A FRACTURE MECHANICS APPROACH FOR FAILURE PREDICTION OF A RESTORED TOOTH

R. de Groot*, H.C. van Elst^{\$}, M.C.R.B. Peters*, Y.M. de Haan[†]

This study reports parts of a research project aimed at prediction of mechanical failure of a restored tooth. The restored tooth can be considered as a construction with an internal crack. Experiments were accompagnied by relevant finite element analysis (FEA). The critical values of stress intensity factor ${\rm K_{Ic}}$ and J integral ${\rm J_{Ic}}$ were measured. Single edge notched bend (SENB) specimens were used made of either dental composite, to test the composite, or dental composite bonded to tooth tissue (enamel), to test the bond. The J integral was also calculated by FEA to predict failure of SENB specimens for various notch depths. Slices cut from composite restored premolars were loaded until fracture. To predict failure, the experimental set up was evaluated using 2-D FEA. Qualitative agreement was obtained.

INTRODUCTION

Problem

After failure of preventive dentistry the dentist is confronted with a patient whose teeth are affected by caries. Besides extraction there is a range of possible treatments available in restorative dentistry. These all start with removal of affected tooth tissue, whereafter the remaining part of the tooth is prepared to receive the restorative material. The restorative material can be either shaped outside, like a cast gold crown and inlay, a fired porcelain crown and jacket, or inside the oral cavity like an amalgam filling and a composite filling. In general, materials shaped outside the mouth are more expensive but also more durable. The economical factor may explain the extensive use of amalgam as a restorative material. Since its introduction amalgam has been improved until nowadays its quality has reached a level which matches almost all clinical requirements. One of

^{*} Dept. Cariology & Endodontology, Subfaculty of Dentistry, University of Nijmegen, PO Box 9101, 6500 HB NIJMEGEN, The Netherlands. \$ TNO-IWECO, PO Box 29, 2600 AA DELFT, The Netherlands.

⁺ Materials Science Group, Dept. Civil Engineering, Delft University of Technology, Stevinweg 1, 2628 CN DELFT, The Netherlands.

its main disadvantages, besides the lack of adhesive properties, is its black colour and for this reason the demand for tooth coloured restorative materials has speeded up the development of dental composite. For front teeth esthetics is perhaps the most important factor.

After the successful development of composites for anterior use and the acid etch technique, by which it is possible to adhere composite to enamel, there is a growing demand for tooth coloured materials which are also applicable in the posterior region. However, proper use in premolars and molars is more demanding with respect to material properties as wear resistance, mechanical strength, and polymerization shrinkage, because restorations in this region not only tend to be larger compared to those in front teeth but also because mechanical loading (chewing forces for example) is higher. Besides that the composite itself has to be strong, it also needs good adhesive properties to tooth tissue. A good and durable marginal adaptation is necessary to reduce the chance for secundary caries and penetration of bacteria to occur. Wear and mechanical strength are nowadays the two main factors limiting the unrestricted use of composite as a restorative materials in the posterior region. Wear of composites has been extensively studied and the improvement in wear resistance of the recent materials is considerable.

The present study focusses on the mechanical failure of composite restorations and their bond to tooth tissue. Mechanical stresses in restored teeth have been investigated before (Peters (1)) using finite element analysis (FEA) and therefore the next step is prediction of mechanical failure based on stress analysis and material deterioration. When the restored tooth is considered as a structure there are two complementary approaches for failure prediction of this structure. First, when the structure can be considered as a continuum without considerable holes or cracks a failure criterion described by a stress or strain formulation (Von Mises yield criterion or such) will do. Secondly, when these material cracks and holes have a size larger than the critical crack length or an even larger gap or crack is present in the structure, a fracture mechanics approach is needed to predict onset of fatal crack extension in these basically brittle materials.

Through a step by step increase in complexity of the test geometry from rectangular bar specimens to a two dimensional model of slices cut from restored teeth an attempt has been made to establish a proper failure criterion. Experimental testing was always accompanied by FEA of the test geometry so that a failure criterion could be verified or critical values of fracture mechanics parameters could be determined. The last step to be made in the future will be the analysis of a three dimensional model of a restored tooth.

