Evaluation of Polymerization Shrinkage, Polymerization Shrinkage Stress, Wear Resistance, and Compressive Strength of a Silorane-based Composite: A Finite Element Analysis Study

Abstract

Background: Understanding the mechanical properties is important in predicting the clinical behavior of composites. Finite element analysis (FEA) evaluates properties of materials replicating clinical scenario. Aim: This study evaluated polymerization shrinkage and stress, wear resistance (WR), and compressive strength (CS) of silorane in comparison with two methacrylate resins. Settings and Design: This study design was a numerical study using FEA. Materials and Methods: Three-dimensional (3D) models of maxillary premolar with Class I cavities (2 mm depth, 4 mm length, and 2.5 mm width) created and restored with silorane, nanohybrid, and microhybrid; Groups I, II, and III, respectively. Loads of 200–600 N were applied. Polymerization shrinkage was first determined by displacement produced in the X, Y, and Z planes. Maximum stress distribution due to shrinkage was calculated using ANSYS software. 3D cube models of composite resins were simulated with varying filler particle size. Similar loads were applied. WR and compressive stress were calculated: \( K W L/H \) and load/cross-sectional area, respectively. Statistical analysis done using one-way ANOVA, Kruskal–Wallis, and Tukey’s honestly significant difference test (\( P < 0.05 \)). Results: Polymerization shrinkage (0.99%) and shrinkage stress (233.21 Mpa) of silorane were less compared to microhybrid (2.14% and 472.43 Mpa) and nanohybrid (2.32% and 464.88 Mpa). Silorane (7.92\times10^{11} \mu m/mm \) and nanohybrid (7.79\times10^{11} \mu m/mm \) showed superior WR than microhybrid (1.113\times10^{11} \mu m/mm \). There was no significant difference in compressive stress among the groups. Conclusion: Silorane exhibited less polymerization shrinkage and shrinkage stress compared to methacrylates. Silorane and nanohybrid showed greater WR compared to microhybrid. CS of all groups was similar.

Keywords: Compressive strength, finite element analysis, polymerization shrinkage, silorane, wear resistance

Introduction

Most of the research in composite resin material has been concentrated on filler particles. revolutions in filler technology resulted in vast combinations of filler particle sizes that improved the mechanical properties of composites; however, the resin matrix has almost remained methacrylate based.

The field of nanotechnology led to the development of nanocomposites with zirconium/silica nanofillers (25–75 nm in size). Filler distribution in the resin matrix was thus increased to 90%–95% further enhancing the physical properties of the material and reducing polymerization shrinkage with improved mechanical properties.

However, shrinkage in methacrylates cannot be totally eliminated. Recent research in resin technology led to the discovery of nonmethacrylate, ring opening resin monomers such as oxiranes, spiro-orthoesters, spiro-orthocarbonates, and siloranes.\(^4\)\(^1\) Weimann et al. in 2005 described the synthesis of a new monomer system-silorane (3,4-epoxycyclohexyl cyclopolymerethyl siloxane). The term silorane (siloxane-oxirane hybrid) refers to the siloxane core and four oxirane functional groups attached to it.\(^5\)\(^1\) Polymerization process occurs through a cationic ring-opening reaction with activation of the initiator (camphorquinone), which opens the oxirane ring and generates a new acidic center. After the subsequent attraction to a new oxirane monomer, the epoxy ring is

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opened to form a chain. In the case of interaction among multiple monomers, a network is formed. This process gains space and counteracts the volume loss that occurs when chemical bonds are formed, thus leading to a reduced overall volumetric shrinkage.\(^6\)

Finite element analysis (FEA) is known to be one of the best methods to evaluate properties of a material replicating clinical scenario that would otherwise be difficult to simulate in vitro. In practice, FEA usually consists of three principal steps: preprocessing, analysis, and postprocessing. The model to be analyzed is geometrically divided into a number of discrete subregions or elements that are connected at discrete points called nodes. These nodes have fixed displacements under prescribed loads, for which the individual deformation (strain and stress) can be more easily calculated than for the whole undivided larger area. From these calculations, the values as a whole can be obtained. This comprehensive in vitro investigation allows the researcher to reduce the time and cost required to bring a new idea from concept to clinical application.\(^7\)

There are very few FEA studies in literature comparing the mechanical properties of siloranes with methacrylate-based resins. Hence, the aim of the present study was to evaluate the polymerization shrinkage, polymerization shrinkage stress, wear resistance (WR), and compressive strength (CS) of a silorane composite in comparison with a microhybrid and a nanohybrid composite using FEA.

Materials and Methods

Polymerization shrinkage and polymerization shrinkage stress

Different cross-sectional images of a maxillary right first premolar were obtained using micro-computed tomography by scanning into 0.5 mm thin sections. These cross-sections were scanned to create solid three-dimensional (3D) models using ProScan software (Technicolor, USA).\(^8\) Standardized Class I cavities of dimensions 2 mm depth, 4 mm length, and 2.5 mm width were simulated. Intact tooth models without cavity preparation \((n = 10)\) and prepared but unrestored models \((n = 10)\) were taken as negative and positive controls, respectively.

