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CAD-CAM resin composites: Effective components for further development

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ABSTRACT

Objective: This paper summarizes the effective components of computer-aided design and computer-aided manufacturing (CAD-CAM) resin composites that contribute to achieving greater mechanical properties and further development.

Methods: In silico multi-scale analysis, *in silico* nonlinear dynamic finite element analysis (FEA), and artificial intelligence (AI) were used to explore the effective components of CAD-CAM resin composites. The effects of the filler diameter and silane coupling ratio on the mechanical properties of CAD-CAM resin composites have been clarified through multi-scale analysis. The effects of the filler contents, and filler and monomer compositions have been investigated by AI algorithms. The fracture behavior of CAD-CAM composite crown was analyzed using *in silico* non-linear dynamic FEA. The longevity of CAD-CAM composite crown was assessed through step-stress accelerating life testing (SSALT).

Results: As the filler diameter decreases, there is an increase in elastic moduli and compressive strengths at the macroscale. At the nanoscale, a decrease in the filler diameter results in a decrease in the maximum value of the maximum principal strain. When the silane coupling ratio decreases, there is a decrease in the elastic modulus and compressive strength. According to the exhaustive search and feature importance analysis based on the AI algorithm, the combination of certain components was narrowed down to achieve a flexural strength of 269.5 MPa. The *in silico* non-linear FEA successfully detected the sign of the initial crack of the CAD-CAM composite molar crown. The SSALT revealed that CAD-CAM resin composite molar crowns containing nanofillers with a high fraction of resin matrix demonstrated great longevity.

Significance: This paper summarized the effective components of CAD-CAM resin composites for their further development. The integration of *in vitro* and *in silico* approaches will expedite the advancement of CAD-CAM resin composites, offering benefits such as time efficiency and reduction of material waste for researchers and manufacturers.

1. Introduction

The success of computer-aided design and computer-aided manufacturing (CAD-CAM) technologies, led by early pioneers such as Mörmann [1], Duret [2], and Rekow [3,4] in the late 1980 s, has dramatically evolved CAD-CAM materials used in dentistry over the past 40 years. These materials include yttria stabilized tetragonal zirconia polycrystals [5,6], lithium silicate glass ceramics [7], and CAD-CAM resin composites [8].

The first machinable CAD-CAM resin composites were fabricated by factory polymerization, and their mechanical properties have been improved through polymerization under varying temperatures and pressures, compared to conventional resin composites for filling [9]. Further improvements in the mechanical properties of CAD-CAM resin composites were achieved through high pressure and temperature polymerization [10]. In 2014, Okada *et al.* [11] invented the filler press and monomer infiltration method to increase the nano-filler content of CAD-CAM resin composites.

In Japan, the restoration of premolars using CAD-CAM composite crowns has been covered by the National Health Insurance system since 2014 [12], and this coverage has been expanded to include the restoration of the first molars in 2017 and the anterior teeth in 2020.

However, despite the evolution of CAD-CAM resin composites and manufacturing techniques, crown fractures and chipping can still occur

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under clinical service, resulting in a limited lifespan for restorations [12,13]. Additionally, CAD-CAM composite crowns cemented on human dentin tend to induce debonding within six months [12]. According to a retrospective cohort study over four years, 106 out of 362 crowns showed complications, with crown debonding being the most frequent (74.5%), followed by crown fracture (4.7%) and chipping (1.9%) [12]. The main factors for debonding were the vertical dimension of the abutment teeth, the taper of the abutment teeth, and the thickness of the crown occlusion surface [14]. The occlusal load during chewing, in combination with a low elastic modulus or insufficient occlusal thickness of the CAD-CAM composite crown, leads to transverse expansion, which tends to spread the crown margin, leading to the destruction of the adhesive interface [15,16]. Therefore, improving the mechanical properties of CAD-CAM resin composites has always been a topic of great interest.