Structure

A tooth (fig. la) mainly exists of a bone like substance called dentine. That part of the dentine that protrudes into the mouth, the crown, is covered with enamel, a highly mineralized inorganic material. The rest of the dentine, the root, is covered with a layer of cementum, which is connected to the surrounding alveolar bone by the periodontal ligament, a layer of fibrous connective tissue. The pulpchamber, enclosed in the dentine containes soft tissue, nerves, and blood vessels, entering through a hole at the apex of the root (Waters (2)). It has been shown that stress analysis of different cavity designs can be restricted to the crown of the tooth with an empty pulpchamber (Peters et al (3)).

According to reference (2) enamel being the most inorganic material (content: inorganic 97%, organic 1%, water 2% by weight) of the body has a structure built up with rods or prisms (thickness about $4\,\mu\,\text{m}$), which are oriented from the dentino-enamel junction to the outer surface of the enamel. The usual key-hole like cross-sectional shape of the prisms locks them together. The inorganic material exists of hexagonal shaped hydroxyapatite crystallites, which can be represented chemically by the empirical formula Ca₁₀(PO₄)₆(OH)₂ (thickness 25 nm, width 40-120 nm, and length 160-1000 nm). The enamel structure has a preference to fracture parallel to the direction of the prisms (Rasmussen et al (4)).

Dentine (content: inorganic 69%, organic 20%, water 11% by weight) can be characterized by the dentinal tubules directed from pulp to the dentino-enamel junction. Their diameter varies between $4\,\mu$ m near the pulp to $1\,\mu$ m at the other end. They are filled with odontoblast cells and surrounded by a highly calcified layer: the peritubular dentine. The hydroxyapatite crystals are much smaller than in the enamel: diameter 3 nm and length 64 nm. The organic substance between the tubules contains collageneous fibrils (thickness 0.3 μ m), generally lying in planes perpendicular to the tubules, and a ground substance of proteoglycans. There is a small preference for dentine to fracture parallel to the aforementioned planes (reference (4)).

Dental composites are a mixture of organic resin from monomers with a high molecular weight and inorganic filler particles. A commonly used monomer is Bis-GMA or Bisphenol A glycidyl methacrylate. According to Lutz and Phillips (5) composites can be classified as conventional composites, containing silica particles (average size 5-30 μm , up to 70% by weight), microfine composites (average particle size 0.04-0.1 $\mu\text{m}\text{,}$ content 50-70% wt.) and hybride composites (average particle size 1-10 $\mu\text{m}\text{,}$ content 80% wt.). The polymerization reaction is either initiated by a chemical or a photo-chemical system. The chemically initiated composite exists of two pastes which are mixed together during 30 seconds, whereafter the dentist has a working time of 90 seconds to insert the mixture into the cavity. After a 5 minutes setting time the restoration is ready to be finished by polishing of its surface. A photochemically initiated composite exists of only one paste and has some advantages. Mixing, resulting in incorporation of air bubbles, is not necessary. Theoretically the dentist has an unlimited working time whereafter he commands the setting with a light source, a commercially available device with a halogen lamp.

The mechanical properties of enamel, dentine, and composite like modulus of elasticity (E), Poisson's ratio (ν), tensile strength ($\sigma_{\rm c}$), compressive strength ($\sigma_{\rm c}$), critical crack length ($\sigma_{\rm c}$ = 1/ π ($\kappa_{\rm Ic}/\sigma_{\rm t}$)²) are given in table 1.

TABLE 1- Mechanical properties of enamel, dentine, and composite.

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	E	ν	[♂] c	σt	^a c
	(10 ⁹ Nm	⁻²)	(10^6Nm^{-2})	(10^6Nm^{-2})	(10 ⁻³ m)
enamel dentine composite	50 13 10	0.3 0-0.3 0.3	300 340 230	10-35 50 40	2 1 0.2

From a mechanical point of view three interfaces between different materials are of interest. The natural bond between dentine and enamel is strong enough to ensure proper functioning of the tooth under normal conditions. At the composite enamel interface resintags have penetrated into the enamel, which has been acid etched using phosphoric acid to clean the surface and to make small holes in or between the enamel prisms. This micromechanical interlocking results in a firm bond (tensile bond strength 10-20 MPa, Gottlieb et al (6)). Agood composite—dentine bond is almost impossible to obtain and to maintain because of fluids present in vital dentine. Techniques in which adhesion to the collagen part of the dentine is promoted lead to, although low, bond strength (0.6-3.4 MPa, Beech (7)).

