Frontiers of Fracture Mechanics

Adhesion and Interfacial Fracture

Contact Damage

Biology, Medicine & Dentistry – The Next Frontiers For Mechanics

- One of the current challenges in materials & mechanics is how to make adequate connections to biology and medicine
- This requires new knowledge and teaming approaches beyond the boundaries of our current efforts
  - medicine, dentistry
  - biology, chemistry, physics
  - materials and mechanics

The Benefits of The Mechanics Approach

- Theoretical/computational mechanics enable quantitative predictions of cause and effect
  - However biological systems are complex
  - Two approaches are often needed
- Experimental mechanics provides new insights and measurements
  - Enables model validation
  - Enables new clinical solutions

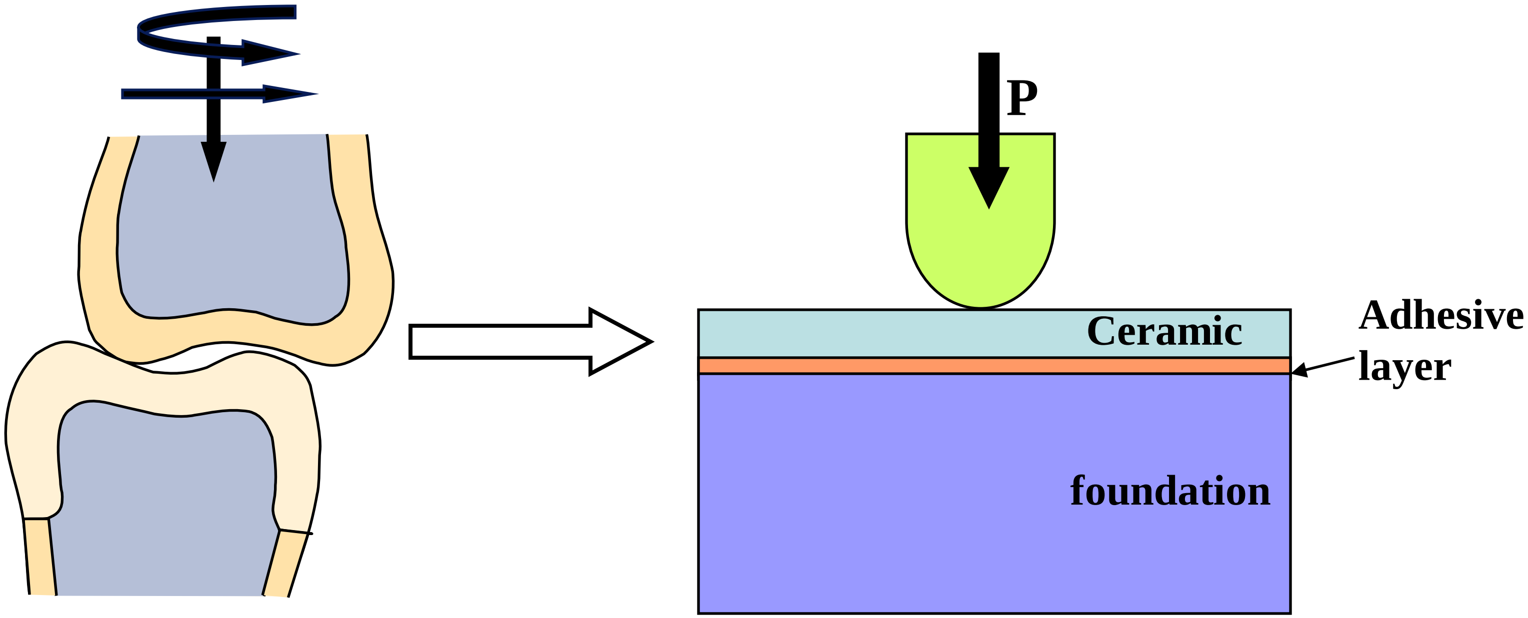
Background and Introduction

- This class presents selected examples at the frontiers of fracture mechanics
- These include:
  - Problems involving adhesion and interfacial fracture
  - Problems involving contact damage
- This focus is on applications of fracture mechanics in biomedical applications

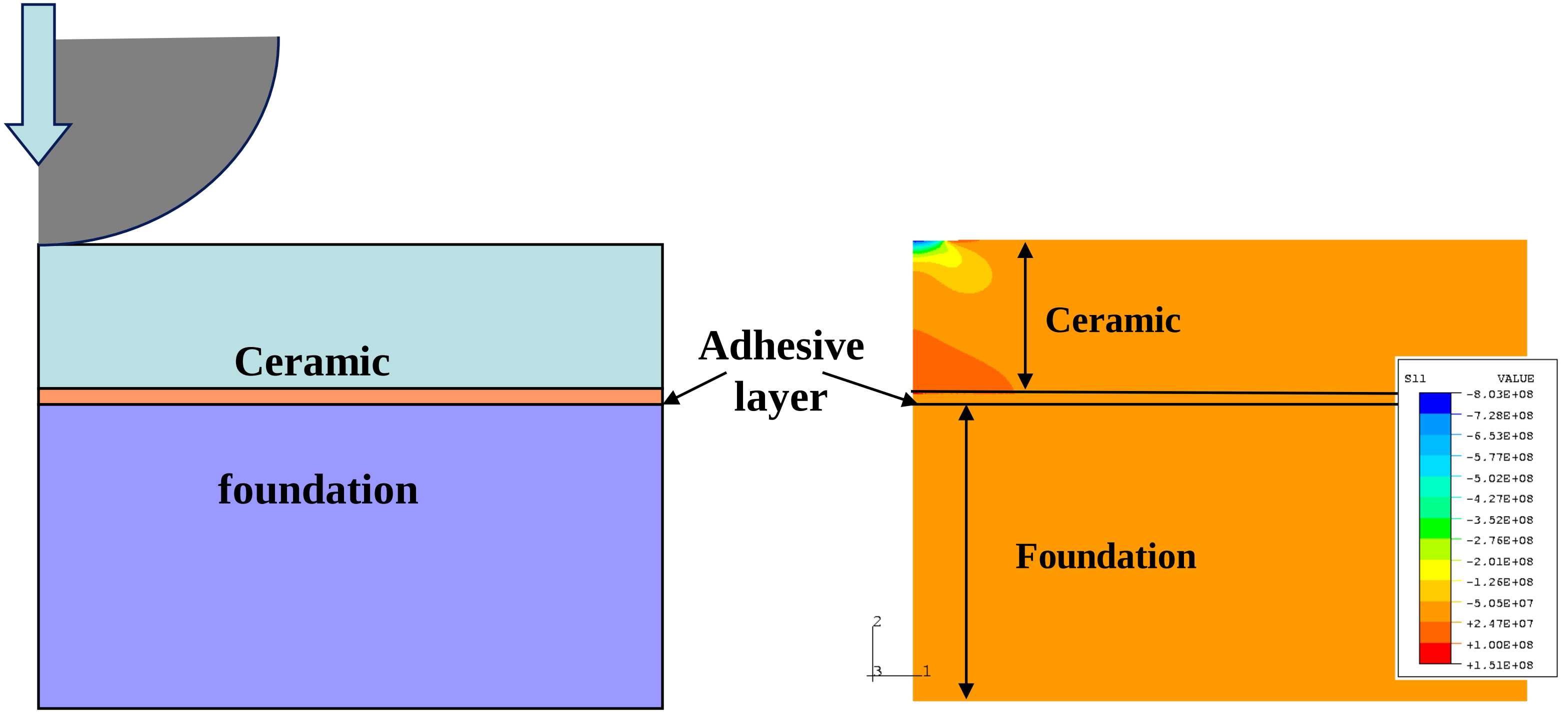
Path to understanding the effects of multiple loadings on dental structure

Tooth on tooth contact

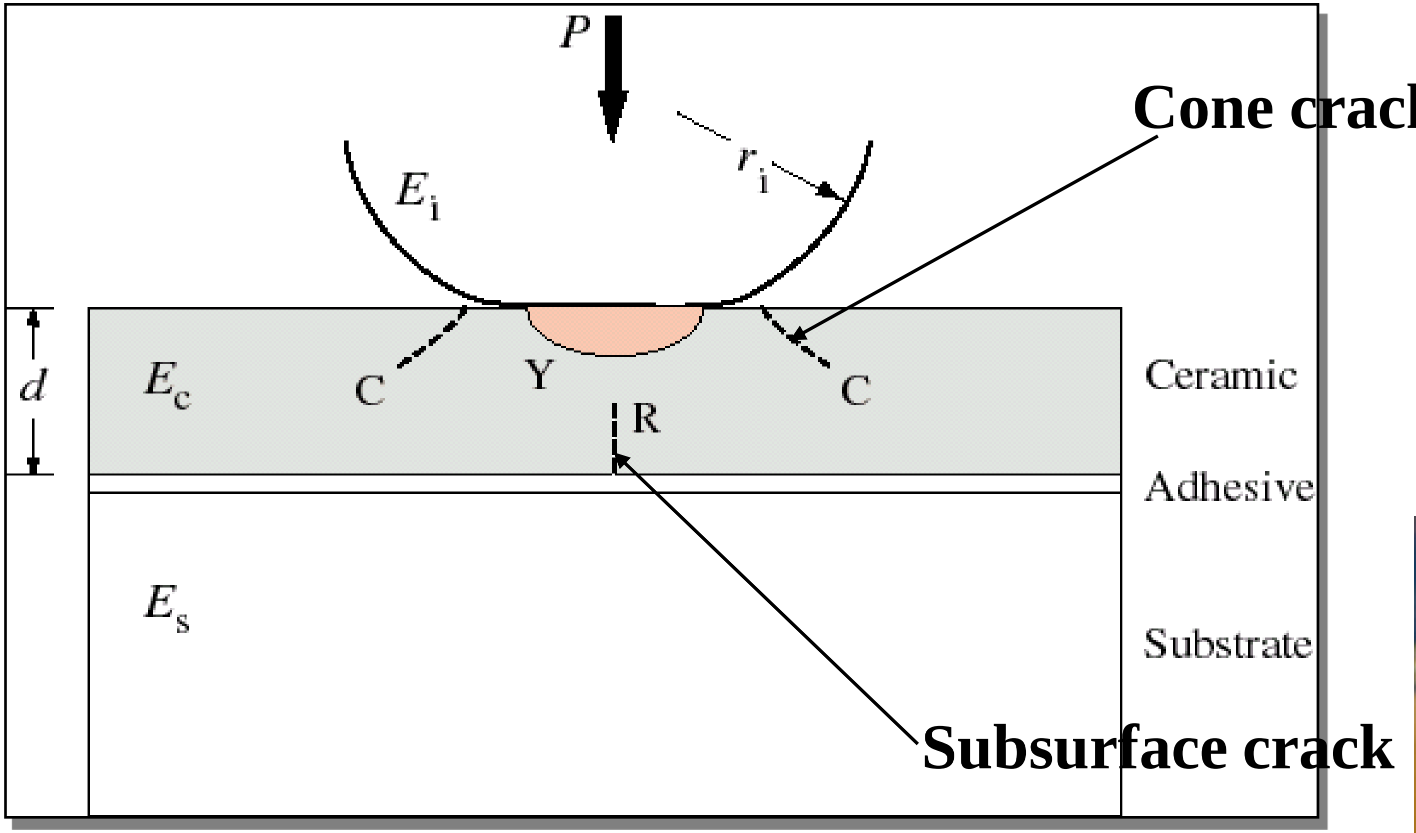
Hertzian contact on idealized Multilayer Structure

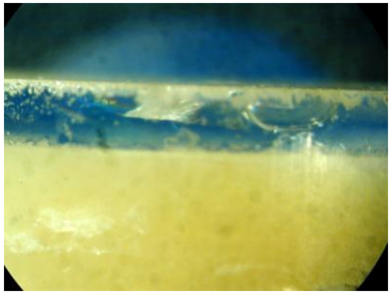


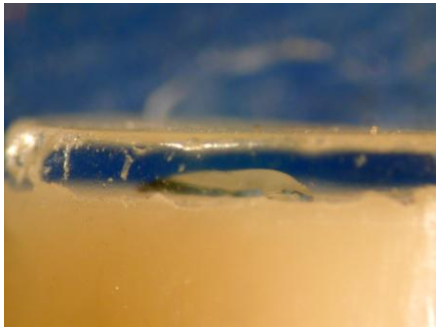
Basic FEA on idealized 3-layer structure



FAILURES CAUSED BY HERTZIAN INDENTATION

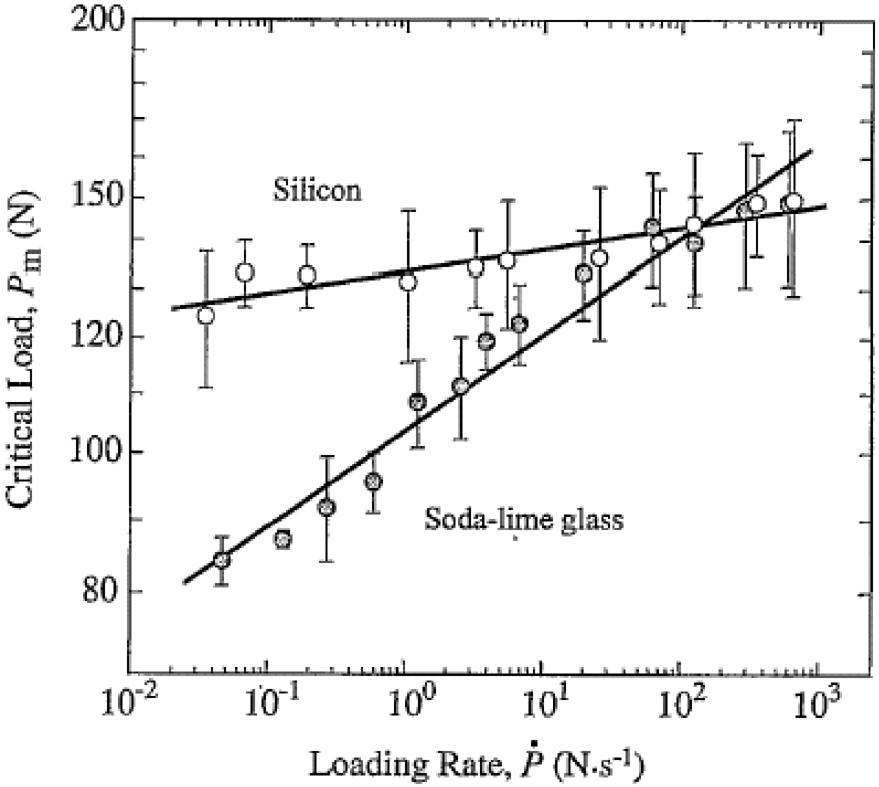






Sub-surface crack is the major clinical failure mode.

Loading rate effects on 3-layer structure



Plot of critical load P_m for radial cracking as function of loading rate P for coatings of soda-lime glass (filled symbols) and silicon (unfilled symbols) bonded to polycarbonate substrates.

