical axis. After this number of cycles, the displacement components rise again up to 240 µm always maintaining the same verse and direction. In other words, during these first cycles, the aligner undergoes a displacement relative to the cast fitting due to initial settlement. As the cycles progress, this displacement decreases, indicating that the aligner adheres to the cast. After that, for high numbers of cycles, the aligner again loses adherence with the resin dental cast walls exactly as it occurs during the stages. This loss of adherence could be associated with the aligner wear which can occur with cracks initiation and propagation.

The experimental results reported in Figure 6 show instead, that the most deformed portion of the material was the one close to the contact area with the opposite tooth (note that the most deformed bands are the purple and blue ones); whereas, on the lateral part of the tooth the entity of strain is quite slight.

It is also interesting to note that the thickness of the observed strain band corresponds perfectly to the thickness of the aligner (0.88 mm). This behavior is clearly highlighted by the graph in Figure 6e which shows the trend of the principal compressive strain along the height of the 1st molar. The curves show an almost constant value along the entire height of the tooth, from 0, close to the gum, up to about 4.5 mm, after which the curves become steep in correspondence with the contact area with the opposite tooth. In addition, it is possible to observe that as the number of cycles increases *n*, the strain band moves along the profile of the tooth, as a function of the area of contact that occurs between the crowns of the upper tooth with the lower one as the number of cycles increase.

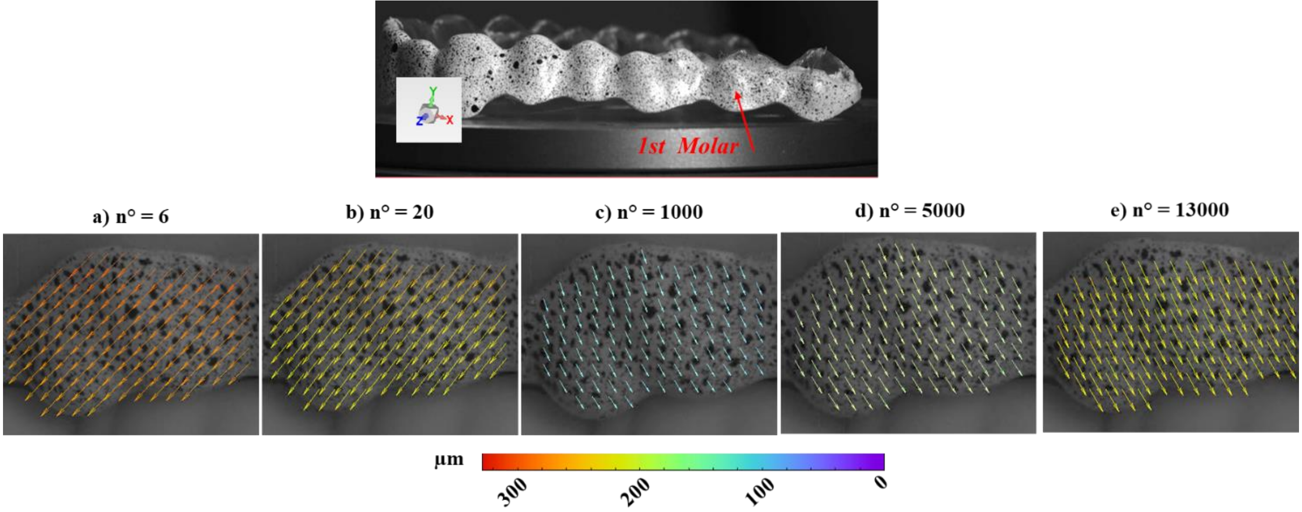

Figure 5. Total displacement direction analysis during the; a) 6nd, b) 20th, c) 1000th, d) 5000th and f) 13000th cycle.