When a tooth has been affected by caries (fig. lb) this part must be removed. In case amalgam will be used as a restorative material the preparation must be extended to ensure macromechanical retention (fig. lc). However, a composite restoration does not need such an extension as it has adhesive properties to enamel (fig. ld). Less sound tooth tissue is lost with such an adhesive preparation form (Lutz et al (8)).

Load situation

A tooth is subjected to several types of mechanical loading. The first to think of are the mastication or chewing forces, occurring at a rate of about 3000 per day, but also bruxism can not be neglected. Reference (2) gives in his review a maximum achievable biting force for one single tooth of 265 N, however, the normal force on a single tooth is in the range of 3-18 N.

In a composite restored tooth one also faces the residual stresses induced by polymerization shrinkage, which develop during the hardening process of the composite. Furthermore the coefficient of thermal expansion of the composite, which is higher than that of enamel and dentine, introduces stresses in the structure during thermocycling processes, like the daily consumption of hot and cold food.

NUMERICAL AND EXPERIMENTAL APPROACH

Polymerization shrinkage and thermal loading

It was decided to estimate the influence of polymerization shrinkage on the stresses at the composite-dentine interface, where perhaps a weak bonding might be present. A tooth was modelled for FEA as an axisymmetric cylinder (diameter 8 mm, length 8 mm) with an occlusal filling (diameter 4 mm, depth 3 mm) (fig. 2). A coefficient of linear free polymerization shrinkage (0.8%), obtained from literature (Davidson and de Gee (9); Bowen et al (10)) was used. Afterwards a kind of stress relaxation, due to viscous flow of material during the early stages of the hardening process, was accounted for, because such a flow is supposed to take place when the shrinkage is not entirely restricted by the boundaries of the cavity. In the most favourable case stresses may reduce to about 5% of those, that can be expected from the coefficient of linear free shrinkage. However, even this resulted in normal stresses at the composite dentine interface (3.8 MPa), which were equal or larger than the possibly obtainable dentine bond strength. The calculated stresses at the composite enamel interface (5.2 MPa) are below the compositeenamel bond strength. The conclusion is that after the composite has set there is good adhesion to the enamel but between composite and dentine there is no connection. The thermally induced stresses per OC were about ten times smaller. The Jintegral (Rice (11) calculated by FEA (using the virtual crack extension method Parks (12); Hellen (13); DeLorenzi, (14)) in the same axisymmetric tooth model but now without connection between composite and dentine resulted in a value ($J_I = 1.8 \text{ Jm}^{-2}$) far below the critical value of the J integral for the composite-enamel bond (J $_{\rm IC}$ = 89 \pm 15 Jm $^{-2}$ de Groot et al (15)). This implies that the composite-enamel bond is not lost by sudden shrinkage induced crack growth starting from the composite-dentine gap. However, the occurrence of fatigue crack growth can not be excluded.

Stress criteria

A pilot study (de Groot et al (16)) on failure of the compositeenamel bond revealed failure both in the composite and at the interface. Attention was then directed to find a failure criterion for composite based on a continuum mechanics stress analysis (de Groot et al (17)). Von Mises yield criterion (criterion #1), which states that the second invariant of the deviatoric stress tensor has a critical value, has been used before to analyse the stresses calculated in a FEA model of a restored tooth (Peters and Poort (18)). Its applicability to brittle composite was now investigated. Also a modification of Von Mises criterion (criterion #2), probably more appropriate for brittle materials, was obtained by adding the first invariant of the stress tensor (Williams (19)), thereby having the possibility to account for the difference in compressive and tensile failure properties: (1)

tensile failure part (1)
$$p J_1 + q J_2^2 = 1$$

with p and q: constants and J_1 : the first invariant of the stress tensor and J_2 : the second invariant of the deviatoric stress tensor. In the experimental set up rectangular bars (RB) and single edge notched bend (SENB) specimens with a chevron notch at midspan were tested in a three point bend test (span S = 12 mm). The specimens' dimensions were $16 \times 2 \times 2$ mm. Relevant 3-D FEA (fig. 3a, 3b) was performed to calculate the value of the two criteria in the region were fracture initiates. It appeared that the modified criterion is a better indication for fracture in the two types of specimens tested.