(Lee *et al.* 2002)

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Contribution of Lawn's approach

- **Experimental study demonstrates the existence of loading rate effect**
- **Silicon does not exhibit slow crack growth (SCG) but silicon tri-layer shows loading rate effect**
- **SCG model can only explain part of loading rate effect**
- **Material properties of the foundation and join layers may play important role**

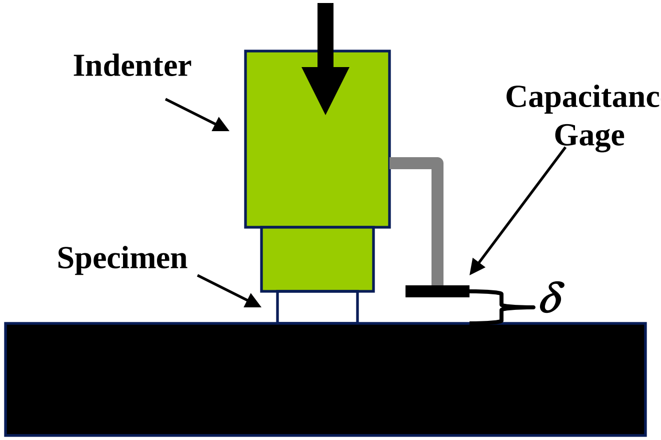
Approach of the Current Work

- Develop understanding of the constitutive behavior of individual layers
- Integrate the constitutive behavior into mechanics models
- Predict critical loads in multilayer structure
- Develop understanding of loading rate effects on deformation and cracking

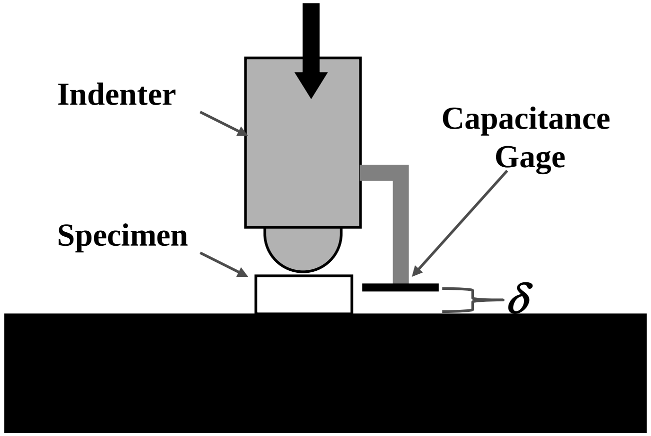
Experiments

- Studied joins, foundations & multilayers with *real dental materials*
- Measured constitutive behavior for individual layers (monotonic compression tests)
- Studied cracking of multilayers (monotonic Hertzian contact tests)

<u>Compression Tests</u>



<u>Hertzian contact Tests</u>



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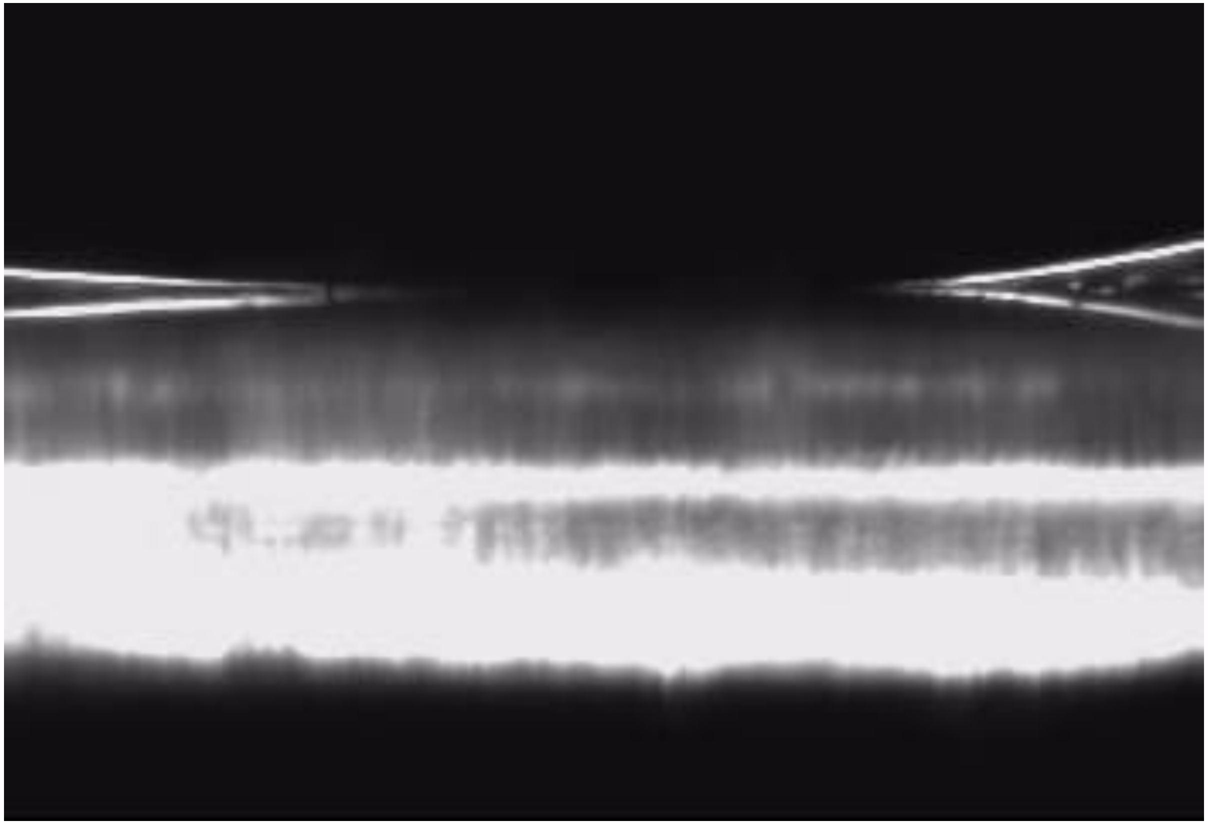
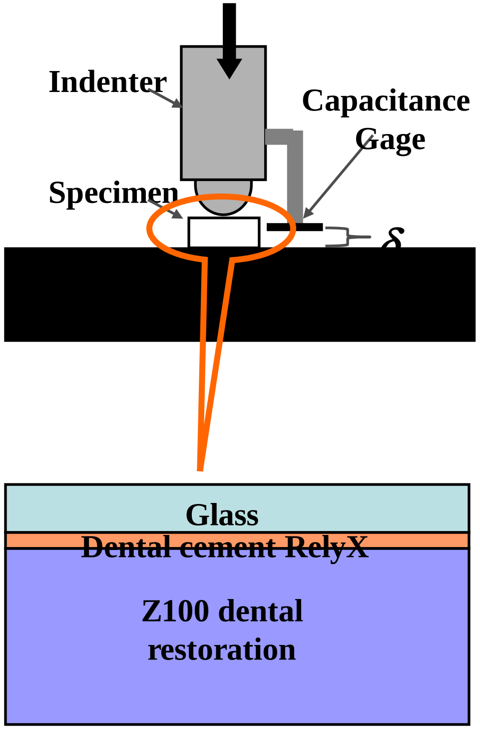
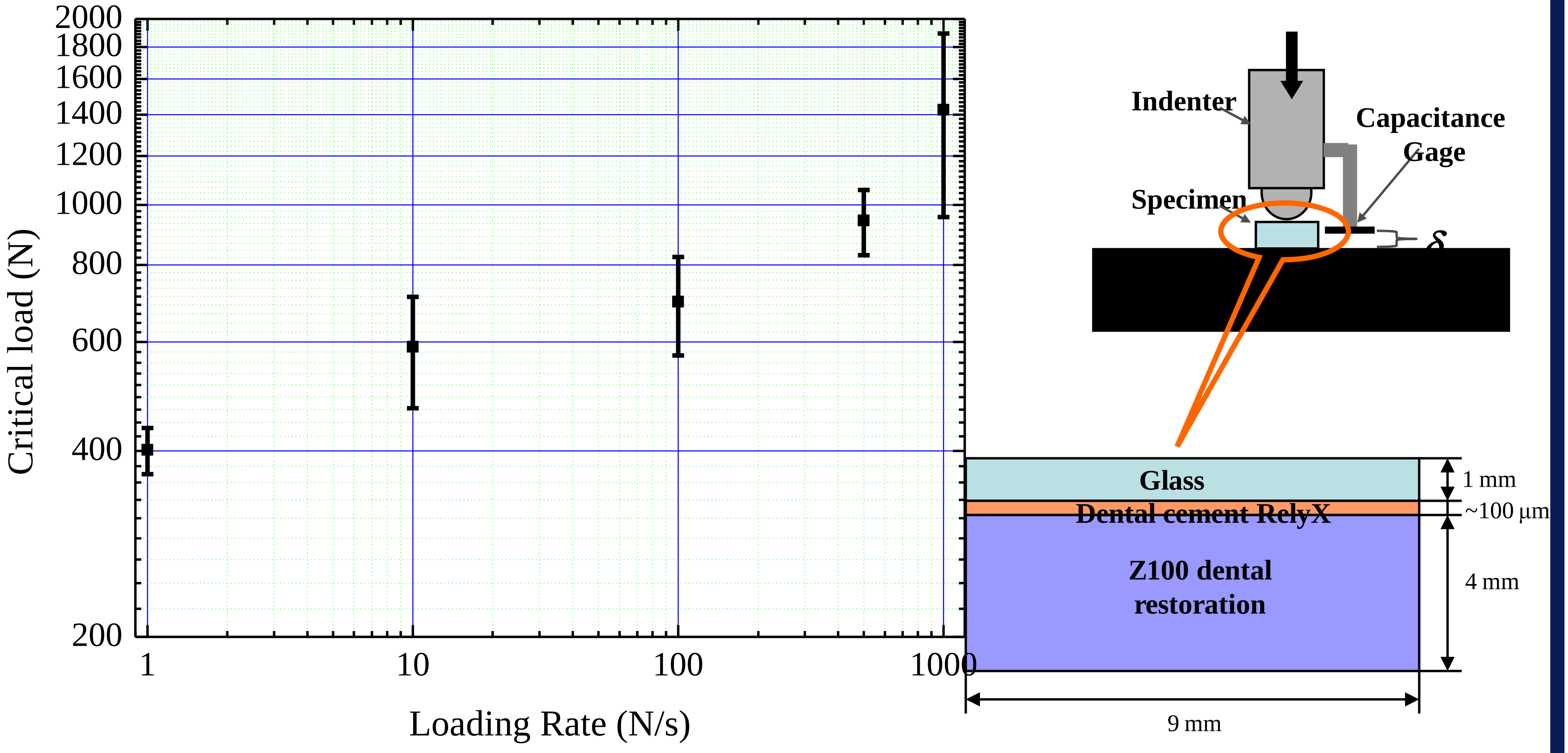
Loading rate effect of critical load measurements



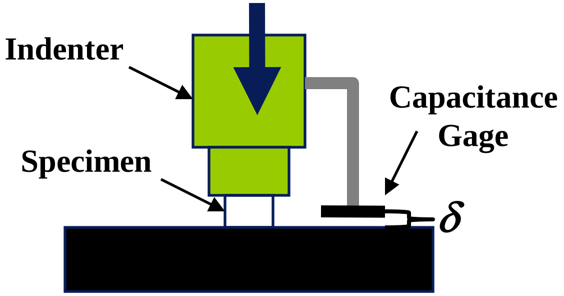


Loading rate 100 N/s

Loading rate effect of critical load on dental multilayer

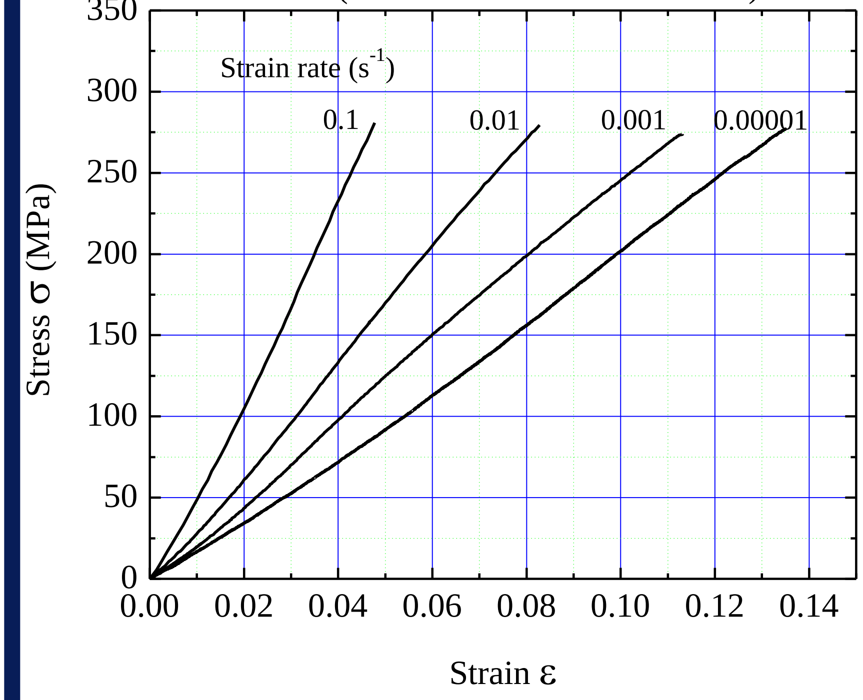


Rate Dependent Young's Moduli of Cement & Foundation Layers



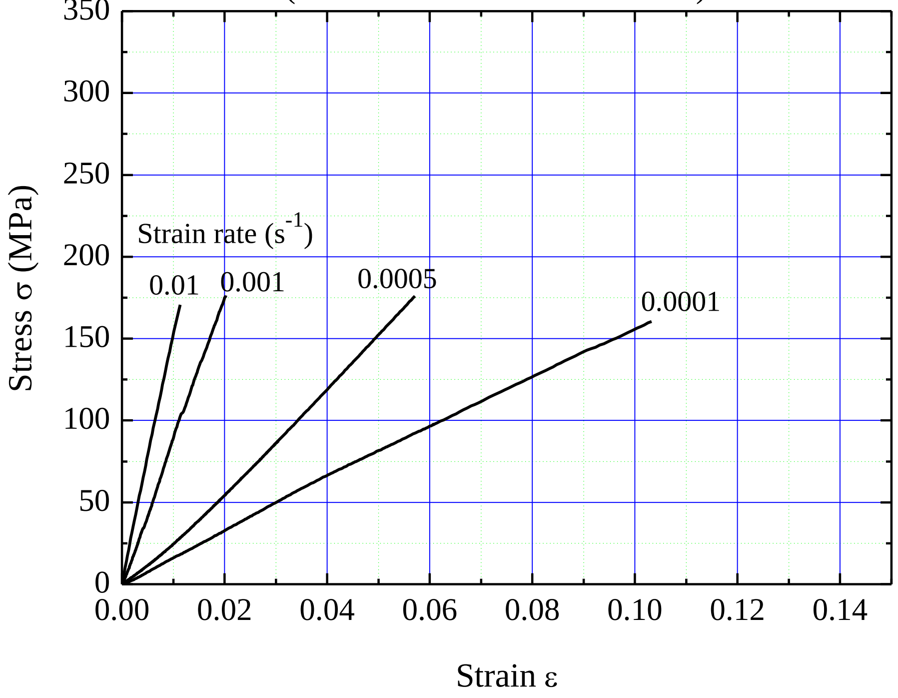
Dental Cement RelyX ARC

(1 mm thick and 7 mm diameter)



Dental Restoration Z100

(4 mm thick and 9 mm diameter)



