Research paper

Fracture origin and crack propagation of CAD/CAM composite crowns by combining of *in vitro* and *in silico* approaches

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ABSTRACT

Purpose: Fractographic analysis has been used to investigate the fracture behavior of Computer-aided design/computer-aided manufacturing (CAD/CAM) composite crowns by subjecting them to compression tests. However, it is difficult to investigate details of the fracture, including its initiation and propagation, using *in vitro* tests. The aim of this study was to determine the fracture origins and the order of crack initiation of CAD/CAM composite crowns using *in silico* nonlinear dynamic finite element analysis (FEA).

Material and Methods: The following materials were used: Cerasmart (CS), Katana Avencia Block (KA), and Shofu Block HC (HC) as CAD/CAM crowns, Panavia SA Cement Plus (SA) as a luting material, and Clearfil DC Core Plus (DC) as an abutment. The elastic moduli and fracture strain of each material were obtained from the stress–strain curve of *in vitro* three-point bending tests. The fracture origins and order of crack initiation of the materials were determined by *in silico* nonlinear dynamic compression analysis. Load-displacement curves were statistically compared with the results of the *in vitro* compression tests (Pearson's correlation test, α=0.05).

Results: The nonlinear dynamic FEA demonstrated that crack initiation was primarily observed near the lingual side of the CAD/CAM crowns and immediately propagated to the central fossa. The models were fractured following the *in vitro* fracture strains, showing the same order for the products tested (CS/KA/HC, SA, and DC). Load-displacement curves with the use of CS, KA, and HC were significantly correlated to the corresponding *in vitro* compression tests results (CS: r=0.985, $p<0.05$, KA: r=0.987, $p<0.05$, and HC: r=0.997, $p<0.05$).

Conclusions: The *in silico* model established in this study clarified the crack initiation of the CAD/CAM composite crowns and the order of crack initiation among the investigated products, suggesting that the present approach is useful for analyzing the fracture behavior of CAD/CAM composite crowns in detail.

KEYWORDS

CAD/CAM resin composites, Fracture initiation, Crack propagation, Compressive tests, Finite element analysis

1 INTRODUCTION

Computer-aided design/computer-aided manufacturing (CAD/CAM) technologies have introduced a new era and accelerated the evolution of dental restorations (Rekow, 2020; Sulaiman, 2020). CAD/CAM-fabricated resin composite blocks (RCBs) containing nano-filler particles are available for use in anterior (Zacher et al., 2020) and posterior (Yamaguchi et al., 2018a) restorations. The pre-polymerized resin matrix under high pressure or high temperature (Ruse and Sadoun, 2014), providing stable and excellent mechanical performance such as flexural strength (Dry: ~206 MPa, Aged: ~172 MPa (Lucsanszky and Ruse, 2020)), hardness (62–102 VHN (Lawson et al., 2016)), Weibull modulus (11.2–31.5 (Choi et al., 2019)), and fracture toughness (~1.47 MPa·m$^{1/2}$ (Lucsanszky and Ruse, 2020)) compared with conventional photo-polymerized resin composites used in fillings. Additionally, less antagonist enamel wear (0.056-0.061 mm^3) of CAD/CAM RCBs compared with polymer infiltrated ceramics (0.108-0.280 mm^3) and glass ceramics (0.276-0.420 mm^3) has been reported (Lawson et al., 2016). CAD/CAM RCBs are attracting attention as an alternative material to such ceramics because their cost is less [4].

Given the recent market releases of CAD/CAM RCBs, only a few long-term evaluations of CAD/CAM composite crowns are available (Rosentritt et al., 2019). Debonding and fracture of CAD/CAM composite crowns have been reported as the main complications of implant-supported crowns (Lohbauer et al., 2017) and removable partial denture abutment premolar teeth (Miura et al., 2019). Artificial intelligence technology established in our previous study demonstrated considerably good performance in terms of predicting the debonding probability of CAD/CAM composite crowns (Yamaguchi et al., 2019). The fracture of CAD/CAM composite crowns should be investigated to ensure the longevity.

As observed clinically, crack initiation and chipping of CAD/CAM ceramic crowns occur mostly at the crown margins (Scherrer et al., 2008). The edge strength is a useful criterion to characterize the chipping force close to the edge specimens such as the margin of crowns (Pfeilschifter et al., 2018). Fractographic analysis has been used to investigate the fracture behavior of CAD/CAM composite/ceramic crowns, including the direction of the crack propagation (dcp), hackle, and arrest line (Lohbauer et al., 2017; Scherrer et al., 2008; Yamaguchi et al., 2018a; Zacher et al., 2020). However, it is difficult to determine the crack initiation and crack propagation by *in vitro* tests.