Fracture mechanics parameters

Because the structure of interest, the composite restored tooth, has a crack-like gap, which might be the initiator of ultimate mechanical failure of the structure, fracture mechanics parameters such as critical stress intensity factor ($\rm K_{IC}$), critical strain energy release rate ($\rm G_{IC}$) and critical value of the J integral ($\rm J_{IC}$) were determined.

These parameters were first measured with SENB specimens ($16 \times 2 \times 2$ mm, notch depth-width ratio a/W=1/4, 2/4 and 3/4) in a three point bend test for composite (de Groot et al (20)) according to:

$$K_{\rm I} = \frac{P S}{B W^{3/2}} \frac{3(a/W)^{1/2} [1.99-a/W(1-a/W)(2.15-3.93a/W+2.7(a/W)^2]}{2(1+2a/W)(1-a/W)^{3/2}}$$
(2)

(Srawley, 21), with P: load, S: span, a: notch depth, B: thickness, and W: width of the specimen.

$$G_{I} = (1 - v^{2}) K_{I}^{2} / E$$
 (3)

for the relevant plain strain situation (ν : Poisson's ratio, E: Young's modulus).

$$J_{I} = \frac{2 \int P \, du}{B \, (W-a)} \qquad \text{for a/W > 0.5}$$

(Rice et al (22); and Srawley (23)). When the load at fracture (P_c) is substituted the critical values of these parameters (K_{Ic}, G_{Ic}, and J_{Ic}) are obtained.

A 2-D mesh (fig. 4a) of the SENB specimens was modelled using second order isoparametric, distorted, eight noded, plain strain elements. Linear elastic materials properties were assumed. The virtual crack extension method was employed to calculate the J integral ($J_{\delta_{\mathbf{C}}}$). The determined $K_{\mathbf{IC}}$, $J_{\mathbf{IC}}$ and $J_{\delta_{\mathbf{C}}}$ (reference (20)) are given in table 2. From table 2 it can be seen that indeed the condition a/W > 0.5 for $J_{\mathbf{IC}}$ must be fulfilled. The other data are quite consistent except for those measured with a/W = 3/4, which are lower. Another way to present these finding is based on $J_{\delta_{\mathbf{C}}}$ measured with a/W = 1/2. It is possible to predict

TABLE 2- Fracture mechanics parameters (critical stress intensity factor (K $_{\rm Ic}$), critical strain energy release rate (G $_{\rm Ic}$), critical value of J integral J $_{\rm Ic}$, and J $_{\delta c}$ determined with composite (Silux $^{\rm R}$ and P-30 $^{\rm R}$) SENB specimens (average + standard deviation).

0.0				
specimen	K _{Ic} (MNm ^{-3/2})	G _{Ic}	J _{Ic} (Jm ⁻²)	^J δc (Jm ⁻²)
Silux 1/4 1/2 3/4 P-30 1/4 1/2 3/4	$\begin{array}{c} 0.98 \ \pm \ 0.03 \\ 0.99 \ \pm \ 0.03 \\ 0.72 \ \pm \ 0.06 \\ 1.82 \ \pm \ 0.03 \\ 1.88 \ \pm \ 0.12 \\ 1.38 \ \pm \ 0.12 \end{array}$	$ \begin{array}{r} 188 + 17 \\ 190 + 17 \\ 101 + 18 \\ 272 + 78 \\ 291 + 43 \\ 156 + 30 \end{array} $	$ \begin{array}{c} 286 + 24 \\ 203 + 11 \\ 136 + 40 \\ 410 + 100 \\ 310 + 37 \\ 196 + 35 \end{array} $	200+ 29 197+ 31 136+103 279+ 53 289+ 47 145+ 58

the load at fracture of composite specimens with a/W=1/4 and 3/4 using the critical value of the Jintegral measured with a/W=1/2. The predicted load was compared with the measured load (fig. 5).

 $K_{\rm IC}$ and $J_{\rm IC}$ were also measured according to equation (1) and (3) for the interfacial layer between composite and enamel with SENB specimens containing a piece of tooth tissue (using a/W = 1/2, fig. 4b) (reference (15)). Three types of failure could be distinguished, which were failure in the enamel, failure in the composite, or failure at the interface. The results are summarized in table 3.