This paper summarizes the effective components of CAD-CAM resin composites that contribute to achieving greater mechanical properties and further development.

2. *In silico* approaches in dentistry

To explore the effective components of CAD-CAM resin composites, an *in silico* approach, which involves the use of computer simulation, is useful. This approach can save time and reduce the waste of *in vitro* testing materials that often results from the trial-and-error approach.

Multi-scale analysis, a coupled method for analyzing physical properties or behaviors across different scales, has been used to predict the mechanical properties of CAD-CAM resin composites [17]. Through homogenization, the mechanical properties of CAD-CAM resin composites can be predicted from their nanostructure. This multi-scale analysis is utilized to compare factors such as filler size, composition, and the coupling condition with the resin matrix. By localization, the points of crack initiation at the nanoscale can be predicted by the stress or strain distribution in the CAD-CAM resin composites at the macroscale.

Finite element analysis (FEA) is widely used to assess stress or strain distribution and is a powerful tool for predicting the points of fracture initiation in CAD-CAM composite crowns [18]. However, conventional static FEA or fractographic analysis does not provide a way to represent fracture behavior such as crack propagation or the order of fracture. Thus, Yamaguchi *et al.* [19] have established an *in silico* non-linear dynamic FEA to mimic the *in vitro* fracture behavior observed in a three-point bending test. The combination of *in vitro* and *in silico* approaches is useful for analyzing the fracture behavior of CAD-CAM composite crowns using various preparation designs, loading conditions, and occlusal contacts that coincide with clinical situations [20].

Artificial intelligence (AI) technologies have become widely accepted in society and have been preliminarily implemented in dentistry [21,22]. Machine learning (ML), a subfield of AI, is a powerful tool for finding meaningful regularities in high-dimensional data, which allows for predictions of unknown data [23]. ML has recently become a major tool in the Materials Informatics (MI) research field and has been used for predicting material properties as a solution to a direct problem from unknown features (compositions, experimental conditions, *etc.*) [24].

3. Components of CAD-CAM resin composites

As shown in Fig. 1, factors such as the filler diameter, the silane coupling ratio with the resin matrix, filler contents, and filler and monomer compositions can influence the mechanical properties of CAD-CAM resin composites.

The effects of the filler diameter and silane coupling ratio on the mechanical properties of CAD-CAM resin composites at both the nanoscale and macroscale have been clarified through homogenization and localization. As the filler diameter decreases (from 100 nm to 20 nm),

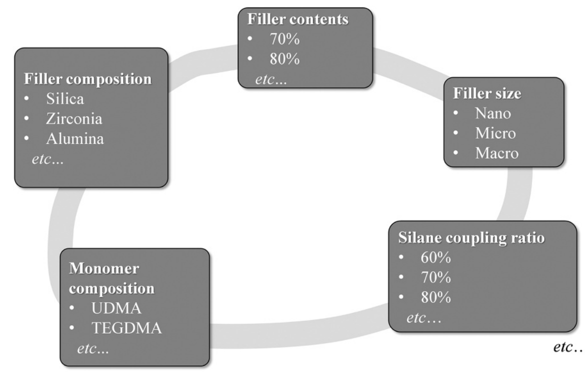

Fig. 1. Schematic illustration of the components of CAD-CAM resin composites. UDMA: urethane dimethacrylate, TEGDMA: triethylene glycol dimethacrylate.

there is an increase in elastic moduli and compressive strengths, while Poisson's ratios decrease [17] at the macroscale. At the nanoscale, a decrease in the filler diameter results in a decrease in the maximum value of the maximum principal strain [17].

When the silane coupling ratio (the ratio of filler surface coverage) decreases (from 100% to 75.5%), there is a decrease in the elastic modulus and compressive strength [25]. The relationship between the silane coupling ratio and the compressive strength is non-linear, suggesting that there is potential for improving the compressive strength by increasing the silane coupling ratio to over 94.4% [25].