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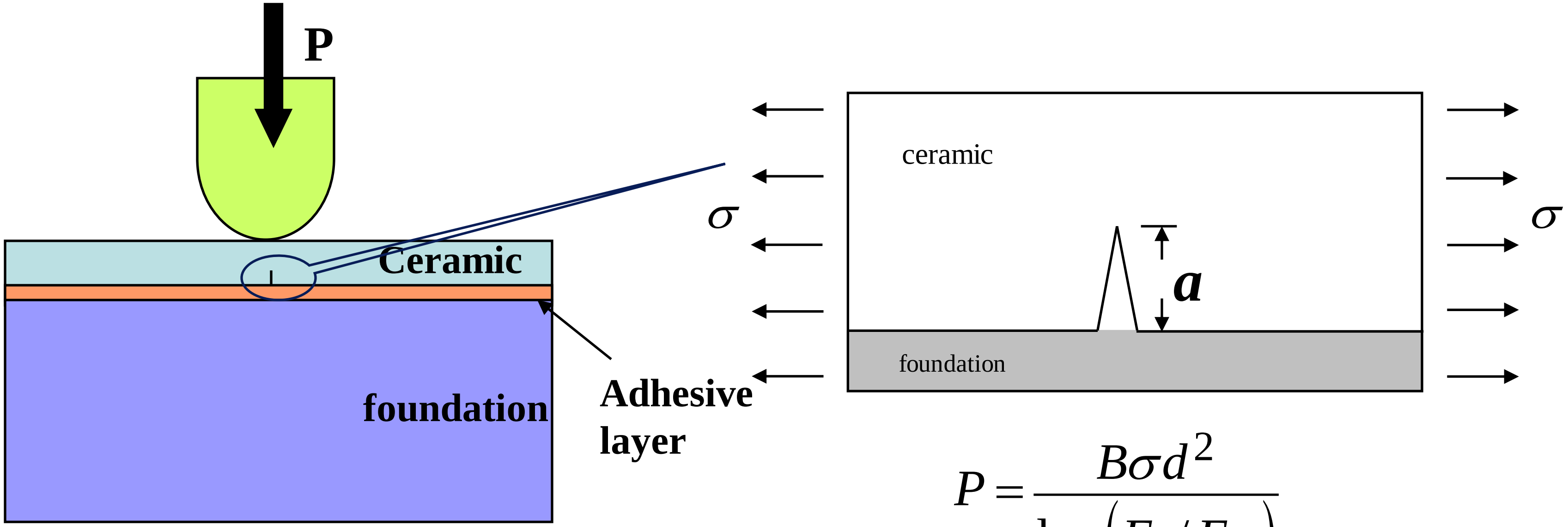
Elasticity Analysis

- Coating/substrate bi-layer model



$$P = \frac{B\sigma d^2}{\log\left(E_t / E_f\right)}$$

  - *B* and *d* are dimension coefficients

Bi-layer Slow Crack Growth solution

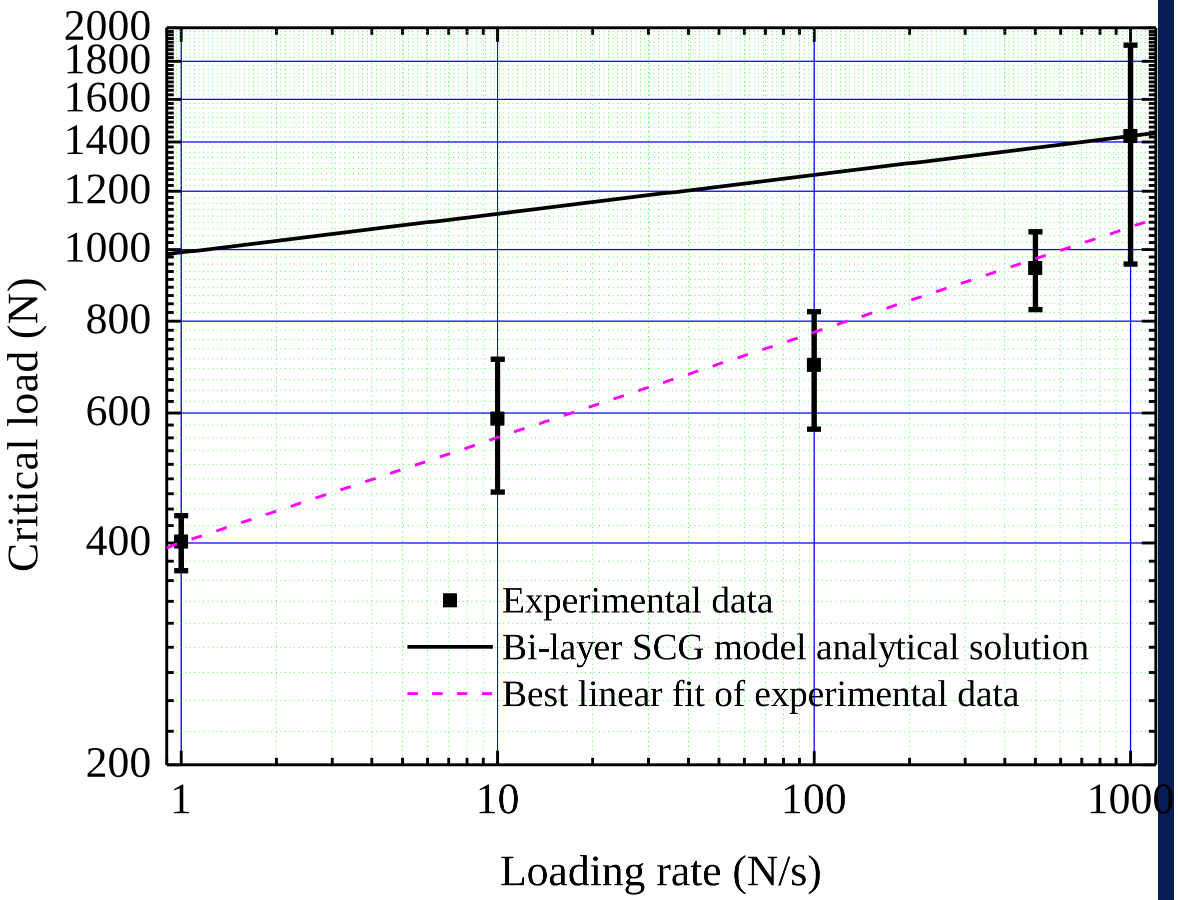
- Power law crack growth model

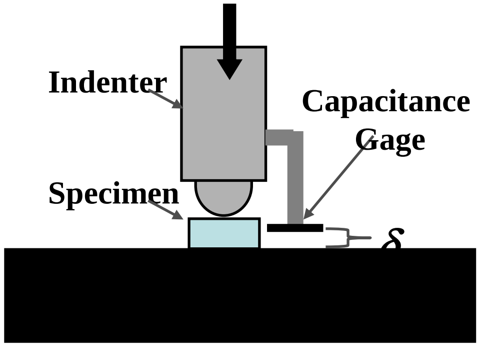
$$v = \frac{da}{dt} = v_0 \left(\frac{K}{K_{IC}} \right)^N$$

  - *K* is stress intensity factor = $\psi \sigma a^{1/2}$
  - *N* and v_0 are determined through four point bending tests

- Bi-layer SCG analytical solution (Lee. et al)

$$P_m = \left(A(N+1)\dot{P} \right)^{\frac{1}{N+1}}$$





Herztian contact Test data

D

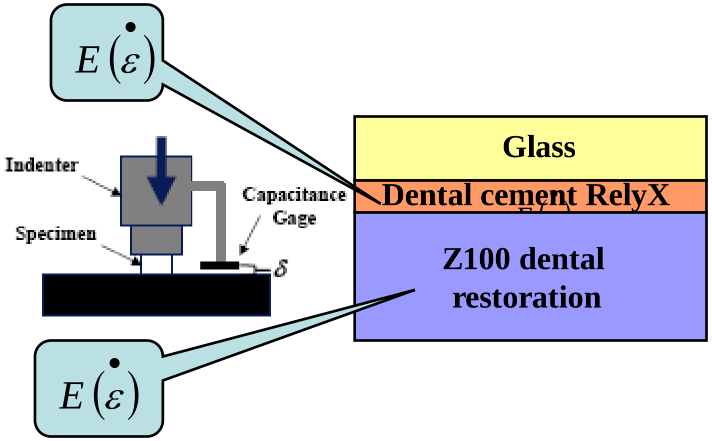
$$D=\frac{K_{Ic}^{N}\left(c_0^{1-N/2}-c_f^{1-N/2}\right)}{\left(N/2-1\right)v_0\beta^{N}}$$

SCG model for top glass layer

$$\int_0^{t_R}\sigma\left(t\right)dt=D$$

Glass

Z100 dental restoration



Finite element analysis (FEA)

$\sigma\left(t\right)$

Integration

Rupture time t_R

$$P_c=\dot{P}\bullet t_R$$

Critical load P_c

RDEASCG Model (Rate Dependent Elastically-Assisted SCG)

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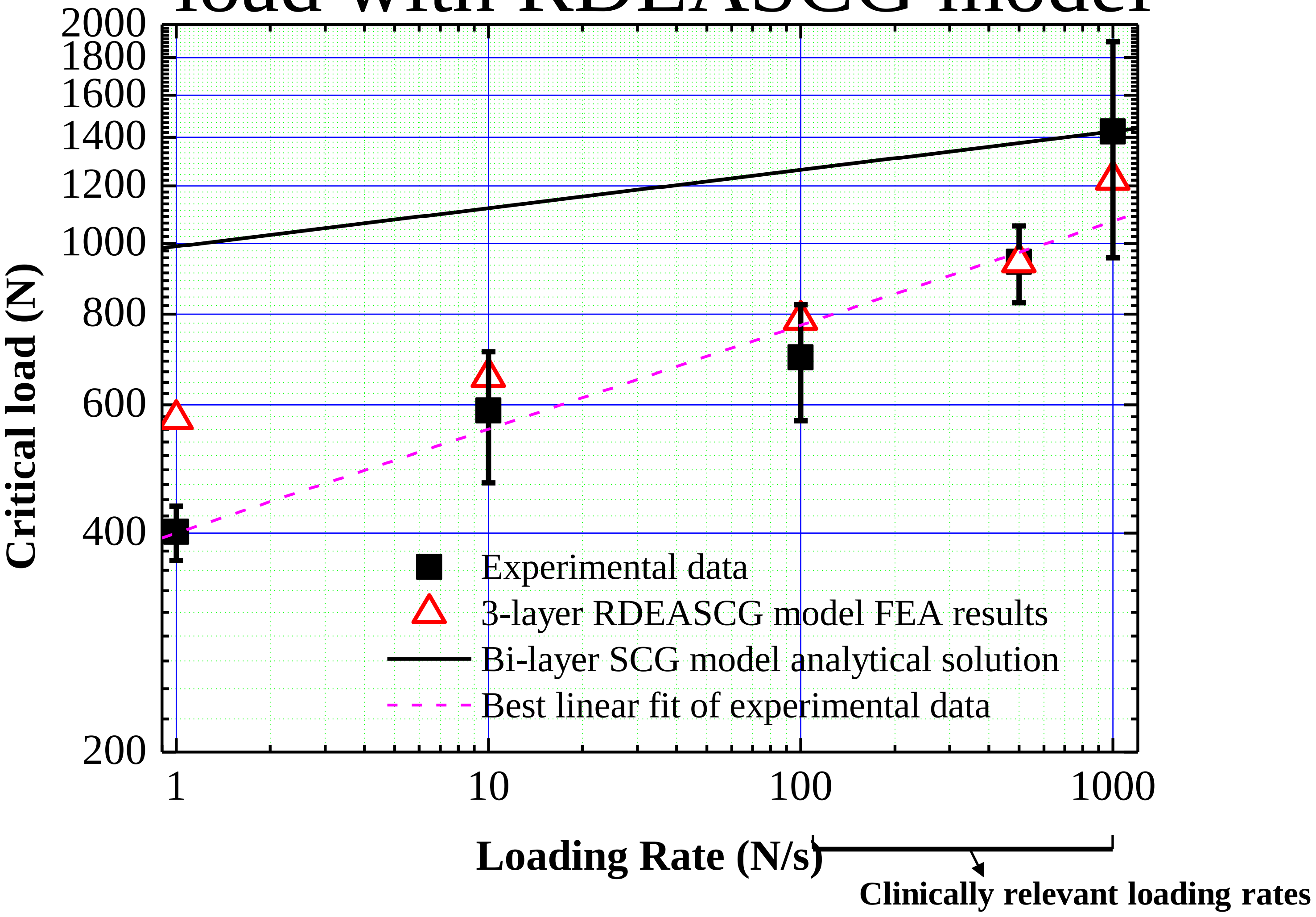
Prediction of Loading rate effect of critical load with RDEASCG model



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Summary – Loading Rate Effects

- Experimental

  -- studied constitutive behavior of individual layers

  -- studied rate-dependent critical loads in multilayer structure

  -- *in situ* study gives good observation of deformation and cracking in dental multilayer

- Modeling

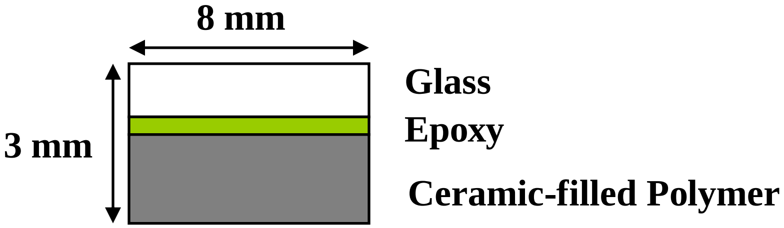
  -- implemented rate-dependent Young's modulus into multilayer structure with *real dental material*

  -- developed analytical model for reasonable prediction of deformation and cracking in dental multilayer under monotonic loading

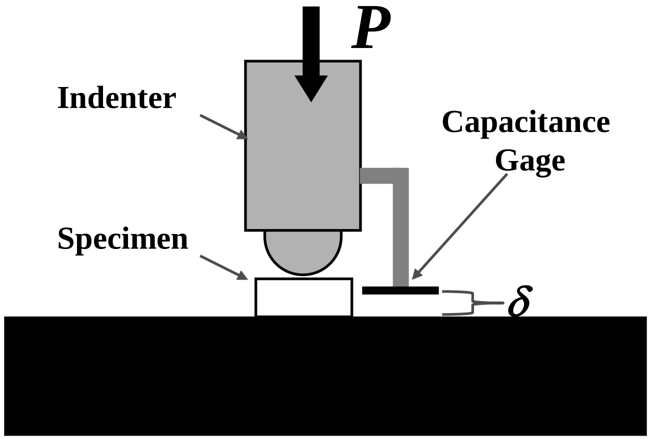
CYCLIC CONTACT EXPERIMENTS

- Model multilayers are subjected to cyclic Hertzian indentation for 10^6 cycles
- Peak load levels lower than observed crack initiation loads under monotonic loading