TABLE 3- Measured J_{IC} and K_{IC} values (average + standard deviations) for bond test specimens (in case of one measurement the estimated accuracy of the measurement is given). (N: number of specimens).

-1				
failure type	J _{Ic}	N	K _{Ic} (MNm ^{-3/2})	
enamel	137 + 11	1	0.81 + 0.01	
composite/ interface enamel composite interface	$ \begin{array}{c} 145 + 35 \\ 87 + 12 \\ 166 + 10 \\ 143 + 16 \end{array} $	5 8 3 1	$\begin{array}{c} 0.84 & + & 0.16 \\ 0.75 & + & 0.10 \\ 1.05 & + & 0.06 \\ 0.94 & + & 0.02 \end{array}$	
	enamel composite/ interface enamel	enamel 137 ± 11 composite/ interface 145 ± 35 enamel 87 ± 12 composite 166 ± 10	enamel 137 ± 11 1 1 composite/interface 145 ± 35 5 enamel 87 ± 12 8 composite 166 ± 10 3	

Application to 2-D structure

Next crowns of extracted upper premolars, either sound (fig. 6ab), prepared (fig. 7ab), or restored with an occlusal composite filling (fig. 8ab) or a composite palatal cusp (fig. 9ab), were sliced (thickness 2 mm)

perpendicular to the mesio-distal direction. Slices were photographed before and after testing. The slices were mechanically tested by indenting a cylinder (diameter 4 mm) between the two cusps until failure. The load was recorded.

Failure occurred as compressive fracture by chipping of the enamel and the composite (where these materials contact the cylinder), as cleavage of the structure from the fissure between the two cusps downward, or as interfacial failure of the composite-enamel junction.

Based on the photograph of each slice a 2-D FEA input deck with fixed number of elements (plain strain, four nodes) and appropriate boundary conditions was generated. The stress distribution was calculated and the three principal stresses were combined using the two failure criteria. The Jintegral calculated by FEA was used as parameter for extension of the crack present between composite and dentine.

High stresses calculated by FEA according to criterion #2 (figs. 6c, 7c, 8c, 9c) combined with highly probable crack extension according to the J integral explain the cleavage and interfacial failures observed in the experiments. The measured load at fracture ($P_{\rm c}$), the highest stress calculated according to criterion #2 ($\sigma_{\rm eqm}$) and the Jintegral at the left or right end of the composite-dentine gap are given in table 4.

TABLE 4- Measured load at fracture (P_c), highest stress calculated according to criterion #2 (σ_{eqm}), and the Jintegral at the left (J₁) or right (J_r) end of the composite-dentine gap for the slices given in figures 6 to 9.

	P _c	°eqm (10 ⁶ Nm ⁻²)	J ₁ (Jm ⁻²)	J _r (Jm ⁻²)
sound prepared occusal cusp	471 233 498 528	225 11 26 95	223 21	30 163

Although criterion #2 takes into account the ratio of compressive and tensile strength, it does not predict the contact failure type. Probably because the presence of local stress concentration due to cracks, and materials inhomogeneities in the contact area and deviation from the assumed idealized contact are not accounted for in the coarse FEA modelling. Using criterion #1 always resulted in spots with high stresses in the contact area. However, for the same reason as given above this cannot be used to predict the compressive failure starting from the contact points

The measured fracture loads of the slices with a preparation for an occlusal filling (230 N) are half the fracture loads of the sound slices (500 N). The fracture loads of the restored slices (200-600 N) reach the

values of the sound slices and are within the same range of the highest physiological chewing forces. A complete restored tooth is expected to withstand such masticatory loading.

CONCLUSIONS

It has been shown that application of fracture mechanics concepts to the field of restorative dentistry gives promising results. Combination of experiments using well-defined specimens and FEA of the test situation opened the possiblity to determine appropriate failure criteria. Both stress criteria based on continuum mechanics and fracture mechanics parameters like J integral were necessary to understand the mechanical failure of slices of restored teeth.

Future research will be directed to refinement of the modelling and failure criteria and their application to the 3-D structure of a restored tooth.