The functionalization of fillers with thiourethane oligomer silanes [26] could potentially serve as an alternative to functionalization with 3-methacryloxypropyl trimethoxysilane (γ-MPS), which is the gold standard silane coupling agent in dentistry.

Lee *et al.* [27] developed an *in vitro* and *in silico* approach to predict the silane coupling ratios of CAD/CAM resin composites. After immersing a CAD-CAM resin composite (Katana Avencia Block, Kuraray Noritake Dental, Niigata, Japan) in water for seven days, the predicted silane coupling ratio decreased from 78.2% to 68.4%, suggesting that 9.8% of the silane coupling layer was hydrolyzed [27]. A hydrophobic silane coupling agent [28] may be useful in inhibiting the degradation of CAD-CAM resin composites.

Concerning filler contents, Nguyen *et al.* [29] conducted an analysis on experimental CAD-CAM resin composites and affirmed that an increase in filler content led to enhanced mechanical properties. Ling *et al.* [30] reported that a relatively high loading (82.5 wt%) of a novel experimental block also augments flexural strength. It is important to note that in literature, filler content is occasionally represented in volume fraction and predominantly in weight percentage. This inconsistency in measurement units hinders direct comparisons among different products.

In relation to the filler compositions, fillers can be synthesized from various raw materials that contain elements such as Si, O, Al, Ba, Zr, and C [31–33]. This is based on both findings from literature and technical information provided by individual manufacturers. However, only a limited number of studies have explored the influence of specific filler types on the mechanical properties of CAD-CAM resin composites [23].

With respect to monomer compositions, Nguyen *et al.* [29] reported that when fillers were kept constant, urethane dimethacrylate (UDMA) used independently exhibited superior flexural strength compared to a mixture of different ratios of UDMA and triethylene glycol dimethacrylate (TEGDMA). Furthermore, Szczesio *et al.* [34] suggested that monomer mixtures of UDMA/ ethoxylated bisphenol A-glycol dimethacrylate (Bis-EMA)/TEGDMA are characterized by higher flexural strength compared to UDMA/TEGDMA. Li *et al.* [23] successfully predicted the flexural strength of CAD-CAM resin composites and identified the effective components that affected flexural strength using a ML approach on an available data set. According to the exhaustive search and feature importance analysis, the combination of certain components was narrowed down to achieve a flexural strength of 269.5 MPa. The corresponding chemical compositions for the flexural strength mentioned above were SiO_2, barium glass, methacrylate mixed filler, with or without Al_2O_3 for fillers, and UDMA used independently for monomers. At the same time, the filler content ranged from 82 to 85 wt %.

The overall relationship between filler content, types of fillers, and monomers used in relation to the flexural strength of CAD-CAM resin composites seems to present a non-monotonic and nonlinear problem that necessitates further investigation. The ML approach, along with *in vitro* experiments, holds significant potential as a crucial tool for identifying effective components to modify the mechanical properties of CAD-CAM resin composites, provided that a sufficient dataset is available.

4. Fracture behavior analysis

Fractographic analysis has been utilized to investigate the fracture behavior of CAD-CAM composite crowns, which is led by occlusal wear and fatigue fracture [13,35]. However, determining the fracture origin and its dynamic propagation, which are essential for understanding clinical failure, remains challenging. Yamaguchi *et al.* [20] clarified the fracture origin of CAD-CAM composite crowns and the order of crack initiation among the tested products using an *in vitro* and *in silico* approach. This approach is useful for analyzing the fracture behavior of CAD-CAM composite crowns using various preparation designs, loading conditions, and occlusal contacts that coincide with clinical situations.

The fracture origin was initiated by a concentration of tensile stress (maximum value of maximum principal stress) at the lingual side of the CAD-CAM composite crown for the restoration of the mandibular right first molar. Subsequently, the cement layer at the lingual side fractured. The order of fracture depends on the material properties of each component for a compression test. The *in silico* non-linear FEA successfully detected the sign of the initial crack of the CAD-CAM composite crown due to the high calculation cycle, while the *in vitro* experiment with the crosshead speed of 1.0 mm/sec did not show such a sign in the load-displacement curve.