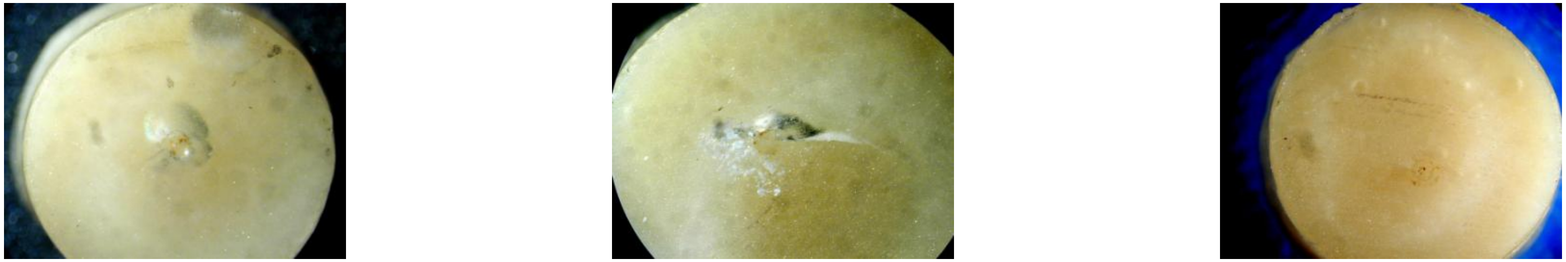
Model multilayer



Experimental set-up



CYCLIC HERTZIAN INDENTATION



0.8 mm, P=60 N

3.18 mm, P=70 N

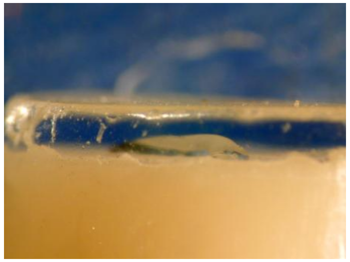
8 mm, P=90 N

Surface deformation after crack nucleation

0.8 mm, P=60 N

3.18 mm, P=70 N

Hertzian cone crack

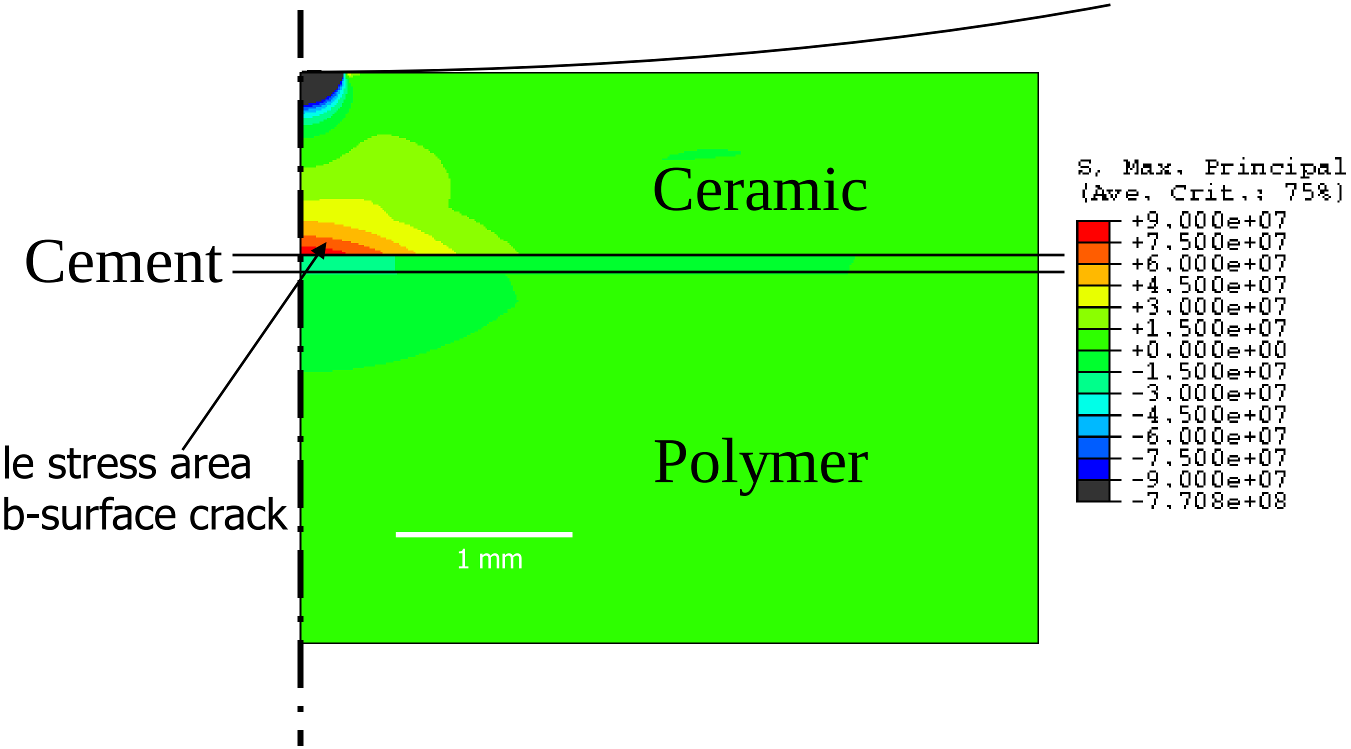


8 mm, P=90 N

Subsurface crack

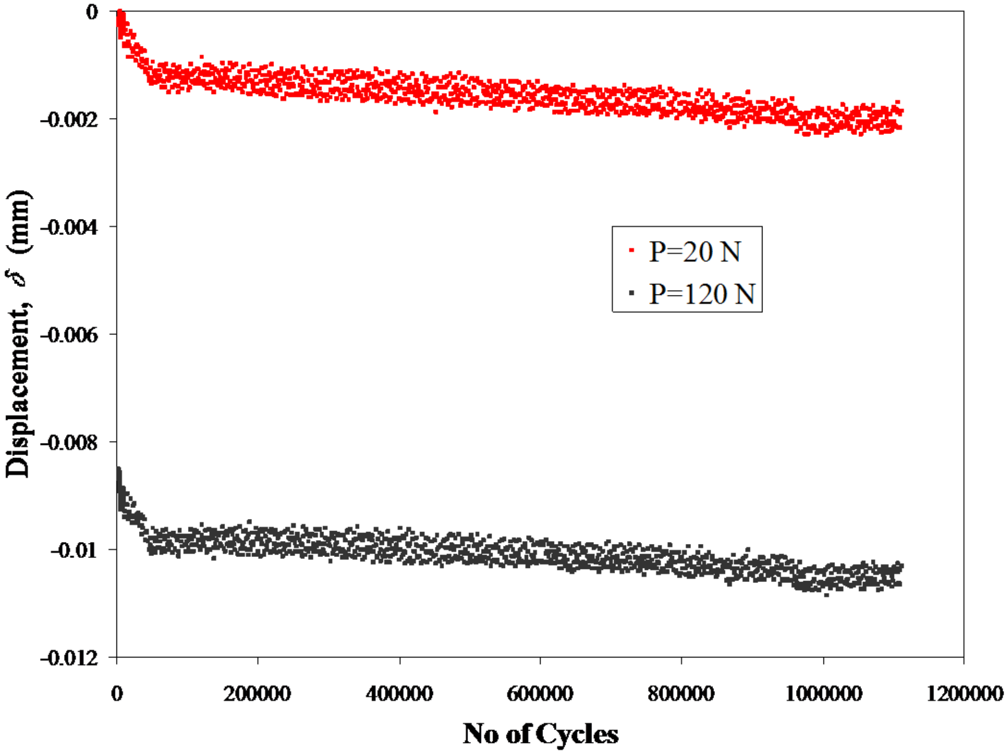
(Soboyejo et al, 2001)

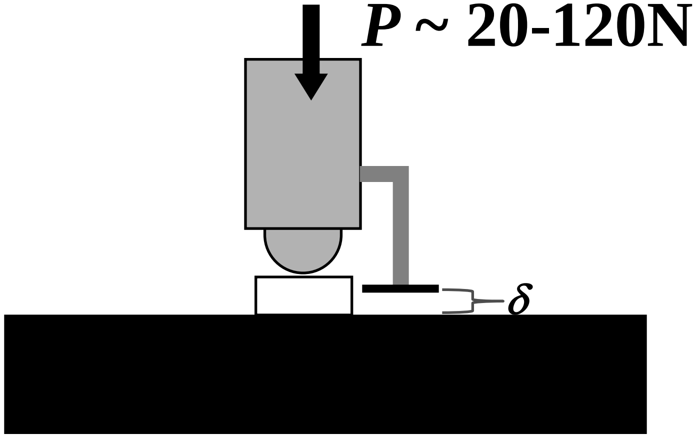
MAXIMUM PRINCIPAL STRESS DISTRIBUTION



high tensile stress area
causes sub-surface crack

DEFORMATION DURING CYCLIC LOADING





200 mm Indenter

$\delta_1(120) \sim -.0085$ mm

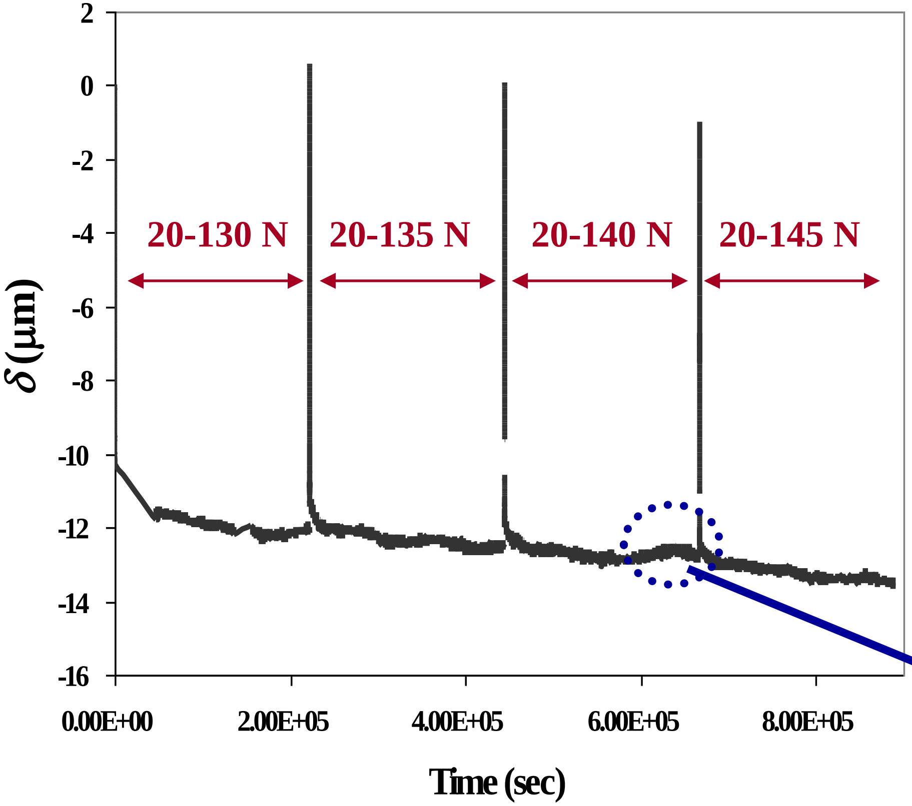
$\delta_{200}(120) \sim -.0089$ mm

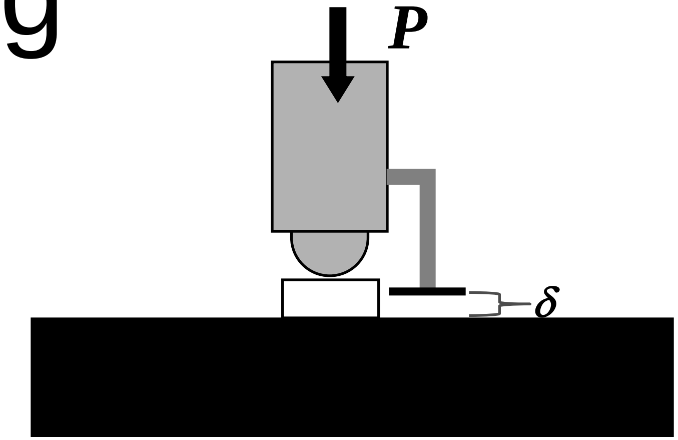
$\delta_{1100000}\,(120) \sim -.0105$ mm

Two Sources — Time dependent response of epoxy layer

— Accumulation of plastic strain in epoxy layer

Deformation During Cyclic Loading



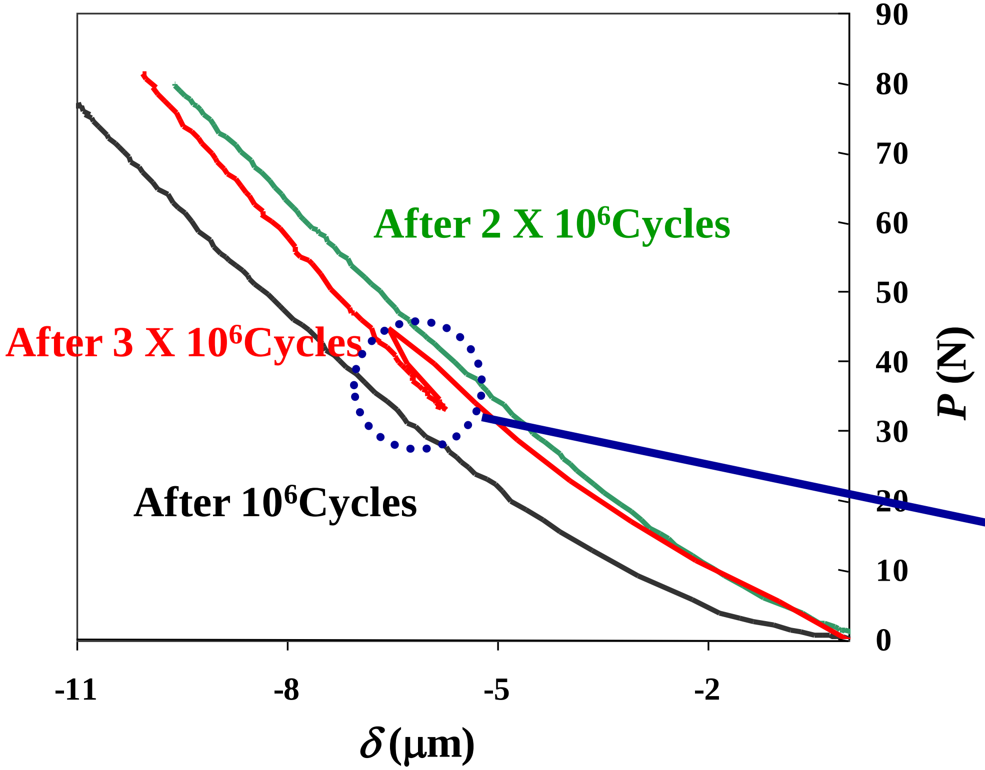


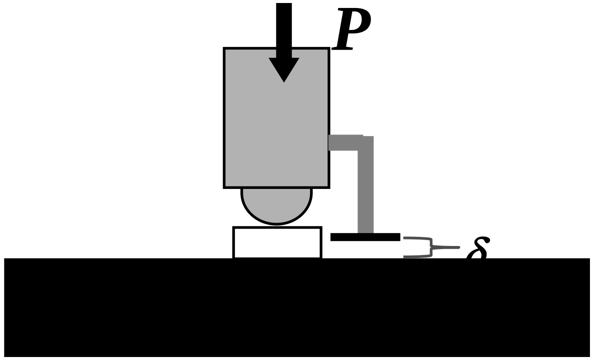
200 mm Indenter

Sharp Change in sample compliance

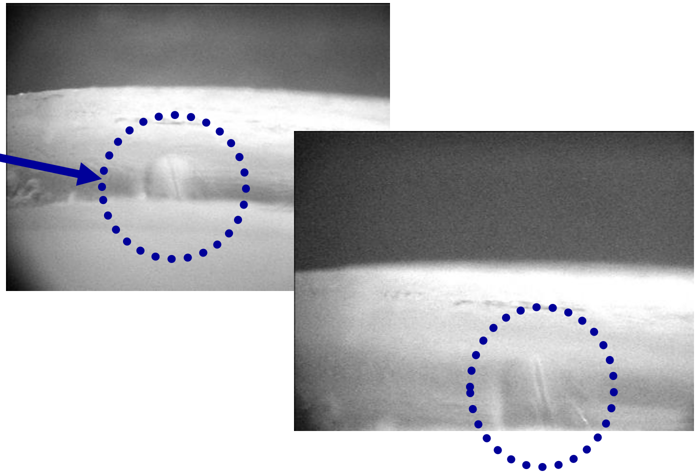
Sample loaded for million cycles at each load level at 5 Hz loading rate

