Design parameters for all-ceramic dental crowns

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CHAPTER 4

Finite element analysis model to simulate the behavior of luting cements during setting.

4.1 Abstract

Introduction: Beside the fixation of the restoration, an important function of dental luting cements is to seal the gap between tooth and restoration. However, as a result of adhesion, the curing contraction is hindered, creating stresses. To maintain the seal these stresses may not exceed the bond nor the cohesive strength of the cement. The aim of this study was to evaluate a rather simple model, which mimics the setting behavior of luting cements based on the division of the setting process into a liquid, visco-elastic and elastic phase, for its suitability to predict in Finite Element Analysis (FEA) the magnitude of the setting stresses occurring clinically.

Material and methods: Commercial luting cement, RelyX ARC, was used in this study. In a dynamic test setup the stresses, the elastic strain, and the shrinkage were determined. Two layers with different thicknesses and different ratios between bonded and free surface (C-factor) were examined. The parameters, found in these experiments, were used in models in a three-dimensional FEA program. The experimental contraction stresses were compared with the results of the FEA.

Results: The smallest plastic deformations and contraction stresses were found in the thinnest layer. The studied model showed to be reliable for predicting the experimental stresses.

Significance: The results of this study may be used for the prediction of the actual stresses occurring in dental restorations with FEA.
4.2 Notations

<table>
<thead>
<tr>
<th>Table 4.1</th>
<th>The variable names and indices used.</th>
</tr>
</thead>
<tbody>
<tr>
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4.3 Introduction

During the last decade, the popularity of dental resin composite luting cements has increased due to their good adhesive properties. Like resin composite restoratives these cements contract during setting, which causes stresses in the thin adhesively bonded cement layer [1-3]. These stresses may exceed the cohesive or the bond strength, placing its longevity at risk [4]. Therefore, knowledge of the polymerization shrinkage stress development, distribution and height is of main importance for a reliable risk assessment of the durability of dental indirect restorations. To reveal this process is hard to perform, as the setting of resin composites is a complex time depending process, throughout which material properties undergo a dramatic change in a relatively short period. Moreover, the complex geometries found clinically are rather difficult to imitate in a laboratory setup. As a consequence, the stress found in simplified laboratory test setups may not fully mimic the complex clinical cases.

Finite Element Analysis (FEA) software has been developed as a tool to reveal the magnitude and distribution of stresses in complex geometries. The setting process of resin composites is well described in literature [5]. However, an FEA-based algorithm for the handling of the setting process is not available and powerful FEA software, applying multi step approach, may be required for it, which is not available in standard software.

In literature many FEA studies are reported where the setting process is simplified to a single step process in which the thermal expansion mode of the FEA-software is used to mimic the shrinkage, assuming pure elastic behavior of the restorative material [6, 7]. Winkler et al. [8, 9] divided the curing process in several steps with increasing curing depth also assuming single step elastic behavior for the cured part. For this approach, during FEA processing, parts made of the material are simply scaled down in all directions (x, y, z) according to its free linear shrinkage. Obviously deformations and stresses will occur now, because the shrunk part stays bonded to the fixed surfaces. The single step approach assumes that all deformations develop at the same pace, which is certainly not true in many dental restorations.

So the multi step approach requires sophisticated software and difficult material property determination, while the single step can only be used in very limited cases. Nevertheless, it may be possible to use existing FEA features to mimic the complex process of setting stress development in a rather simple way. Much standard FEA software has the possibility of dealing with elastic - plastic behavior.
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This generally means that the material may be characterized by two linear stress-strain relations: one giving the angle of the elastic part, the Young's modulus $E$, and a second one to approximate the angle of the more horizontal part beyond the elastic limit the hardening modulus $H$. The transition between these two moduli is marked by an amount of strain rather than a point in time marking the progression of the setting process.