The elastic modulus is one of the material parameters required to conduct the *in silico* non-linear dynamic FEA. In the case of CAD-CAM resin composites, the *in vitro* three-point bending test is conducted to evaluate flexural properties due to the limited block dimension. However, the flexural modulus obtained from the three-point bending test is not equal to the elastic modulus obtained from the tensile test, which is required for the FEA. Thus, Yamaguchi *et al.* [20] established an *in silico* model to mimic the *in vitro* fracture behavior by the three-point bending test of each component for a compression test of the CAD-CAM composite crown. The *in vitro* and *in silico* approach was available for fracture toughness tests [19], biaxial flexural strength tests [36], tensile tests [37], and shear tests [37], not only the three-point bending test. This approach can be used to assess other key properties, such as edge strength [38], to characterize clinically related behavior. The guidelines provided by the Academy of Dental Materials [39] can serve as a reference for further consideration on CAD-CAM resin composites. The digital twin [40] of these *in vitro* specimens will accelerate the digital transformation of *in vitro* testing.

Step-stress accelerating life testing, which mimics mouth-motion and sliding contact, is reliable for predicting the longevity (reliability and failure mode) of porcelain–zirconia all-ceramic crowns [41], yttria-tetragonal zirconia polycrystals crowns [42], and CAD-CAM resin composites [43]. Yamaguchi *et al.* [18] revealed that CAD-CAM resin composite molar crowns containing nanofillers (62 wt%/55 vol%) with a high fraction of resin matrix demonstrated great longevity. However, the low elastic modulus and the high fraction of the resin matrix lead to transverse expansion, which tends to spread the crown margin leading to the destruction of the adhesive interface [15,16], while it contributes to improving the fracture toughness of CAD-CAM resin composites. The trade-off between the low elastic modulus and great longevity should be resolved for the further development of CAD-CAM resin composites. To solve this trade-off, an adaptive experimental design method with Bayesian optimization as an MI approach [24] or the combination with Taguchi's method and the genetic algorithm [44] will be useful for finding effective components of CAD-CAM resin composites. A repetitive cycle of the *in vitro* experiments and the feedback of results to the developed AI improve the prediction accuracy of AI. It is effective for finding unknown components hidden in the extrapolate region to achieve desirable performance. To obtain reliable prediction results from such AI, it is important to utilize unified input data that aligns with *in vitro* test settings (*e.g.*, specimen dimensions and testing speed), following standards such as ISO, ASTM, ANSI/ADA, and DIN.

5. Clinical implications and potential

The exceptional fracture toughness of CAD-CAM resin composites has brought significant benefits to pediatric dentistry. In this field, primary posterior teeth with extensive caries have traditionally been restored with ready-made full metal crowns due to their superior mechanical properties compared to resin composites. However, due to their non-aesthetic appearance, parents may prefer to avoid stainless steel crown restoration for their children.

Nakase *et al.* [45] developed a CAD-CAM resin composite that incorporates surface pre-reacted glass (S-PRG) filler [46] for primary teeth crowns. This composite demonstrated promising physical properties and wear resistance, exhibiting greater fracture toughness and wear resistance compared to a commercially available CAD-CAM resin composite and two resin composites designed for primary teeth.

The high fracture toughness of this composite is particularly useful for the restoration of thin primary molar teeth. It contributes to clinically acceptable fatigue behavior and bonding performance, even when glass ionomer cement is used as a luting material [47].

6. Summary

This paper summarized the effective components of CAD-CAM resin composites for their further development. The integration of *in vitro* and *in silico* approaches will expedite the advancement of CAD-CAM resin composites, offering benefits such as time efficiency and reduction of material waste for researchers and manufacturers.

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