In silico finite element analysis (FEA) is used to assess the crack initiation of CAD/CAM composite crowns/ceramics from stress or strain concentrations (Dal Piva et al., 2018; Dartora et al., 2019; Yamaguchi et al., 2018a). However, there is no way to represent crack propagation by conventional static FEA without changes in time. Our previous study confirmed that *in silico* non-linear dynamic FEA could predict the fracture toughness of CAD/CAM RCBs, reflecting the *in vitro* fracture behavior (Karaer et al., 2020). By combining *in vitro* tests and *in silico* non-linear dynamic FEA, the crack initiation and crack propagation of a CAD/CAM composite crown specimen subject to *in vitro* compression tests may be clarified.

The aim of this study was to determine the crack initiation and order of fracture of each component during an *in vitro* compression test of CAD/CAM composite crowns by combining *in vitro* tests and *in silico* non-linear dynamic FEA.

2 MATERIALS AND METHODS

2.1. CAD/CAM resin composite crowns specimens

The materials for the CAD/CAM resin composite crown specimens for *in vitro* compression tests were Cerasmart (CS, GC, Tokyo, Japan), Katana Avencia Block (KA, Kuraray Noritake Dental, Tokyo, Japan), and Shofu Block HC (HC, Shofu, Kyoto, Japan) as CAD/CAM crowns; Panavia SA Cement Plus (SA, Kuraray Noritake Dental) as a luting material; and Clearfil DC Core Plus (DC, Kuraray Noritake Dental) as an abutment. The material composition of the CAD/CAM resin composites are summarized in Table 1.

2.2.*In vitro*/*in silico* three-point bending tests

In vitro three-point bending tests of the CAD/CAM resin composites (4.0- × 1.2- × 14.0-mm specimen, n=10), luting material and abutment (2.0- × 2.0- × 25.0-mm, n=10) were conducted after the samples were stored in water for 24 h. The samples were tested using a universal testing machine (EZ-SX, Shimadzu, Kyoto, Japan) with a 1.0-mm/min crosshead speed. The flexural moduli and fracture strains were determined by the obtained stress–strain curves. The density of each material was calculated by dividing the volume obtained by micro-CT analysis (R_mCT2, Rigaku, Tokyo, Japan) by the weight. The flexural modulus and elastic modulus were not equal. By using flexural modulus as the initial elastic modulus of the *in silico* non-linear dynamic three point bending analysis (LS-DYNA, LSTC, Livermore, CA, USA), the *in silico* stress–strain curve was obtained and compared with the corresponding *in vitro* curve. The initial elastic modulus was repeatedly updated until both curves converged and the elastic modulus of each material was obtained (Karaer et al., 2020). The maximum principal strain reflecting to the fracture strain was used as the failure criteria (Yamaguchi et al., 2018b). The Poisson's ratio of each material was set to 0.38 according to that of dental composites (Greaves et al., 2011).

2.3. *In vitro*/*in silico* single compression tests

In vitro compression tests were conducted for each material (n=3) after specimens were stored in water for 24 h. Testing was conducted using a universal testing machine (AGS-500D, Shimadzu, Kyoto, Japan) with a 0.5-mm/min cross head speed. The preparation of the CAD/CAM resin composite crowns specimens were previously described (Yamaguchi et al., 2018a). The occlusal surface and margin were designed to be greater than 1.5 mm and 1.0 mm, respectively. The taper angle of abutment ranged from 6° to 10°. The cement layer was homogeneously seated under the crown with a minimum thickness of 50 μm (Gressler May et al., 2015). The load-displacement curves after *in vitro* single compression tests were obtained and the fractured specimens were observed with stereomicroscopy (SMZ-745T, Nikon, Tokyo, Japan). All FEA models of the indenter, crown, luting material, abutment, acrylic resin, and polyvinyl chloride (PVC) tube were designed from scanned stereolithography data (Fig. 1) of the *in vitro* compression tests and analyzed using *in silico* non-linear dynamic FEA software (LS-DYNA). The PVC tube was fixed as indicated by yellow tetrahedrons (Fig. 1). Axial displacements (1.0 mm) along to tooth axis were applied to the occlusal surface of the crown by the indenter, and the crack initiation and order of the fracture were analyzed. The number of elements for the indenter, crown, luting material, abutment, acrylic resin, and PVC tube were 10625, 105467, 37774, 141983, 124229, and 30254. All analysis was conducted under dynamic explicit method. The crown, luting material, and abutment were defined as the piecewise linear plastic material (MAT_024) using the effective stress-strain curve according to each material. The indenter was defined as the rigid material (MAT_020). The acrylic resin and PVC tube were defined as the kinematic plastic material (MAT_003).

2.4. Statistical analysis

Load-displacement curves obtained by *in vitro* compression tests were statistically compared with the results of the *in silico* compression analyses by Pearson's correlation test (PASW Statistics 18, IBM, Somers, NY, USA). *P*-values of less than 0.05 were considered statistically significant.