In the case of uniform cement layer thickness, all in-plane shrinkage may be assumed to be converted to the direction perpendicular to the gap and will always be restrained uniformly resulting in defined shrinkage conditions in the cement layer. Consequently, in gaps with uniform layer thickness this amount of shrinkage will be representative of the progression of the reaction. With this assumption the setting process of a resin composite cement can be expressed as a stress-shrinkage plot, which is time independent and exists of a liquid phase where the materials shrinks but no stress develops, a visco-elastic phase, where the shrinkage partly leads to stress formation and partly is relieved by viscous flow, and an elastic phase where all shrinkage is transferred into stress.

The aim of this study was to evaluate the use of such an elastic-plastic FEA element for its ability to be used for the visualization of the setting stresses. It was hypothesized that time dependent dynamic setting behavior of resin composite luting materials in cement gaps with uniform thickness could be mimicked by a time independent static FEA model by making use of elastic-plastic element behavior.

4.4 Materials and Methods

The material used was dual-curing luting cement RelyX ARC (batch AEAE, 3M, St. Paul, MN, USA) a two-paste BisGMA-TEGDMA-based resin composite. According to the supplier zirconia/silica filler is used to impart radiopacity, wear resistance and strength. Filler loading of the mixed cement is approximately 67.5 % by mass. The average particle size for the filler is approximately 1.5 $\mu$m. The cement was handled and mixed according to the manufacturer's instructions, no light cure was used.
Methods

To assess the stress - shrinkage relation of the material during the early stage of setting, bonded luting cement discs (Ø 9.45 mm) with thickness of 0.140 mm (C = 33, n = 2x5) (C-factor as described by Feilzer et al. [10]) and 0.250 mm (C = 19, n = 2x5), were cured in a simple, straightforward tensiometer test setup (Hounsfied, Perrywood Business Park, Salfords, Redhill Surrey, UK) as described earlier by Alster et al. [11] (Fig. 4.1).

The surfaces of two steel cylinders (Ø 9.45 mm), one connected to the moving crosshead with the load cell and one to the fixed base of the tensiometer, were coated with a thin silica layer and subsequently silanized (Silicoater, Kulzer GmbH, Wehrheim, Germany) to ensure optimal bonding between steel cylinder and the freshly mixed samples inserted between the two cylinders.

Any axial displacement of the adhesive surfaces was determined with the aid of an extensometer (LVDT type 1304K, Millitron, Feinprüf Perthen GmbH, Göttingen, Germany) consisting of two inductive probes that were fixed as close as possible to these surfaces. In this way any possible measuring error caused by canting of the probe holder or the contact plane holder was excluded.
Two conditions were tested: one in which the curing contraction of the samples was hindered (strain=0) and one in which the samples were free to contract in axial direction (unhindered condition; load=0). In the hindered condition the moving crosshead compensated automatically any axial displacement of the adhesive surface to maintain the original sample height, while in the unhindered condition the moving crosshead compensated any load recorded by the load cell to maintain a zero load on the sample. In this way the sample was free to contract. With the unhindered condition linear shrinkage data were obtained, while with the hindered condition setting stress data were gathered, both as function of setting time. The combination of both data sets enables the visualization of the setting stress - shrinkage relationship.

To obtain the elastic strain as function of setting time periodically load/strain cycles were performed during the test execution in the hindered condition. Every 200 s the obtained load was reduced to zero in 15 s, held at zero for 30 s. and in 15 s the condition of zero strain was reinstalled.

In this test setup the two inductive probes were fixed as closely as possible to the adhesive surfaces. Nevertheless, a small amount of compliance was inevitable, which may have a relative large influence on the setting stress development in very thin cement layers. In order to determine the compliance of the test setup the two steel cylinders were made out of one piece and the test setup was loaded with a crosshead speed of 200 μm/s in order to find the compliance of the test setup for every load registered. All displacement values measured were corrected for the compliance of the test setup.

A data-acquisition console (Instrumat, Raamsdonksveer, The Netherlands) collected the data (time, load and displacement) simultaneously during the experiment at a sampling rate of 10 /s.