Subsurface Pop-In Conditions

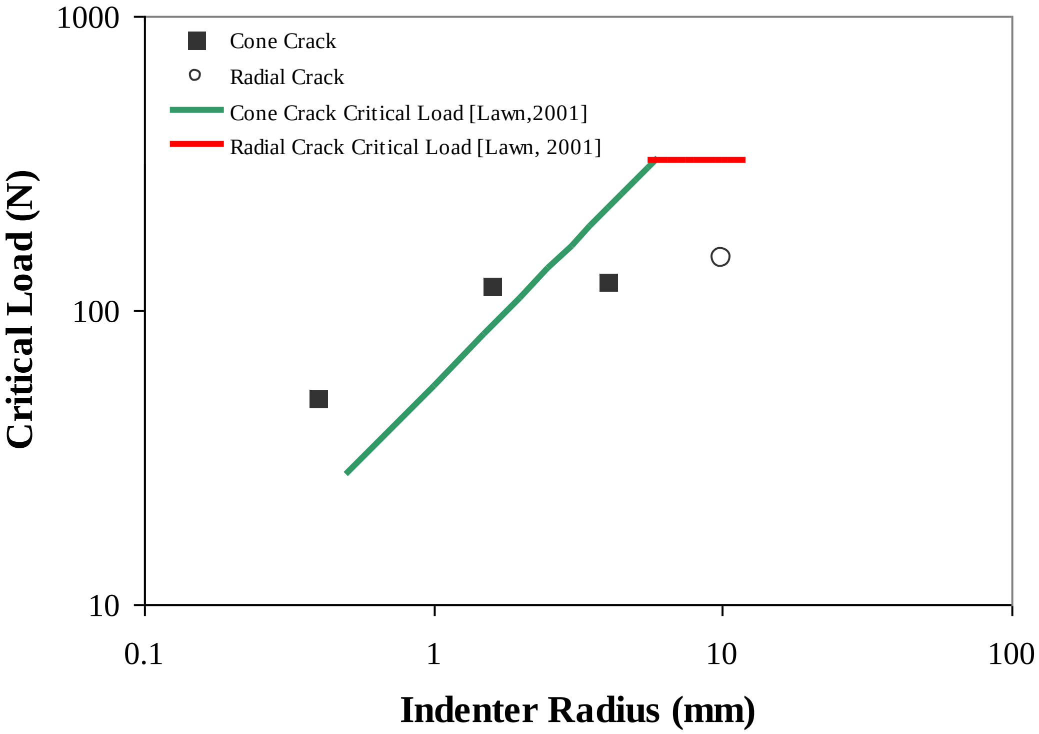




200 mm Indenter



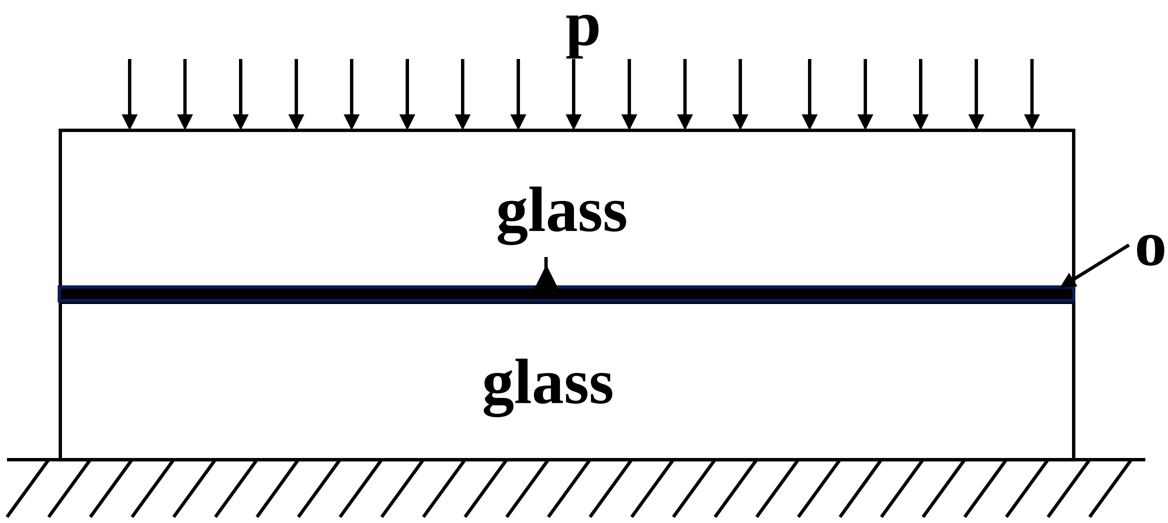
Pop-In Criteria(Lawn, 2001)

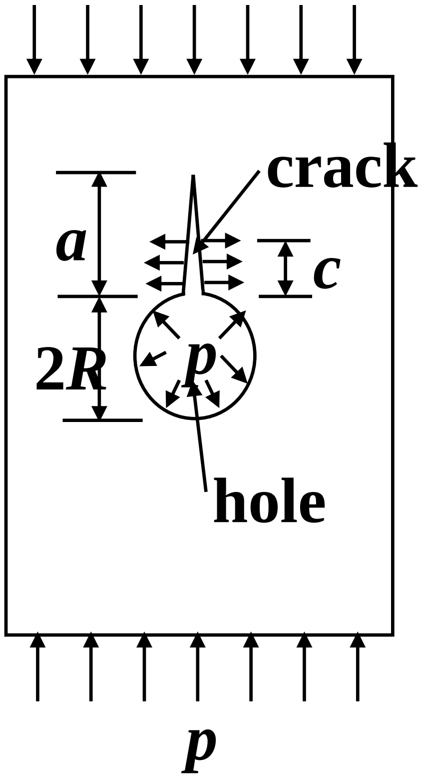


POSSIBLE MECHANISMS OF SUB-SURFACE CRACKING

- Mechanics-driven crack growth – due to flow of the cement into the crack
- Stress corrosion cracking
- Mechanical fatigue

HYDRAULIC FRACTURE TEST

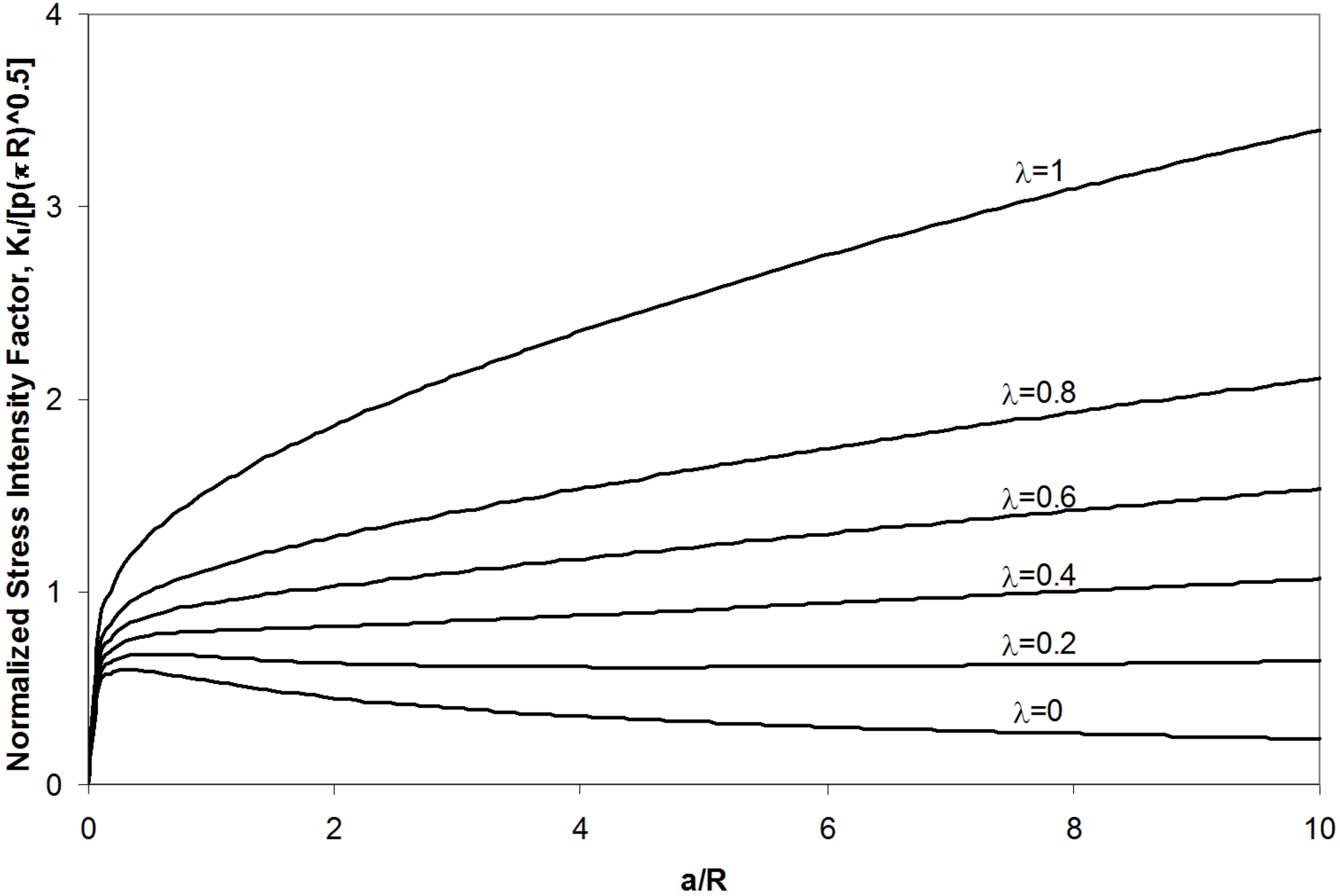




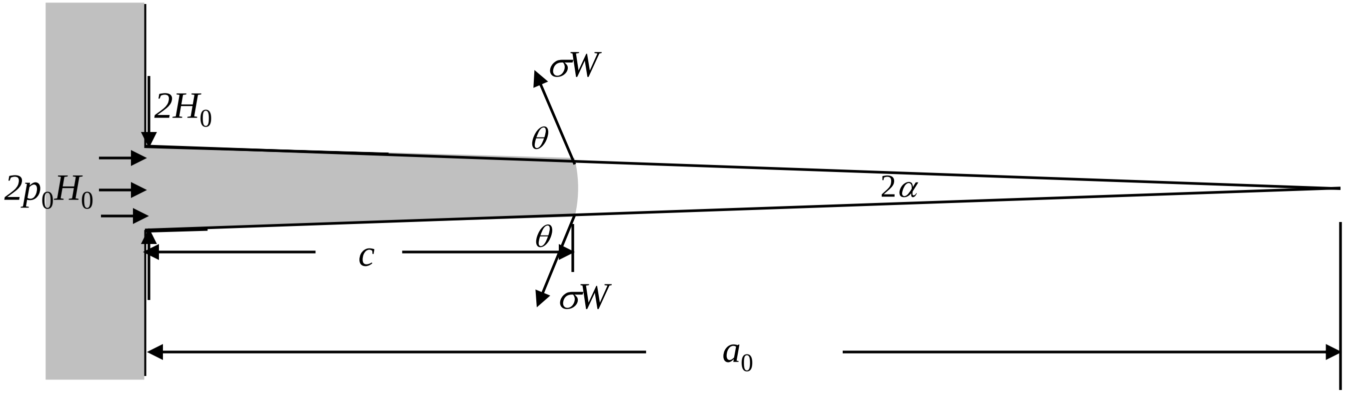
$\lambda = c/a$

Glass cracks under certain pressure.

NORMALIZED STRESS INTENSITY FACTOR



CEMENT FLOWS INTO CRACK



CRACK GROWTH RATE

$$\frac{da}{dt} = \frac{2H^2 p_0}{3\mu a} \cdot \frac{1}{\sin\left[K_c\sqrt{\pi}/\left(p_0\sqrt{a}\right)\right]} \cdot \frac{1}{\tan\left[K_c\sqrt{\pi}/\left(2p_0\sqrt{a}\right)\right] - K_c\sqrt{\pi}/\left(4p_0\sqrt{a}\right)} \cdot \left(1 - \frac{\sigma\cos\theta}{p_0 H}\right)$$

$$\left.\frac{da}{dt}\right|_{a\to\infty} = \frac{8H^2 p_0^3}{3\pi\mu K_c^2} \cdot \left(1 - \frac{\sigma\cos\theta}{p_0 H}\right)$$

If H= 1μm, p_0=2 MPa, K_c=0.5 MPa-s, μ=100 Pa-s, σcosθ=0.005 N/m, then

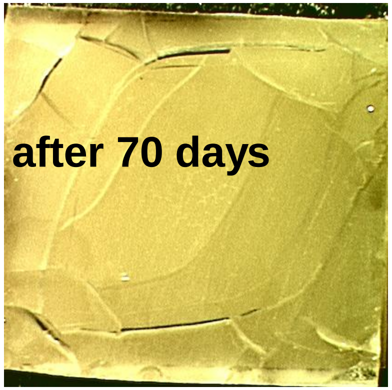
da/dt = 0.27 μm/s

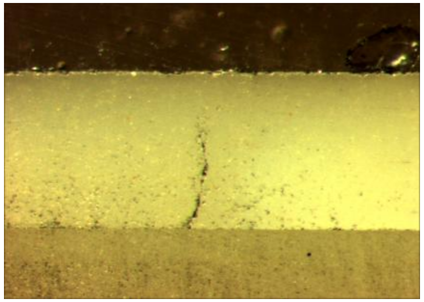
Summary – Cyclic Contact

- Pop-in conditions are strongly influenced by ball size in Hertzian indentation experiments
- Ball size effects explained using simple contact mechanics models
- Hydraulic fracture may be caused by water within cracks
- Mechanics model developed for hydraulic fracture modeling
- Mechanistically-based fatigue model needed

Modeling of Water Diffusion

- Cracking is shown in top ceramic layer after the dental multilayers immersed in water for some time.
- Major observations:
  1. cracking occurs after some time, and becomes more extensive as time increases.
  2. cracking first occurs near the edge of the sample and propagates parallel to the edge.
  3. cracking initiates from the bottom surface of the top layer.