SYMBOLS USED

= notch depth (m) = critical crack length (m) ac = thickness of the bar (m) В = subscript c denotes critical value of parameter = modulus of elasticity (Nm^{-2}) E = finite element analysis = strain energy release rate (Jm^{-2}) G_T = J integral (Jm^{-2}) = J_{I} at left end of composite-dentine gap in slice. (Jm⁻²) J_1 = J_{I} at right end of composite-dentine gap in slice. (Jm⁻²) J_r = J integral from P_c and FEA calculations (Jm⁻²) J = first invariant of stress tensor (Nm^{-2}) J_1 = second invariant of deviatoric stress tensor (N^2m^{-4}) Jo = stress intensity factor $(Nm^{-3/2})$ K_{T} = load (N) = constant in criterion #2 (m^2N^{-1})

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- q = constant in criterion #2 $(m^4 N^{-2})$
- RB = rectangular bar
- S = span of support in three point bend test (m)
- SENB = single edge notched bend specimen
- W = width of specimen (m)
- v = Poisson's ratio
- $\sigma_{\rm c}$ = compressive strength (Nm⁻²)
- σ_t = tensile strength (Nm⁻²)
- $\sigma_{\rm eqm}$ = equivalent stress according to criterion #2 (Nm⁻²)

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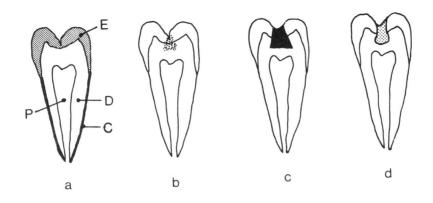


Figure 1 a: Schematic drawing of a tooth, C: cementum, D: dentine, E: enamel, P: pulp; b: Tooth with caries; c: Amalgam filling; d: Composite filling

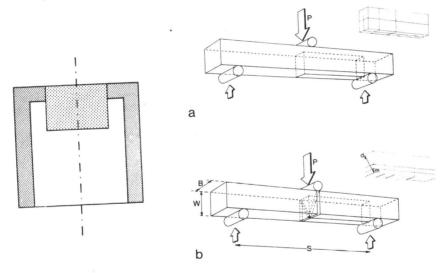
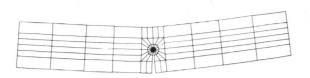
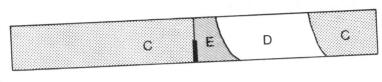


Figure 2: Axisymmetric Figure 3 a: Rectangular bar; b: Single edge model of a tooth (diameter notch bend specimen (chevron notch); 8 mm, height 8 mm) quarter of the bars as used for FEA



a



b

Figure 4 a: FEA mesh of SENB specimen (deformed structure) a/W=1/2 4b: SENB specimen for composite-enamel bond test, C: composite; D: dentine; E: enamel

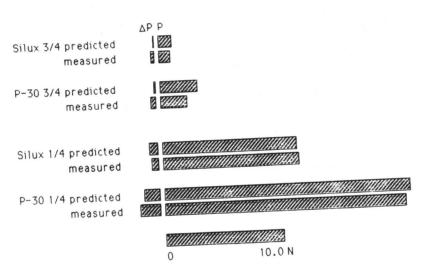


Figure 5: Comparison of predicted and measured fracture load for two composites (Silux $^{\!R}$ and P-30 $^{\!R}$)

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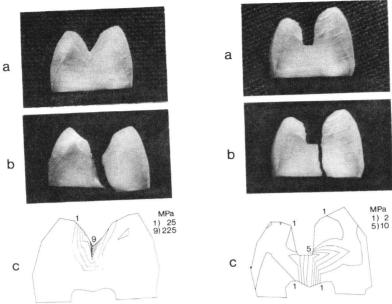


Figure 6 a: Sound tooth
b: Failure; c: Stress levels crit #2
b: Failure; c: Stress levels crit #2

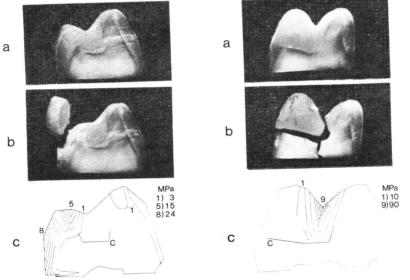


Figure 8 a: Occlusal filling
b: Failure; c: Stress levels crit #2
C: composite-dentine gap

Figure 9 a: Rebuilt cusp
b: Failure; c: Stress levels crit #2
C: composite-dentine gap