The prepared cavities were restored with composite resin \((n = 30)\). Properties of the composite material and their respective bonding agents (as given by the manufacturer) were used to simulate the composite resin material. The teeth models were divided into three groups according to the composite resin used:

- **Group I** - Silorane (Filtek P90, 3M ESPE, India); \((n = 10)\)
- **Group II** - Microhybrid (Z250, 3M ESPE, India); \((n = 10)\)
- **Group III** - Nanohybrid (Z350, 3M ESPE, India); \((n = 10)\)

A mesh was created on the prepared tooth models and opposing forces of 200, 300, 400, 500, and 600 N were applied at the contact points to determine the stress distribution taking into account the vertical and horizontal components of the applied force.\(^9\)

The percentage of polymerization shrinkage of the three composites was determined by the displacement produced in the X, Y, and Z planes according to the formula,

\[
\Delta X, \Delta Y, \Delta Z = \text{shrinkage in mm along the opposite (negative) directions of the X, Y, and Z axis. Shrinkage volume} = (X_i - \Delta X)(Y_i - \Delta Y)(Z_i - \Delta Z)
\]

The displacement produced due to polymerization shrinkage and the maximum principal stress distribution due to polymerization shrinkage were calculated using finite element ANSYS software package.

Wear resistance and compressive strength

3D cube models of the composite materials (length × breadth × height of 0.0375 mm\(^3\)) with resin matrix and filler particles were simulated.\(^10\) The filler shape was kept as a standard sphere, and the distance between the filler particles was also kept constant; only the filler size and percentage and radius of spherical indenter for testing were varied for each group [Table 1].

- **Group I** - Silorane (Filtek P90, 3M ESPE, India); \((n = 10)\)
- **Group II** - Microhybrid (Z250, 3M ESPE, India); \((n = 10)\)
- **Group III** - Nanohybrid (Z350, 3M ESPE, India); \((n = 10)\)

WR was calculated as \((KW L)/H\), where \(K\) is the dimensionless constant, \(W\) - force applied in Newtons, \(L\) - sliding length in mm, and \(H\) - hardness of the material.

For CS testing, instead of a spherical indenter, forces applied by Instron Universal testing machine were

| Groups                 | Filler radius (mm) | Filler loading (%) | Radius of indenter (WR) (mm) | Load applied (WR and CS) |
|------------------------|--------------------|--------------------|------------------------------|--------------------------|
| Group I - silorane     | 0.0025             | 74-76              | 0.9×10\(^{-2}\)             | 200, 300, 400, 500 and 600 newtons |
| Group II - micro hybrid| 0.00175            | 78                 | 0.9×10\(^{-2}\)             |                          |
| Group III - nanohybrid | 0.00001            | 90-95              | 0.9×10\(^{-6}\)             |                          |

WR=Wear resistance, CS=Compressive strength
simulated. The deformation in millimeter on application of increasing loads was obtained, and the compressive stress in MPa was calculated as the load/cross-sectional area.\textsuperscript{[11]}

**Statistical analysis**

Statistical analysis was done using one-way ANOVA and Kruskal–Wallis test. Multiple comparisons between the experimental groups were done using Tukey’s honestly significant difference test. Significance level was kept at 95% ($P < 0.05$).

**Results**

The FEA revealed that there was no significant difference between the mean stress distribution of the positive control (148.37 Mpa) and negative controls (154 Mpa) ($P = 1.000$) at all loads.

Polymerization shrinkage of Group I (silorane 0.99%) was significantly less when compared to Group II (microhybrid 2.14%) and Group III (nanohybrid composite 2.32%) ($P = 0.0001$). Similarly, polymerization shrinkage stress was the least for Group I and significant when compared to Groups II and III [Table 2 and Figure 1].

| Group          | Polymerization shrinkage stress (MPa) | Polymerization shrinkage (%) | WR ($\mu$m/mm$^3$) | CS (Mpa) |
|----------------|-------------------------------------|-----------------------------|-------------------|---------|
| Group I - silorane | 233.21                              | 0.99                        | $7.92 \times 10^{11}$ | 854.98  |
| Group II - microhybrid | 472.43                              | 2.14                        | $1.113 \times 10^{-17}$ | 925.40  |
| Group III - nanohybrid | 464.88                              | 2.32                        | $7.79 \times 10^{11}$ | 731.92  |

WR=Wear resistance, CS=Compressive strength

There was no statistically significant difference between Groups II and III ($P = 1.000$) for all the three parameters.