Courtesy of Prof. V.P. Thompson, NYU Dental School

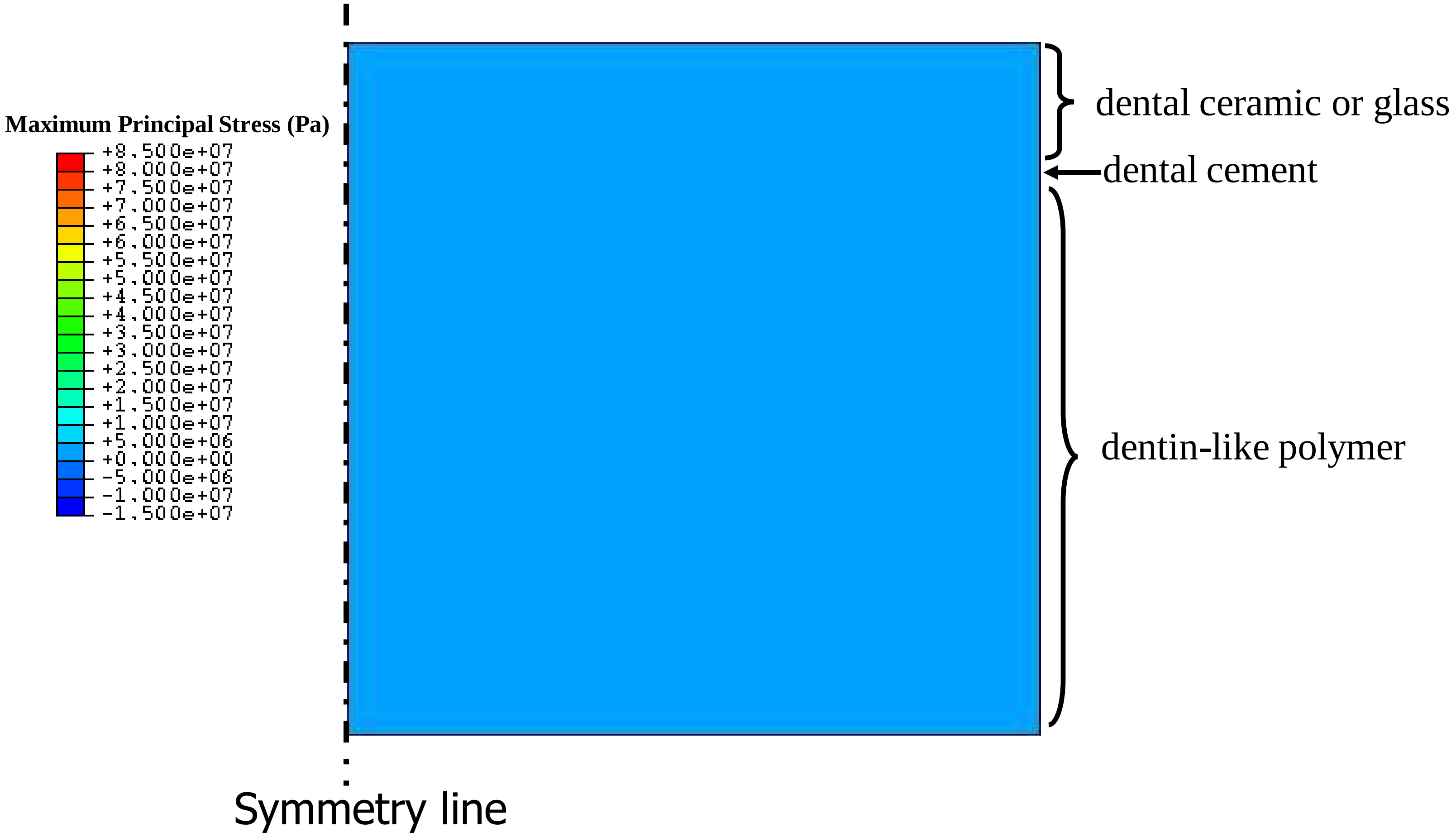
Real Questions

- Is the stress induced by water diffusion high enough to cause the cracking?
- Can the crack pattern be understood by water diffusion induced SCG?

Thermal diffusion analogy

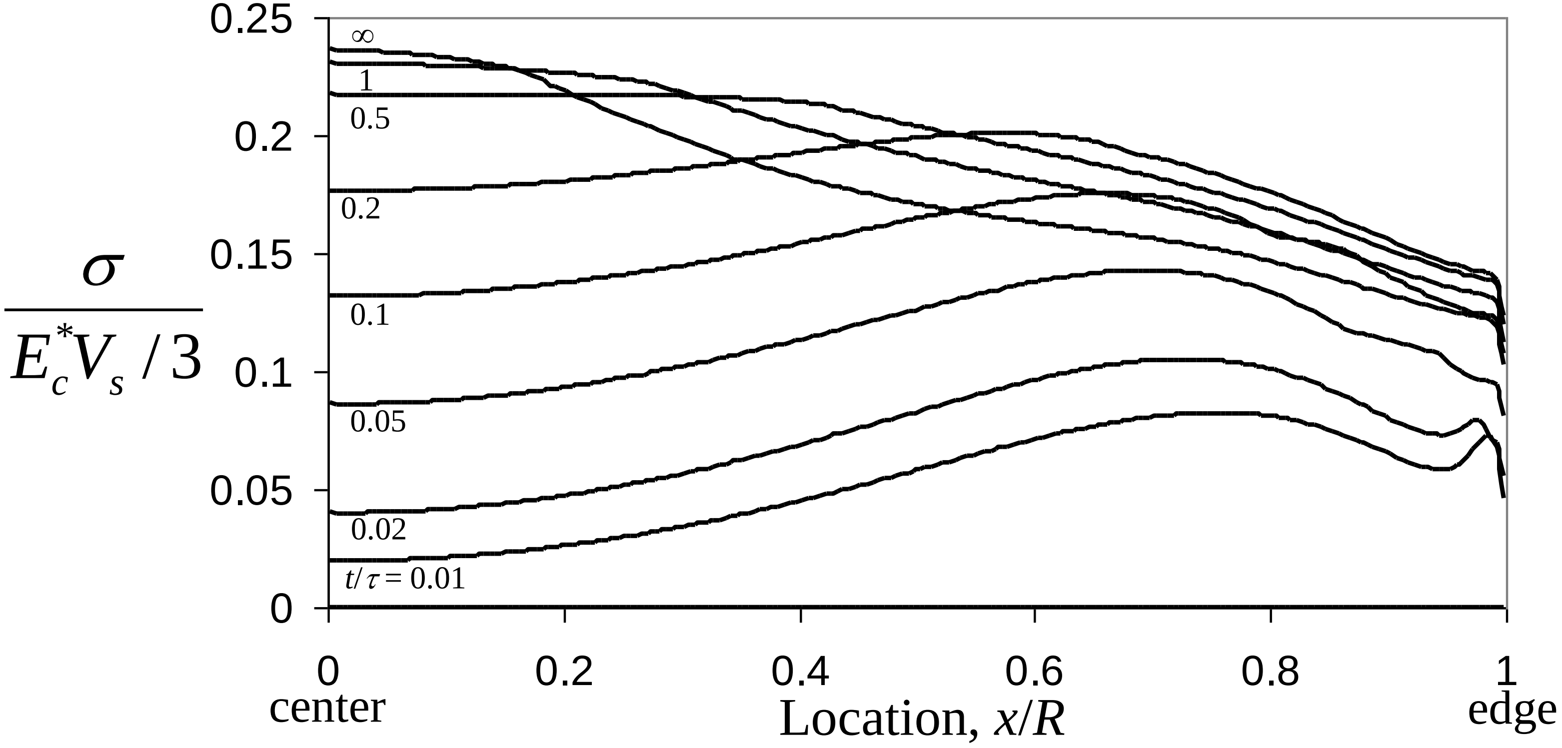
Water diffusion → Heat transfer
Water induced foundation expansion → Thermal expansion

MAXIMUM PRINCIPAL STRESS DISTRIBUTION DURING WATER DIFFUSION



- Maximum tensile stress appears at the bottom surface of the top layer.
- Peak tensile stress first appears near the edge and is parallel to the edge.

Maximum Principal Stress Distributions in Dental Crown Multilayer



$$\tau = \frac{(\text{length scale})^2}{\text{diffusivity}} \sim \frac{\left(5\times10^{-3}\ \text{m}\right)^2}{10^{-12}\ \text{m}^2/s} = 289\ \text{days}$$

$$E_c^* \sim 100\text{GPa} \quad V_s \sim 1\% \quad E_c^* V_s / 3 \sim 300\text{MPa}$$

Slow Crack Growth Theory

Crack growth rate: $da/dt = v_0 \left(K/K_{IC}\right)^N$

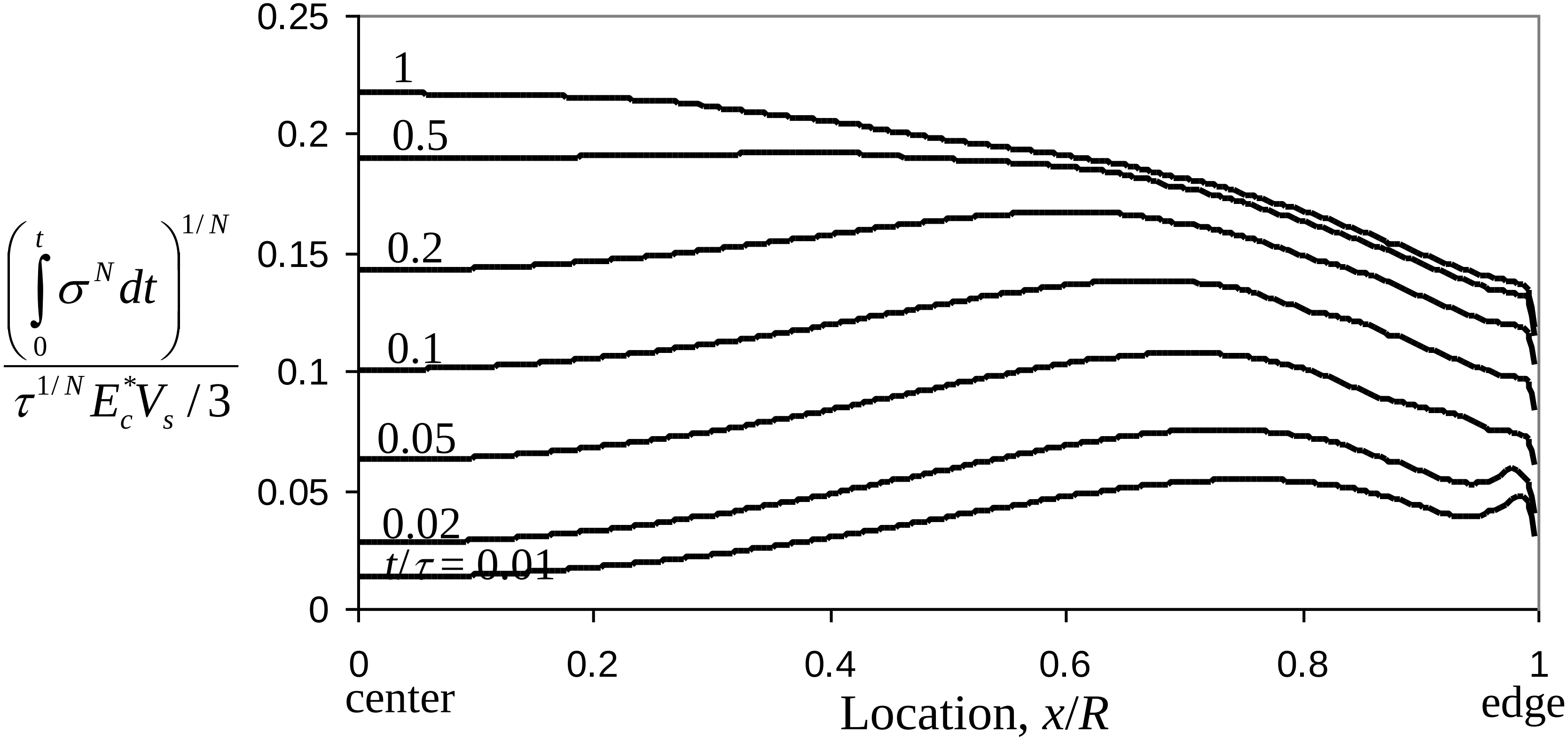
Stress intensity factor: $K = \psi \sigma a^{1/2}$

Criteria to form subsurface crack: $\int_0^{t_R} \sigma(t)^N dt = D$

$D \approx \dfrac{K_{IC}^N}{(N/2-1) v_0 \psi^N a_i^{N/2-1}}$ independent of time and load

Driving force to form subsurface crack: $\boxed{\left[\int_0^t \sigma(t)^N dt\right]^{1/N}}$

SCG in Top Glass Layer Due to Water Diffusion



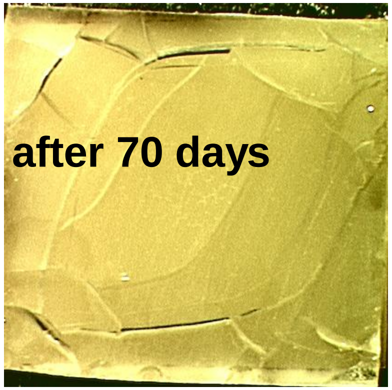
- Water diffusion is very important in determining the lifetime of dental multilayers.

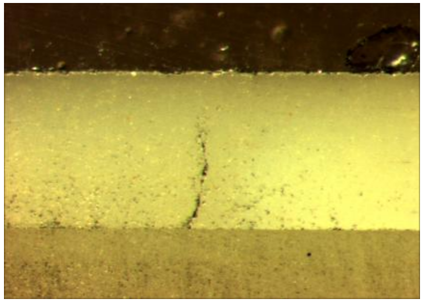
Summary – Modeling of Water Diffusion

- Model predicts the cracking in the top ceramic layer after the dental multilayers immersed in water for some time.
- Model also predicts the major observations:
  1. cracking occurs after some time, and becomes more extensive as time increases (due to stresses associated with water distribution).
  2. cracking first occurs near the edge of the sample and propagates parallel to the edge (consistent with stresses and slow crack growth).
  3. cracking initiates from the bottom surface of the top layer (ditto).


after 6 days

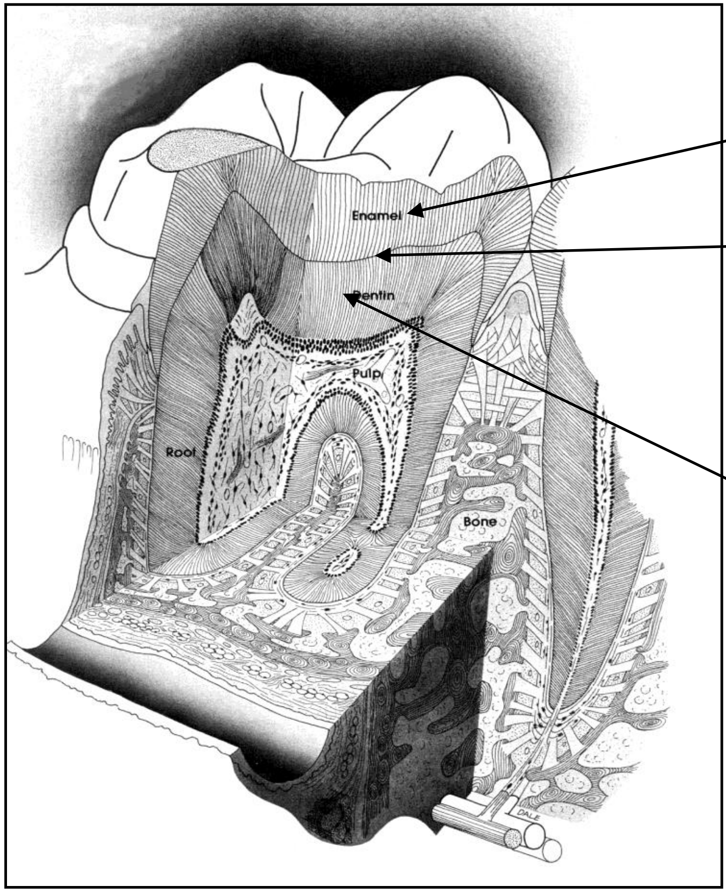

after 15 days


after 70 days



Courtesy of Prof. V.P. Thompson, NYU Dental School

BIO-INSPIRATION - TOOTH STRUCTURE

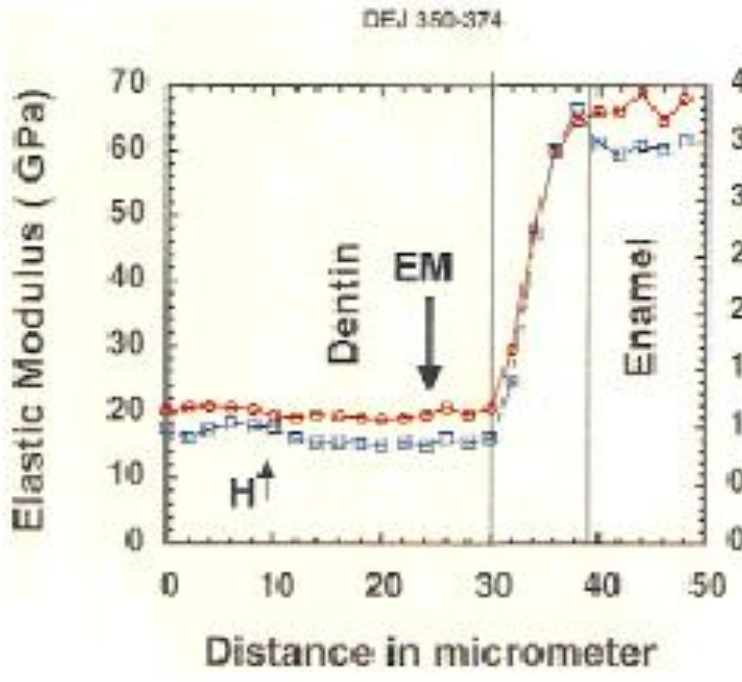


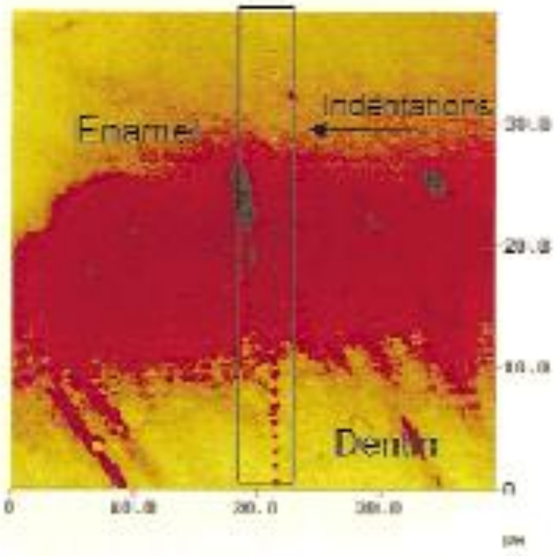
Enamel

Dentin-Enamel-Junction (DEJ)