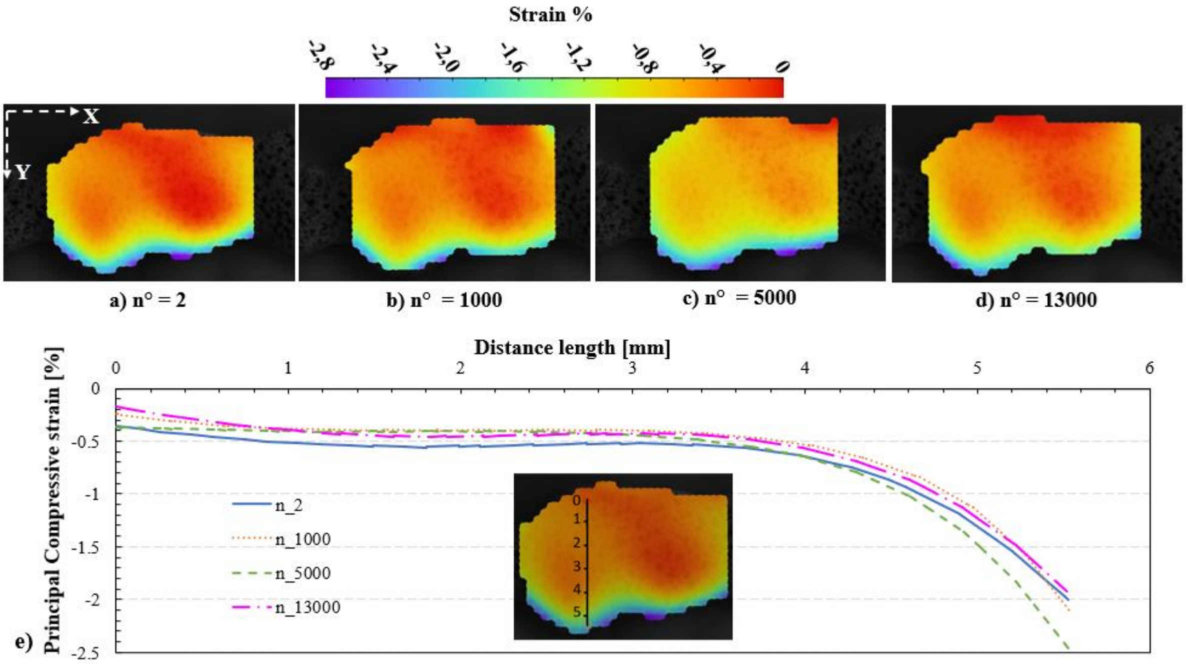

Figure 6. Principal compressive strain performed by DIC technique for the PET-g aligner during the a) 2nd, b) 1000th, c) 5000th. d) 13000th load cycle and e) trend of the principal compressive strain along the length of the tooth in the Y-direction.

Finally, for completeness, Figure 7 shows the results of the displacement analysis along the y and x-axis for the entire aligner. In order to immediately highlight the differences, a monochrome scale was used.

Note that for the chromatic scale along x, the positive direction increases to the left, while, for the one along y, the positive direction increases to the right. By observing Figure 7a-d, it is possible to infer that the largest displacements occur in the anterior part of the teeth: in the incisors. In fact, this is what really happens when the two dental arches, upper and lower, move apart and reconnect; this again confirms that the experiment is faithfully reproduced from start to finish. Furthermore, it can be observed that the displacement ranges affected by the aligner change with the cycles confirming that the crowns of the teeth touch differently during the test. Especially, in the 2nd cycle a range of 168÷468 µm can be observed, at the 1000th cycle a range of 90-327 µm (Figure 7a), at the 5000th cycle a range of 100 ÷ 366 µm (Figure 7b) and finally at the 13000th cycle a range of 185 ÷ 440 µm (Figure 7c). While with regard to the x axis (Figure 7e-h), it can be observed that the displacement is fairly constant for the entire aligner. Particularly, in the contact area of the aligner there is an average displacement of -235 µm for the 2nd cycle (Figure 7e), 86 µm for the 1000th cycle (Figure 7f), 114 µm for the 5000th (Figure 7g) and 144 µm for the 13000th cycle (Figure 7h). It should be specified that these data also include the rigid displacement component, which is important precisely in correspondence with the incisors. If the rigid displacement component is excluded, along X there is a displacement range from +40 µm to -35 µm, while along Y there is a range from 110 µm to -90 µm, with the greatest displacements reached in correspondence of the molars. As a result of the analyses seen above, it is therefore clear how the analysis performed with the DIC is able to detect and describe the real behavior of the aligner allowing at the same time to verify that the test continues according to the imposed operating conditions