**Discussion**

Conventional methods to measure polymerization shrinkage (dilatometer, bonded disc method, strain gauge analysis, and pycnometer), compressive stress (universal testing machine), and wear rate (profilometric analysis) are based on volume or density changes before and after curing. These methods are laborious, besides being sensitive to changes in temperature and specimen weight.\textsuperscript{[12]} FEA has been shown to be a reliable method to evaluate the properties of a material in a simulated \textit{in vitro} model, which would otherwise be difficult to assess under clinical scenario. Therefore, in this study, FEA was used to determine the polymerization shrinkage, polymerization shrinkage stress, WR, and CS.\textsuperscript{[13,14]}

![Figure 1: Stress distribution after application of 600 N force in (a) normal tooth, (b) tooth with class I cavity and polymerization shrinkage stress, (c) silorane, (d) microhybrid, (e) nanohybrid](image-url)
Maxillary first premolar was selected in this study, due to its unfavorable shape, crown/root proportion, crown volume, and anatomic location making it more susceptible to cusp fracture compared to posterior teeth (Bitter K et al., 2010 and Shefiei F et al., 2014).[15,16] In this study, silorane-based composite was compared with two commonly used methacrylate-based resins, microhybrid and nanohybrid composites. Studies have shown that these composites have polymerization shrinkage of 2%–3.5% and 1.5%–2.5%, respectively.

This is one of the first FEA studies comparing the stresses acting on the normal tooth (positive control), the tooth with prepared cavities (negative control), and polymerization shrinkage stress after restoration with the three composites. Composite resins were simulated and directly filled in the Class I cavities created in the 3D models in accordance with the FEA study by Li et al., 2010.[17]

For evaluating the WR and CS, 3D models as simulated by Pramanik et al. in 2007 were used.[10] Symmetric dimensions and boundary conditions were applied to make the model size manageable.

The normal occlusal forces acting in the premolar region range from 222 N to 445 N (50–100 pounds) and the maximum sustainable force ranges from 450 to 580 N.[18] Therefore, the stress distribution was determined by application of forces from 200 to 600N.

Results revealed that there was no significant difference between the mean stress distribution on the normal tooth (148.37 MPa) and the prepared tooth (154.00 MPa) ($P = 1.000$). This may be due to minimal loss of tooth structure after cavity preparation and the presence of intact marginal ridges that minimizes the tooth flexure under specific loading conditions.[15]

Polymerization shrinkage was found to be significantly higher for siloranes, which is in accordance with other similar studies.[6,19,20] The resultant shrinkage stresses of the three groups are given in Table 3. No significant difference was found in the stresses of silorane composites when compared with the control groups, whereas there was a statistically significant increase in the stress of methacrylate groups ($P < 0.001$). This correlates with the percentage of polymerization shrinkage; more the shrinkage, more the resultant stress. Stress buildup depends on the kinetics of the polymerization reaction. The degree of conversion may vary in relation to the composition of the resin material and the curing technique, and an insufficient degree of conversion can reduce the stress development. A lower degree of conversion has been described for the silorane-based composites compared to other methacrylate-based composites by Palin et al. 2005. [21] Moreover, it has been hypothesized that siloranes have a slower polymerization that may allow enough time for stress relaxation through the material flow.[5] In any case, because cationic polymerization continues for extended periods of time due to leaching of the residual unreacted oxirane monomers, the continued curing reaction reduces the polymerization shrinkage stress at the tooth composite interphase.[22]

In the current study, WR of silorane and nanohybrid composites was significantly higher than that of microhybrid composite ($P < 0.001$). The higher filler content (82%–90%) with reduced volume of resin matrix may be the reason for the reduced wear rate in nanohybrids when compared with the microhybrids (66%–72% filler loading). Studies conducted by Ferracane JL 2005 and Cha HS et al., 2004 have shown that higher the filler loading, greater is the WR.[23,24] However, siloranes with a lower filler loading of 76% showed greater WR; this may be due to the hydrophobic nature of the siloxane core, the silorane composite exhibits a low water sorption, this may be one of the reasons for the increased hardness and good WR.[21,25]

Compressive stress for all the three groups was similar with no significant difference ($P = 0.641$). Weinmann et al., 2005, showed that the mechanical properties of silorane-based composites such as CS, flexural strength, and tensile bond strength were similar to methacrylate-based composites.[6]

However, results of our study differ from that obtained by Lien and Vandewalle, where the silorane composite showed relatively low CS and microhardness than the
methacrylate-based composites. This may be due to differences that exist in the chemical bond energy between filler particles and matrix among the methacrylate-based and silorane-based restorative materials. During the cationic ring-opening polymerization reaction in siloranes, the acidic Si–OH groups on the quartz filler particles can potentially result in an undesired initiation of the cationic polymerization process. This unwanted process can increase the overall number of unreacted oxirane monomers and pendant intermediates and can potentially induce failure of the material when subjected to a compression stress.

**Conclusion**

Within the limitations of this FEA study, it can be concluded that:

1. The silorane composite showed less polymerization shrinkage, shrinkage stress, and greater WR compared to methacrylate resins
2. Nanohybrid composite had better WR compared to microhybrid composite
3. There was no significant difference in the compressive stress values among all the three composite resins.

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**Conflicts of interest**

There are no conflicts of interest.

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