Dentin

ELASTIC MODULUS DISTRIBUTION IN DENTIN-ENAMEL JUNCTION (DEJ)

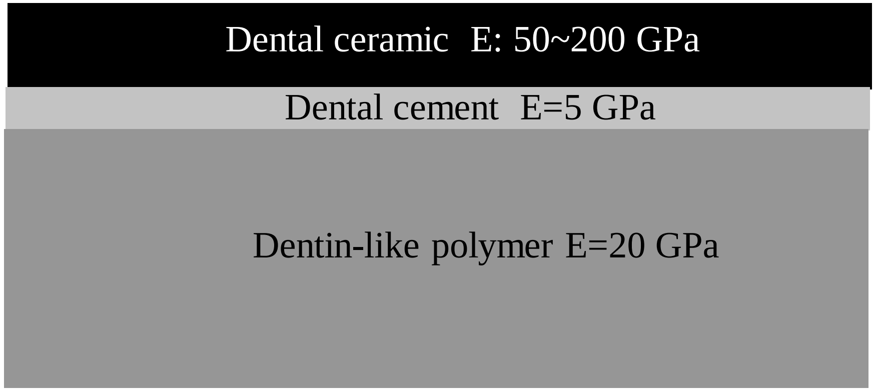




G.W. Marshall Jr., et al. *J Biomed Mater Res* 54, 87-95, 2001

MECHANICAL PROPERTIES OF DENTAL MATERIALS/MULTILAYERS

Dental restoration

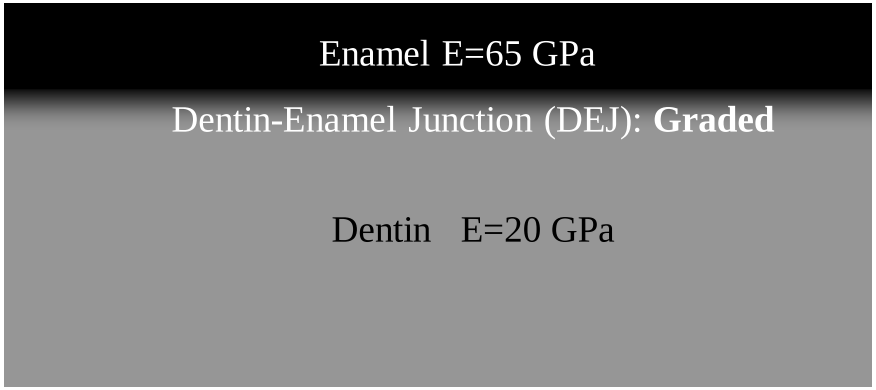


Dental ceramic E: 50~200 GPa

Dental cement E=5 GPa

Dentin-like polymer E=20 GPa

Real tooth

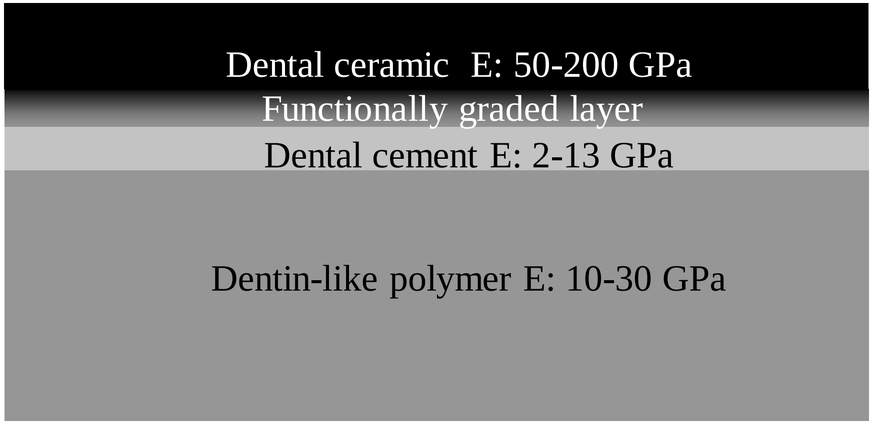


Enamel E=65 GPa

Dentin-Enamel Junction (DEJ): **Graded**

Dentin E=20 GPa

DENTAL CROWN RESTORATION FGM DESIGN



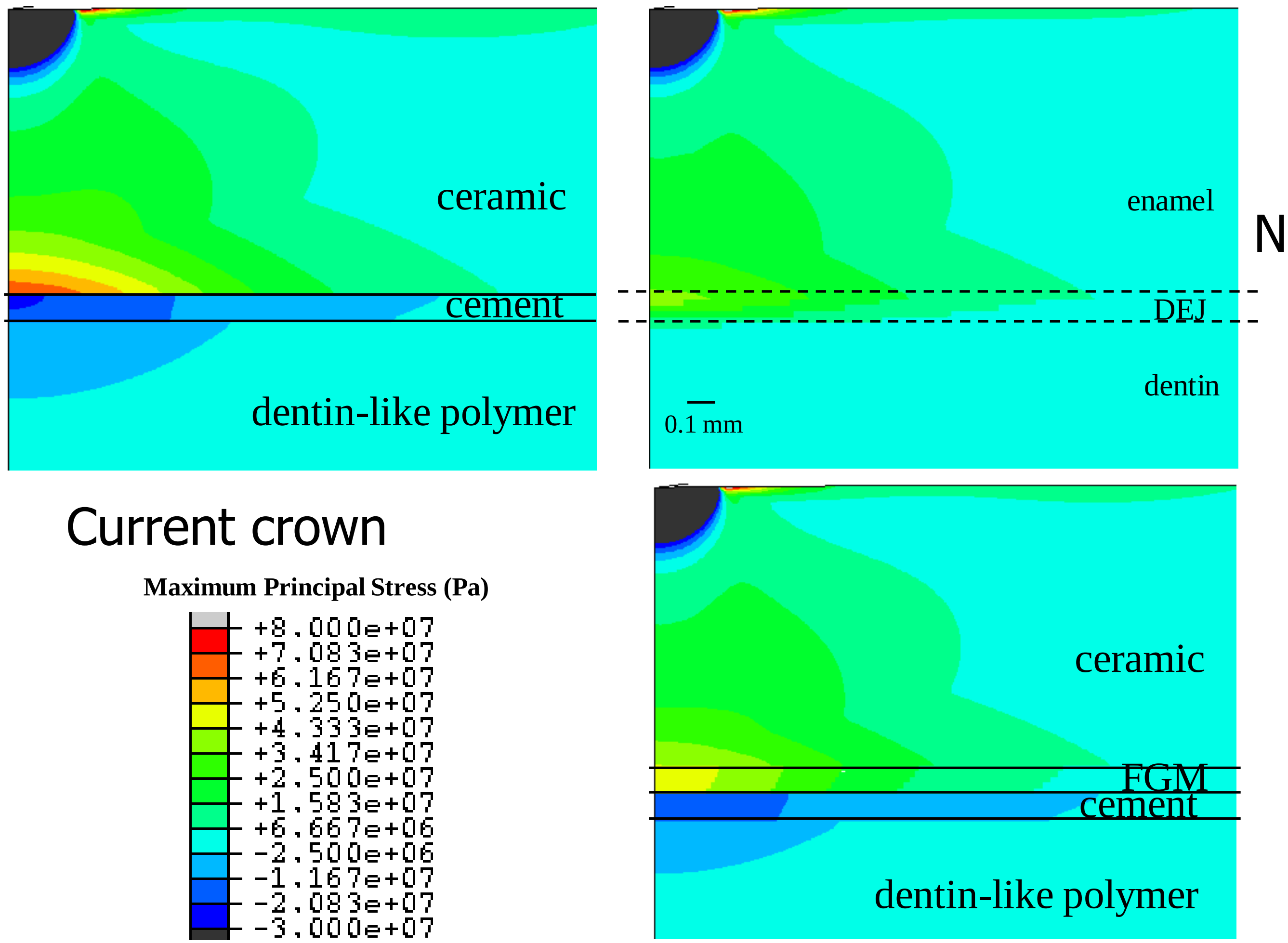
Dental ceramic E: 50-200 GPa

Functionally graded layer

Dental cement E: 2-13 GPa

Dentin-like polymer E: 10-30 GPa

MAXIMUM PRINCIPAL STRESS DISTRIBUTION

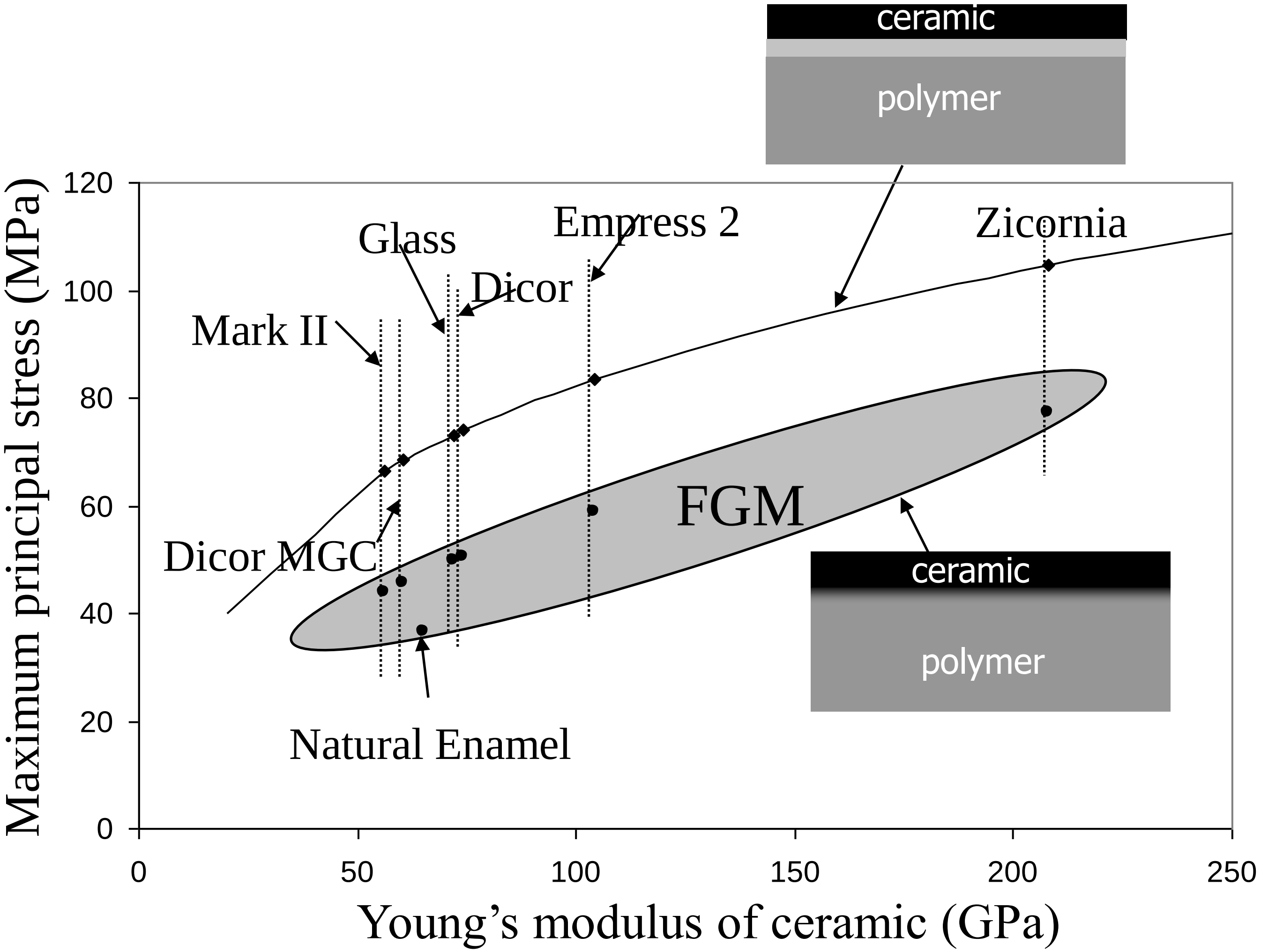


Current crown

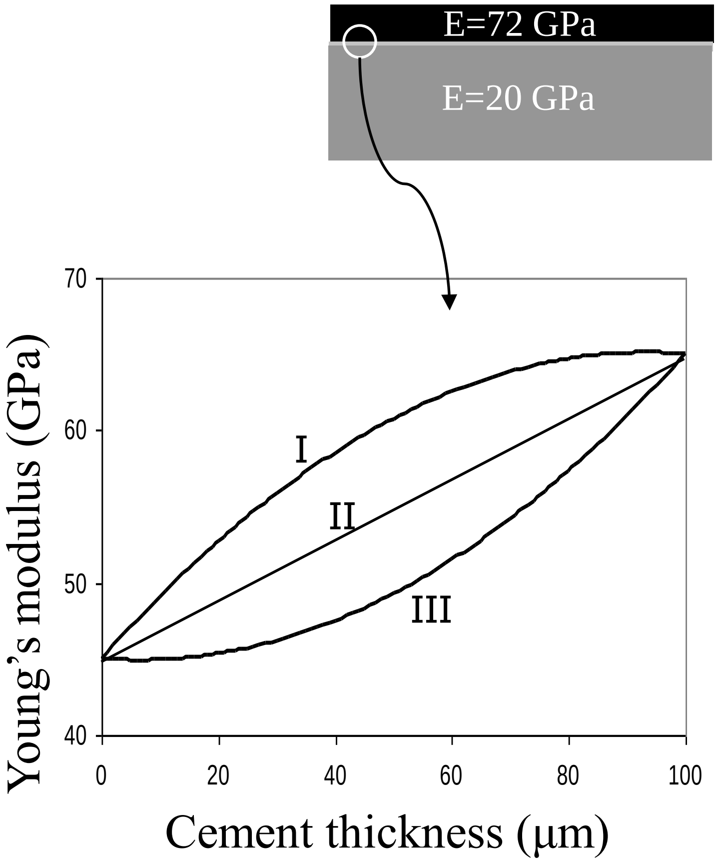
Natural tooth

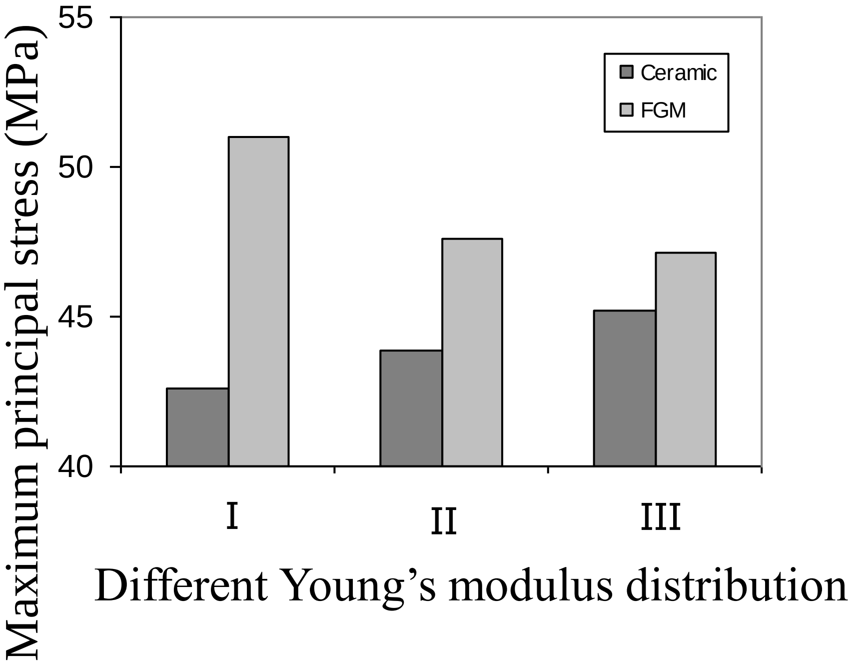
FGM design

Maximum Principal Stress

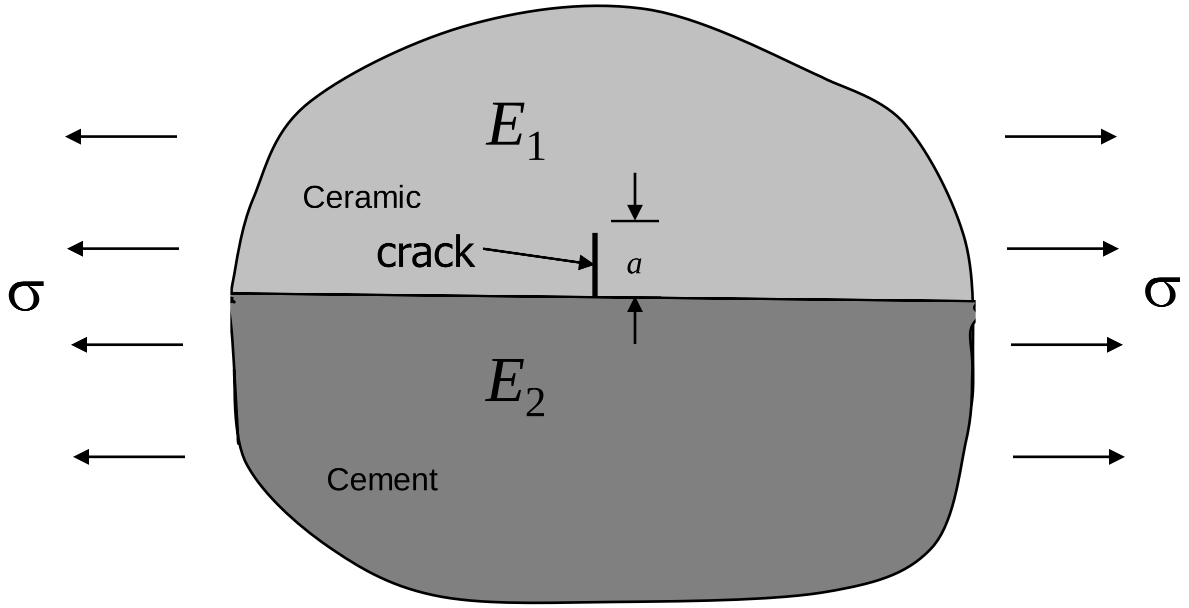