3. RESULTS

3.1. Physical properties of the CAD/CAM composite crown specimens

Load-displacement curves obtained from the *in vitro*/*in silico* compression tests are shown in Fig. 2. The elastic moduli, densities, fracture strains, and fracture stresses of CS, KA, HC, SA, and RC are summarized in Table 2. The fracture stress corresponding to the fracture strain of each material obtained from the *in vitro* three-point bending test was used as fracture criteria for the *in silico* compression analysis.

3.2. Crack initiation and crack propagation

Non-linear dynamic FEA demonstrated that the fracture origin was primarily near the lingual side of the outside surface in CAD/CAM crowns, which immediately propagated to the central fossa (Video 1, Video 2, and Video 3). The models were fractured following *in vitro* fracture strains, showing the same order for the products tested (CS/KA/HC, SA, and DC). Load-displacement curves with the use of CS, KA, and HC, as shown in Fig. 2, were significantly correlated to the *in vitro* compression tests results (CS: r=0.985, $p<0.05$, KA: r=0.987, $p<0.05$, and HC: r=0.997, $p<0.05$). The *in silico* curve could be separated into two phases. In the first phase, the crack initiation was observed at the lingual side of each CAD/CAM composite crown. In the second phase, the crack initiation was immediately propagated to the central fossa and lingual cusps.

3.3. Fracture pattern of the CAD/CAM composite crown specimens

Figure 3 shows the fracture pattern of the *in silico* compression tests for CS, KA, and HC with maximum principal stress distribution from the occlusal surface at each time point. Figure 4 shows the stereoscopic images of the occlusal surface after *in vitro* compression tests for CS, KA, and HC. Crack initiations were observed at the lingual side for all CAD/CAM composite crowns. At that time, there was no fracture in the cement layer or abutment. The abutment in the lingual cusp was fractured and two lingual cusps were separated from the main body of the CAD/CAM composite crowns (Fig. 5). The *in vitro* and *in silico* compression test fracture patterns of each CAD/CAM composite crown matched.

4. DISCUSSION

An *in silico* model of CAD/CAM composite crown specimens subject to *in vitro* compression tests was successfully developed without material waste to clarify the crack initiation and order of fracture of CAD/CAM composite crowns. Crack initiation was observed at the near lingual side of the CAD/CAM composite crowns despite lower fracture stresses of the luting material and abutment than the crowns, suggesting that the stress concentration exerting crack initiation was controlled by tensile stress instead of compressive stress.

Load-displacement curves obtained from *in silico* compression tests were divided into two phases and those of the *in vitro* tests were one phase. The sampling rate of the universal testing machine used in the *in vitro* compression tests was 0.01 s and 10 times slower than those of the *in silico* non-linear dynamic compression analysis. Therefore, the *in silico* non-linear dynamic FEA could clarify two phases and have possibility to find the unknown fracture phenomenon. The velocities of the stress propagation (Yamaguchi et al., 2014) of CA, KA, and HC that were 2,650 m/s, 2,748 m/s, and 2,636 m/s, respectively, which suggest that the velocity of the crack propagation was lower than those velocities. The discrepancy between *in vitro* and *in silico* curves was confirmed. The acrylic resin supporting the crown specimen was defined as the plastic kinematic material using elastic modulus, density, and Poisson's ratio while the crown, luting material, and abutment were defined as the piecewise plastic material using effective stress-strain curve obtained from *in vitro* results. The material property of acrylic resin might be one of reasons for the discrepancy in case of the assembled components and further investigation will be required.

Regarding long-term evaluations, the fatigue behavior of the CAD/CAM composite crowns indicated the fracture load after single compression tests did not match the order of increase in reliability after the fatigue tests because of the different monomer compositions of the crowns (Yamaguchi et al., 2018a). However, similar fracture patterns of each CAD/CAM composite crown were observed between the single compression tests in this study and the fatigue tests in a previous study (Yamaguchi et al., 2018a) even to both tests were different loading condition. The wear scars of the CAD/CAM resin composites uniformly increased and became round craters after sliding contact wear (Wendler et al., 2020), suggesting that the center of the contact points at the occlusal surface is not much change. These results suggest that *in silico* non-linear dynamic FEA of CAD/CAM composite crowns is possibly able to predict crack initiation and crack propagation to contact points corresponding to clinically relevant occlusal contacts such as sliding contact (El Zhawi et al., 2016). The predicted fracture patterns will become crucial indications to develop new CAD/CAM RCBs.