All experiments were repeated five times and performed at room temperature (22 ± 1°C).

The obtained data were used to calculate Young’s modulus E, and the hardenings modulus H.
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**Calculation methods**

The normal stress was calculated by means of: \( \sigma = \frac{F}{A} \), (see table 4.1 for the connotation of the abbreviations)

The elastic strain was calculated from the displacement values to reduce the load to zero in the hindered condition \( \varepsilon_{\text{elast}} = \frac{\Delta_u - \Delta_{\text{rest}}}{h_0} \).

The shrinkage during setting was calculated from the displacement values in the unhindered condition \( \varepsilon_{\text{shrinkage}} = \frac{\Delta_b}{h_0} \).

The plastic deformation was calculated by subtracting the length of the sample, reducing the load to zero in the hindered setting situation, by the length of the unhindered shrinking sample \( \varepsilon_{\text{plastic}} = \frac{(h_0 - \Delta_u) - (h_0 - \Delta_b)}{h_r} = \varepsilon_{\text{shrinkage}} - \varepsilon_{\text{elast}} - \varepsilon_{\text{rest}} \).
Determination of the start of the different phases

The beginning of stress development and the change in stress development in the hindered condition were considered as the beginning of the visco-elastic phase and the beginning of the elastic phase respectively, see Fig.4.2 and Fig.4.3.

Fig. 4.2  Contraction stress - shrinkage relation during hardening in the hindered condition for RelyX ARC in the 0.140 mm layer
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![Graph showing stress-shrinkage relation](image)

**Fig. 4.3** Contraction stress-shrinkage relation during hardening in the hindered condition for RelyX ARC in the 0.250 mm layer.

All parameters in the visco-elastic phase and the elastic phase ($\times_{visco-el}$ and $\times_{el}$, respectively) were taken at the time marking the end of these two phases.

**Young’s modulus $E_c$ and hardenings modulus $H_c$**

Young’s modulus $E_c$ and the hardenings modulus $H_c$ can be calculated as follows:

In all three phases:

$$\Delta_{\text{shrinkage}} = \Delta_{\text{elastic}} + \Delta_{\text{plastic}} + \Delta_{\text{rest}}$$

$$\varepsilon_{\text{shrinkage}} = \varepsilon_{\text{elastic}} + \varepsilon_{\text{plastic}} + \varepsilon_{\text{rest}}$$

(1)

*During the liquid phase*

$$\sigma_{\text{liquid}} = 0$$

(2)
During the visco-elastic phase

With $E = \frac{\sigma}{\varepsilon}$ (for $\varepsilon_{\text{elastic}}$ and $\varepsilon_{\text{restr}}$) the equation (1) can be worked out to:

$$\varepsilon_{\text{visco-el}} = \varepsilon_{\text{plastic,visco-el}} + \frac{\sigma_{\text{visco-el}}}{E_{\text{restr}}}$$

or

$$\sigma_{\text{visco-el}} = H_{\text{visc}} \times \varepsilon_{\text{visco-el}}$$

where

$$H_{\text{visc}} = \frac{\varepsilon_{\text{visco-el}} - \varepsilon_{\text{plastic,visco-el}}}{\varepsilon_{\text{visco-el}}} \times \left( \frac{E_{\text{visco-el}} \times E_{\text{restr}}}{E_{\text{visco-el}} + E_{\text{restr}}} \right)$$

During the elastic phase

For the elastic phase with $\varepsilon_{\text{plastic}} = 0$ equation (3) simplifies to:

$$\sigma_{\text{el}} = E_{\text{el}} \times \varepsilon_{\text{elastic,el}} \cdot \text{where} \quad E_{\text{el}} = \left( \frac{E_{\text{el}} \times E_{\text{restr}}}{E_{\text{el}} + E_{\text{restr}}} \right)$$