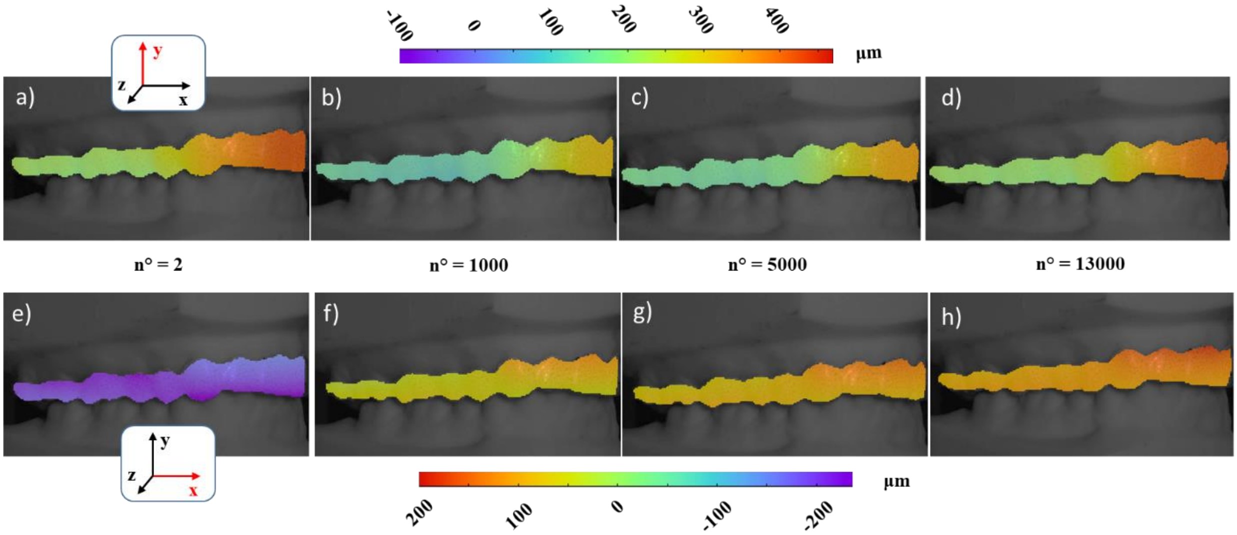

Figure 7. Displacement chromatic maps performed by DIC technique during the: a, e) 2nd, b, f) the 1000th, c, g) the 5000th and d, h) the 13000th load cycle along the load axis *y* and *x*, respectively.

3.3. Optical Microscopy characterization

The OM analysis allowed to corroborate the above results. Figure 8 shows the micrographs of the occlusal plane of the 1st molar. It can be observed that the surface of the aligner is strongly degraded following the 13000 load cycles. It is interesting to note that the most worn area is the central one of the tooth. In particular, in this area, the surface is characterized by the formation of an elevated depression (fracture) and cracks that branch out towards the dental crown starting from the fractured area. The presence of these cracks indicates high degradation kinetics in the central part of the tooth. In addition, it is worth noting that all around the crack surface there is the presence of numerous crazes. It was also observed that the density and size of these crazes decrease as one moves away from the crack surface. While along the crown of the tooth small micro-voids of different morphology and with sizes of 20-50 µm were observed. The micro-voids with acicular morphology observed as well as large voids are generally preferential sites for the nucleation of the fatigue crack, due to the local intensification of the stress dependent on the size and morphology of the voids. The origin of this damage lies in the fact that the elasticity degree of the PET-g thermoplastic material is not enough to counteract the stresses induced by the occlusal load for an exercise period of 13 days. The presence of this degree of wear could compromise the correct transmission of orthodontic forces. Furthermore, the observations under the light microscope show important chromatic variations all around the fractured area. This phenomenon is known as birefringence and is due to the cyclic compressive load which induces internal stresses and important deformations within the aligner.

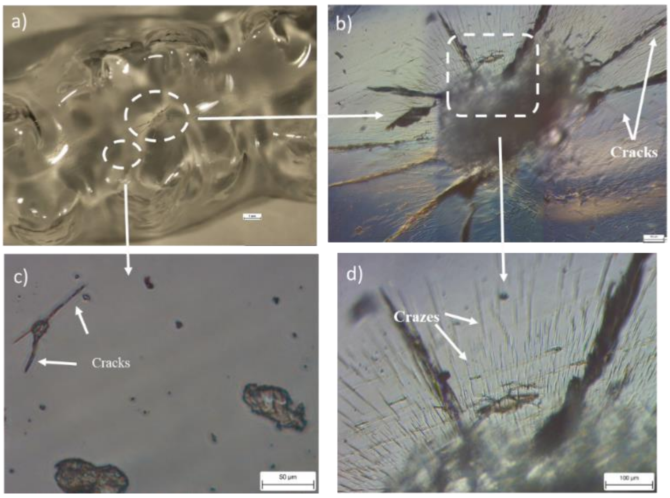

Figure 8. a) overview of the occlusal plane of 1st molar of PET-g aligner at the end of the 13000 load cycles, b) enlargement of the central area of the tooth showing high depressions and cracks, c) enlarged image of the spot fringe of Figure a and d) enlarged image of the spot fringe of Figure b showing the crazes around the crack surface

4. Conclusion

The study of mechanical response of 0.88 mm thick PET-g thermoformed aligners using the DIC technique has brought the following evidences:

- A good correlation was found between the measurements obtained by full-field (DIC) analysis and the analysis of the hysteresis loops obtained from the cyclical tests. Moreover, the DIC analysis helps to understand phenomena that occur in aligner during usage.
- The hysteresis loops reflect a ratcheting displacement reduction in the aligners during loading cycles. At the same time, the orthodontic thermoplastic material become stiffer and less viscoelastic as the aligner was fatigued. The loss of the viscoelastic behavior of thermoplastic material is evidenced by the decrease in viscoelastic energy loss per cycle.
- Local displacement maps show that the quantities derived from the load-displacement cyclic curves, such as energy and stiffness, are influenced not only by the mechanical behavior of the material itself, but also by the complexity of the loading distribution.
- The DIC technique has been found to be an excellent optical method for determining local displacements of an aligner under load, which is fairly new in this field
- The OM analyses showed that the surface of PET-G aligner was affected by significant morphological variations such as high depressions and cracks indicating a significant reduction of functionality after 7 consecutive days of wear.
- From a medical point of view, it is necessary to carefully evaluate possible use of the aligners for a further week due to considerable degradation of the surface

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