Under the same preparations, HC with the lowest elastic modulus indicated the first order of fracture among the three CAD/CAM composite crowns. However, crack initiation was still observed at the crown instead of the luting material or abutment. Owing to the low elastic modulus, CAD/CAM composite crowns have bonding failure from the zirconia abutments in 80% of cases within the first year of clinical service (Schepke et al., 2016). The size of the silica fillers loaded into HC ranged from 2 μm to 15 μm, and those in CS and KA were 20 nm and 40 nm, respectively. The smaller filler particles enhanced the elastic modulus of the CAD/CAM RCBs (Yamaguchi et al., 2017), which prevents bonding failure. The interface between the crowns and luting material, and the luting material and abutment were perfectly bonded as boundary conditions in the *in silico* non-linear dynamic FEA. Low silane coupling ratios decreasing the elastic modulus of the CAD/CAM resin composites (Lee et al., 2020) and boundary conditions reflecting the hydrolysis of silane coupling should be implemented as further study.

Crack initiation and crack propagation on the nano/micro scale level have not yet been clarified. The combination of multi-scale analysis (Yamaguchi et al., 2017) and *in silico* non-linear dynamic FEA (Karaer et al., 2020) can achieve direct observation of the fracture behavior of composites with nano-filler at the nano/micro scale level (Lee et al., 2019).

A machine learning algorithm is under development to identify optimal material compositions for extending the longevity of CAD/CAM resin composites. The composition of commercially available CAD/CAM resin composites are limited for use as input for machine learning. The establishment of new artificial intelligence technologies in dentistry (Grischke et al., 2020) with only the current limited data has still attracted attention to the challenging development issues of innovative materials and contributes to achieving the healthcare mission of Japan’s Society 5.0 for sustainable development goals (Fernandez-Luque and Imran, 2018; Vinuesa et al., 2020).

5. **CONCLUSIONS**

The *in silico* model established in this study clarified the crack initiation of CAD/CAM composite crowns and the order of crack initiation among the tested products, suggesting that the present approach is useful to analyzing the fracture behavior of CAD/CAM composite crowns using various preparation designs, loading conditions, and occlusal contacts that coincide with clinical situations.

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TABLES

Table 1. Material compositions of the computer-aided design/computer-aided manufacturing (CAD/CAM) resin composites. Bis-MEPP: 2,2-Bis [4-(methacryloxy ethoxy)phenyl]propane, UDMA: urethane dimethacrylate, NPG: Neopentyl Glycol Dimethacrylate, TEGDMA: triethylene glycol dimethacrylate

Product name	Code	Manufacturer	Composition		
			Monomer	Filler	Filler (wt%)
Cerasmart	CS	GC, Tokyo, Japan	Bis-MEPP, UDMA, NPG	SiO_2 (20 nm), Ba glass (300 nm)	71
Katana Avencia Block	KA	Kuraray Noritake Dental, Niigata, Japan	UDMA, Methacrylate monomers	SiO_2 (40 nm), Al_2O_3 (20 nm)	62
Shofu Block HC	HC	Shofu, Kyoto, Japan	UDMA, TEGDMA	Silica filler (2–15 μm), Fumed silica (10–40 nm), Zirconium silicate (1–10 μm)	68

Table 2. Physical properties of the CAD/CAM composite crown specimens.

Code	Elastic modulus (MPa)	Density (g/cm^3)	Fracture strain	Fracture stress (MPa)
CS	7300	1.946	0.0256	150
KA	6700	1.661	0.0279	151
HC	6000	1.617	0.0211	118
SA	5000	2.144	0.0221	53
RC	8000	2.013	0.0147	74

FIGURE LEGENDS

Figure 1. Computer-aided design/computer-aided manufacturing (CAD) models and occlusal contacts (red circles) of the *in silico* non-linear dynamic finite element analysis. PVC tube was fixed as indicated by yellow tetrahedrons.

Figure 2. Load-displacement curves obtained by *in vitro*/*in silico* compression tests and maximum principal stress distribution of the occlusal surface for (a) Cerasmart (CS), (b) Katana Avencia Block (KA), and (c) Shofu Block HC (HC) *In silico* curves were separated into two phases. Crack initiation was observed at the lingual side in Phase 1. Crack initiation was immediately propagated to the central fossa and lingual cusps in Phase 2. The stress concentration was released after Phase 1.

Figure 3. Maximum principal stress distribution during crack propagation at each axial displacement of the indenter for (a) CS, (b) KA, and (c) HC.

Figure 4. Stereoscopic images of the fracture patterns at the crown after *in vitro* compression tests for (a) CS, (b) KA, and (c) HC.

Figure 5. Order of crack initiation during *in silico* compression tests in CS. Time lapse images from left to right. The upper series indicates the crack propagation of the crown specimen. The lower series indicates the crack propagation of the luting material and abutment at the same time point corresponding as the upper series.

VIDEO LEGENDS

Video 1. Crack initiation and crack propagation of the occlusal surface for Cerasmart.

Video 2. Crack initiation and crack propagation of the occlusal surface for Katana Avencia Block.

Video 3. Crack initiation and crack propagation of the occlusal surface for Shofu Block HC.