The total contraction stress $\sigma = E_{\text{visc}} \times \varepsilon_{\text{visco-el}} + H_{\text{visc}} \times \varepsilon_{\text{visco-el}}$ (5)

The material properties can be found with a test setup where the compliance of the setup is not influencing the test results, in that case $\Lambda_{\text{restr}} = 0$ i.e. a setup where $E_{\text{restr}} >> E_{\text{v}}$ then

$$E_{\text{visc}} = \left( \frac{E_{\text{visc,el}} \times E_{\text{restr}}}{E_{\text{visc,el}} + E_{\text{restr}}} \right)$$

simplifies to

$$E_{\text{visc,el}} = \frac{\sigma_{\text{el}}}{\varepsilon_{\text{elastic,el}}}$$

and

$$H_{\text{visc}} = \frac{\varepsilon_{\text{visco-el}} - \varepsilon_{\text{plastic,visco-el}}}{\varepsilon_{\text{visco-el}}} \times \left( \frac{E_{\text{visco-el}} \times E_{\text{restr}}}{E_{\text{visco-el}} + E_{\text{restr}}} \right)$$

simplifies to

$$H_{\text{visc}} = \left( \frac{\varepsilon_{\text{visco-el}} - \varepsilon_{\text{plastic,visco-el}}}{\varepsilon_{\text{visco-el}}} \right) \times \left( \frac{\sigma_{\text{visco-el}}}{\varepsilon_{\text{visco-el}}} \right)$$

Equations (6) and (7) have been used to determine out of the experimental results the Young's modulus $E_{\text{v}}$ and hardenings modulus $H_{\text{v}}$. 

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**FEA modeling**

The data, obtained in this way, were used as input of a time independent FEA model of the tensilometer test setup, where the cement was mimicked by an element with an elastic-plastic behavior (finite element modeling and post processing: FEMAP 8.10; ESP, Maryland Height, MO, USA; analysis; CAEFEM 7.3; CAC, West Hills, CA, USA). Two models were built consisting of two steel bars (Ø 9.45 mm) with a length of each half of the length over which the test-setup is complying.

The length over which the test setup is complying can be calculated by

\[ h_{\text{substrate}} = \Delta_{\text{refr}} \times \frac{E_{\text{substrate}}}{\sigma}, \]

where \( E_{\text{substrate}} \) is the Young’s modulus of the steel bolts is 190 GPa [9] and \( \sigma \) is the stress giving a strain of \( \Delta_{\text{refr}} \). In between the two steel bars there is a composite layer with a thickness of 0.140 mm and 0.250 mm, respectively.

Each model consisted of approximately 27,000 brick solid elements. The distribution of the elements in the axial direction was chosen in such a way that both composite layers were four elements high. We assumed four elements to be sufficient to describe accurately the stress-development in the cement layer.

The steel bars were assumed to be homogeneous, linearly elastic and isotropic with a Young’s modulus of 190 GPa and a Poisson ratio of 0.34 [12]. The composite layers were assumed to be homogeneous, elasto-plastic and isotropic. For Young’s modulus \( E \), hardenings modulus \( H \), and \( \sigma_p \), the results out of the tests were used. The used value of 0.27 for the Poisson ratio was found in unpublished experiments with this material and is among values for resin based composite cements indicated in literature [13, 14]. All nodes in the bottom plane of the lower steel bar and the top plane of the upper steel bar were assumed to be fixed; no translation or rotation was allowed in any direction. The composite layer was given a linear shrinkage of \( \varepsilon = \varepsilon_{\text{shrinkage, crev. el}} + \varepsilon_{\text{shrinkage, el}} \).

The FEA model was evaluated by comparing the output data with the results of the tensilometer study.
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Statistical analysis

Statistical analysis was carried out using SPSS statistical software package 9.01 (SPSS Inc., Chicago, IL, USA) on the data with the stress as the dependent and the shrinkage or the time as the independent variable.

4.5 Results

The compliance of the test set-up and the length over which the test set-up is complying.

![Graph showing the relationship between stress and deformation.](image)

**Fig. 4.4** Compliance of the test setup

Fig. 4.4 shows the compliance of the test setup, the change of height of the material between the cement and the strain sensors, at different stress levels. There is a rather linear relation between the deformation and the applied stress.

\[ h_{\text{substrate}} = 48.8 \text{ mm} \]
**Stress-shrinkage relation**

Fig. 4.2 and Fig. 4.3 show the relation between the contraction stress and the shrinkage of the 0.140 mm and the 0.250 mm layer. The two different linear relations for the two phases were found to be significantly different (p<0.05). The visco-elastic phase and the elastic phase started at respectively approximately 60 s and 900 s.

**Elastic strain, shrinkage and plastic deformation**

![Graph showing elastic strain, plastic deformation, and shrinkage development](image)

**Fig. 4.5** Elastic strain, plastic deformation and shrinkage development for RelyX ARC in the 0.140 mm layer

Fig. 4.5 shows the graph of the shrinkage, the elastic strain and the plastic deformation for the 0.140 mm layer. Plastic deformation and elastic strain are greatest during the first 900 s, when the material passes the liquid and the visco-elastic phase. The shrinkage stops after approximately 4000 s.
Contraction stress

Contraction stress development for RelyX ARC in the 0.140 mm and 0.250 mm layer

Fig. 4.6 shows the contraction stresses during setting for the 0.140 mm and 0.250 mm layers. The contraction stresses were significantly lower in the 0.140 mm layer (p < 0.05)
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**FEA model**

![FEA model diagram](image)

**Stress (MPa)**

**Fig. 4.7** FEA model of the 0.140 mm cement layer and two steel bars long 24.4 mm (half the compliance of the test setup)

Fig. 4.7 shows the contraction stress in the FEA model for the 0.140 mm layer using the data found in the experiments. The FEA models give a major principal stress in the steel bars (here equal to the stress in the axial direction) of 15.7 MPa and 21.7 MPa for the final contraction stresses in the 0.140 mm and the 0.250 mm layer respectively. This is a rather good prediction for the final contraction stress as found in the experiments according to Fig. 4.6.
Table 4.2
The different parameters for the FEA model for the 0.140 and 0.250 mm layer

<table>
<thead>
<tr>
<th>Layer</th>
<th>$E_c$ (GPa)</th>
<th>$H_c$ (GPa)</th>
<th>$\sigma_p$ (MPa)</th>
<th>Visco-el. and el. strain ($10^{-3}$)</th>
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<tr>
<td>0.140 mm</td>
<td>5.145</td>
<td>3.125</td>
<td>3.248</td>
<td>38.2</td>
</tr>
<tr>
<td>0.250 mm</td>
<td>5.082</td>
<td>1.552</td>
<td>5.578</td>
<td>37.1</td>
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Table 4.2 shows the parameters found in the experiments and used in the FEA models.

Table 4.3
The contraction stresses found in the experiments and with FEA for the 0.140 mm and the 0.250 mm layer

<table>
<thead>
<tr>
<th>Layer</th>
<th>Contraction Stress (MPa)</th>
<th>Experiments</th>
<th>FEA</th>
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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$\sigma_c$</td>
<td>$\sigma_c$</td>
</tr>
<tr>
<td>0.140 mm</td>
<td></td>
<td>16.1</td>
<td>15.7</td>
</tr>
<tr>
<td>0.250 mm</td>
<td></td>
<td>20.7</td>
<td>21.7</td>
</tr>
</tbody>
</table>

Table 4.3 shows the final contraction stresses in the 0.140 mm and the 0.250 mm layer as found in the FEA compared with the experimentally found values.

4.6 Discussion

During curing of composites a complicated process takes place. In the beginning, the polymer has a glassy stage where it ends as a highly cross-linked material. Its restrained shrinkage induces stress, which in its turn induces plastic deformation. Fig.4.2 and Fig.4.3 show that the process can be divided into three different phases, a liquid phase, a viscoelastic phase and an elastic phase.

During the early stage of setting, the liquid phase no stress increase occurs. The linear stress - shrinkage relation found during the visco-elastic phase is in line with the theory as is the different linear relation during the elastic phase.
Fig. 4.5 shows that plastic deformation and elastic strain are greatest during the first minutes of setting. In layers with these high C-factors nearly all volumetric contraction is converted into linear shrinkage perpendicular to the cement layer [15]. The linear shrinkage for both layer thicknesses was as expected practically the same. After the liquid phase and the visco-elastic phase, after 925 s, the shrinkage continues. The material becomes stiffer causing higher stresses with the same elastic strain.

Fig. 4.6 shows the contraction stress for the same compliance to be the smallest for the thinnest layer. This is because the restraint, \( E_{\text{rest}} = \frac{E_{\text{substrate}} \times h_{\text{f}}}{h_{\text{substrate}}} \), is smaller for thinner layers \( (h_0) \).

This is also in accordance with the findings of Alster et al. [16] and Alster, Venhoven et al. [17], who demonstrated this relation between layer thicknesses, compliance, and contraction stress in thin resin composite layers.

During the visco-elastic phase, the resin network is still soft and relatively flowable and plastic yielding at this stage of setting can be achieved without damage of the internal structure of the resin composite and the adhesive bond [18].

It has to be noted that the recording of data has been started during the experiments 180 s after the start of mixing of the two components.

For clinicians it might be interesting to know that the elastic phase started approximately 18 min after the start of the mixing of the two components, from this moment on the cement may be loaded lightly without further plastic deformation.

Table 4.2 shows the different parameters for the FEA model for the 0.140 mm and 0.250 mm layer. Fig. 4.4 shows the linear relationship of the compliance of the test setup for the load range tested. Even with our system where the compliance was minimized by mounting the two displacement transducers as close as possible to the adhesive surfaces of the test samples, the compliance still has a significant influence on the determination of the elastic strain. The correction of the displacement of the crosshead for the compliance is large in comparison with the displacement and the remaining value is in the order of sub-microns.

The parameters for the 0.140 mm layer may be in line with the clinical condition concerning layers thickness and compliance. Values of the Young's modulus of dentine and the dimensions of elements result in an \( E_{\text{rest}} \) in the same order of magnitude as the used \( E_{\text{rest}} \). Table 4.3 shows the experimental contraction stresses and the contraction stresses found with the FEA model as in Fig. 4.7.
The maximum major principal stress in the cement layer is much greater than the contraction stress; this is caused by the shear stress due to the hindered shrinkage in the transverse direction. The major principal stress is close to the strength of the material. Feilzer et al. [10] found in some cases cohesive failures due to the contraction stress.

In the clinical situation the contraction stresses will depend on the compliance of the substrate materials [17] and the possibility for not hindered shrinkage of the cement layer for example due to movement of the restoration towards the preparation during shrinkage.

The bond strength to dentin as published by Cobb et al. [19] and the bond strength and its development in time of RelyX ARC as published by Braga et al. [20] and the contraction stresses found in this study indicate that in the clinical situation there is a considerable risk of bonding failure, which depends on the possibility of the substrates to comply with developing setting stresses.

Since the influence of the compliance of the substrate materials is greater for thin layers, it may be concluded, that thinner resin composite film may produce a more reliable bond, this confirms the findings of Alster, Venhoven et al. [17].

Additional stresses in the cement like stresses due to bite forces on the cemented restoration will increase the probability of bonding failure. For that reason the design of the cement layer is of importance. However, further research is needed to assess the stresses occurring in the clinical situation.

It may be concluded that, in cement layers with uniform layer thickness, it is possible to predict the contraction stresses with the found parameters. Finite element analysis of clinically placed crowns would be one of the possibilities to do so; the results of this study can then be used as input.

4.7 References


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