Effects of Different Distributions of Young’s Modulus





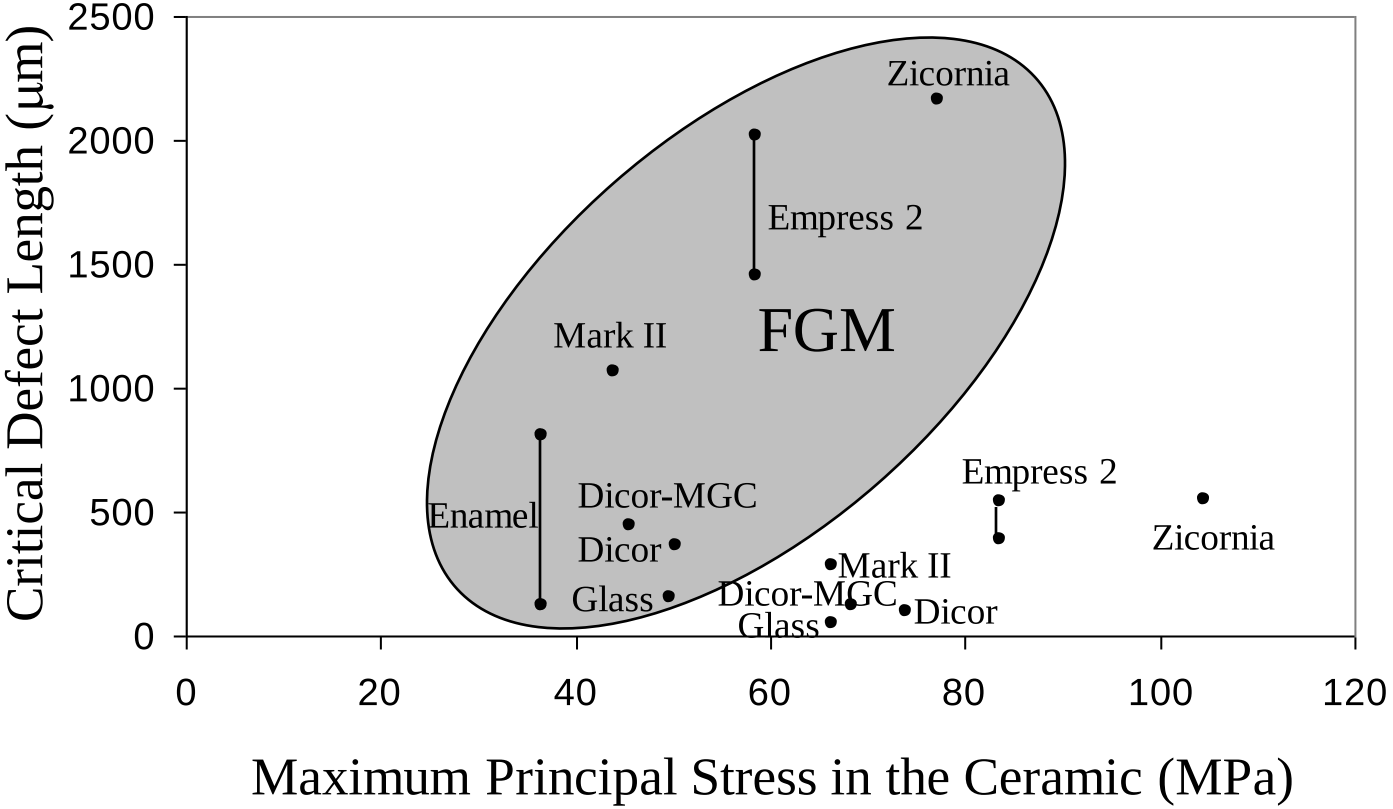
Effects of FGM on Fracture Toughness



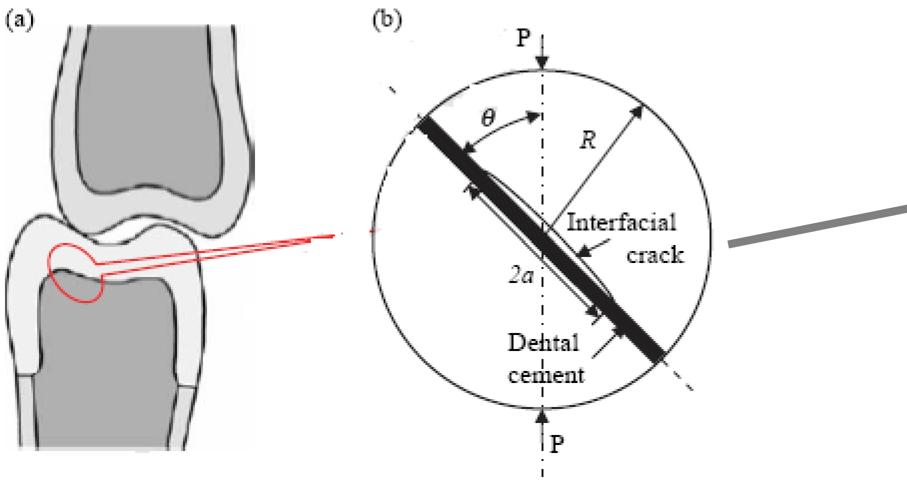
Stress intensity factor: $K_I = \beta \sigma \sqrt{\pi a}, \qquad \beta = f\left(E_2 / E_1, \nu_1, \nu_2\right)$

Critical defect length: $a_c = K_c^2 / \left(\pi \beta^2 \sigma^2\right)$

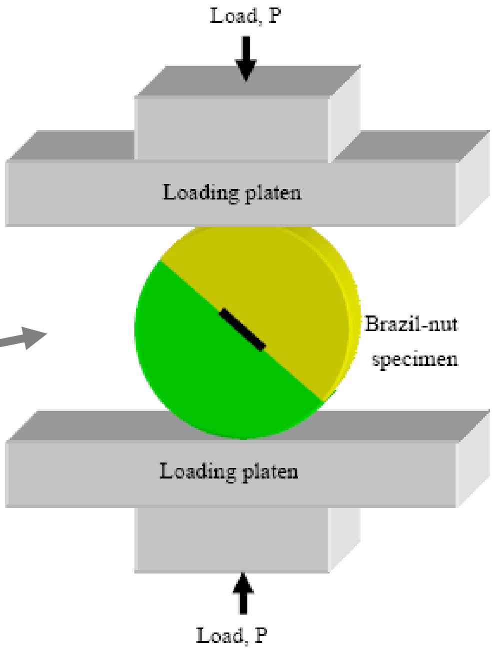
Comparison of Critical Defect Lengths



Brazil-nut Sandwich Sample Test in Determining Interfacial Toughness between a Dental Cement Composite and Glass Substrate



Schematics of (a) teeth contact during chewing and (b) Brazil-nut sandwich samples under contact loading

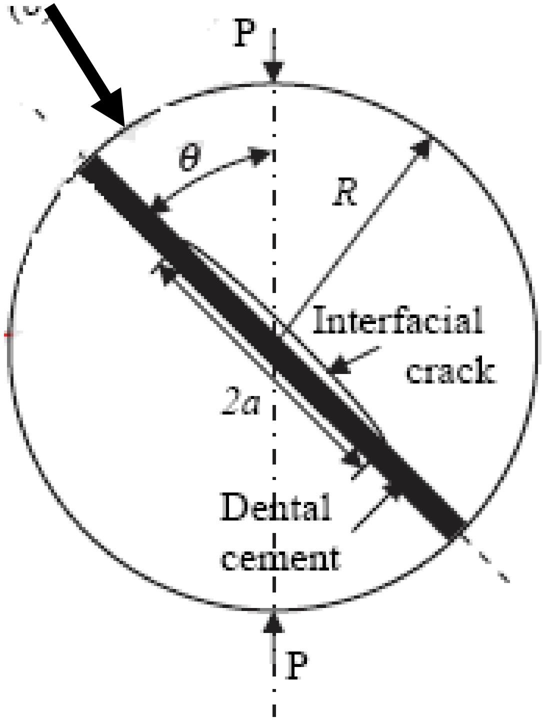


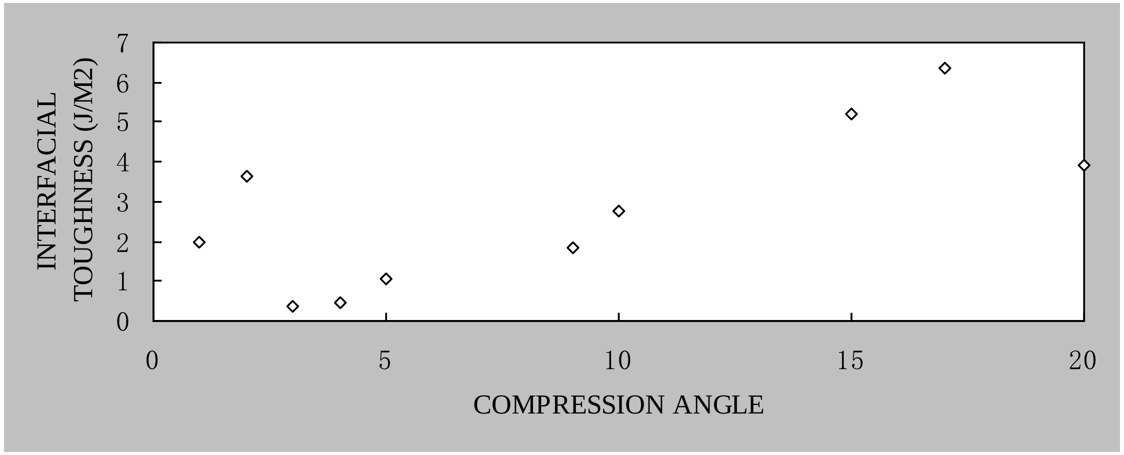
Schematic illustration of Brazil-nut sandwich sample and setup for fracture testing

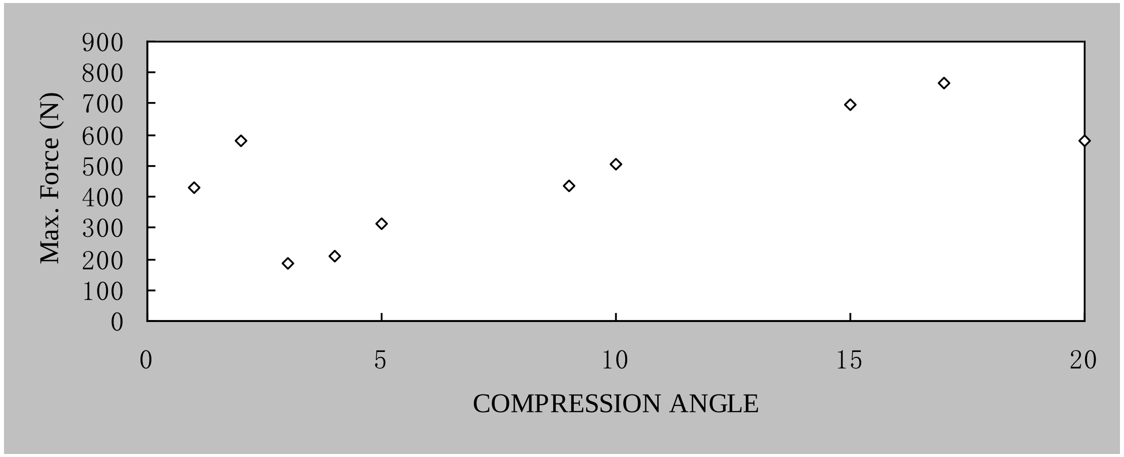
Experimental Results of Brazil-nut Sandwich Sample Test

Compression Angle

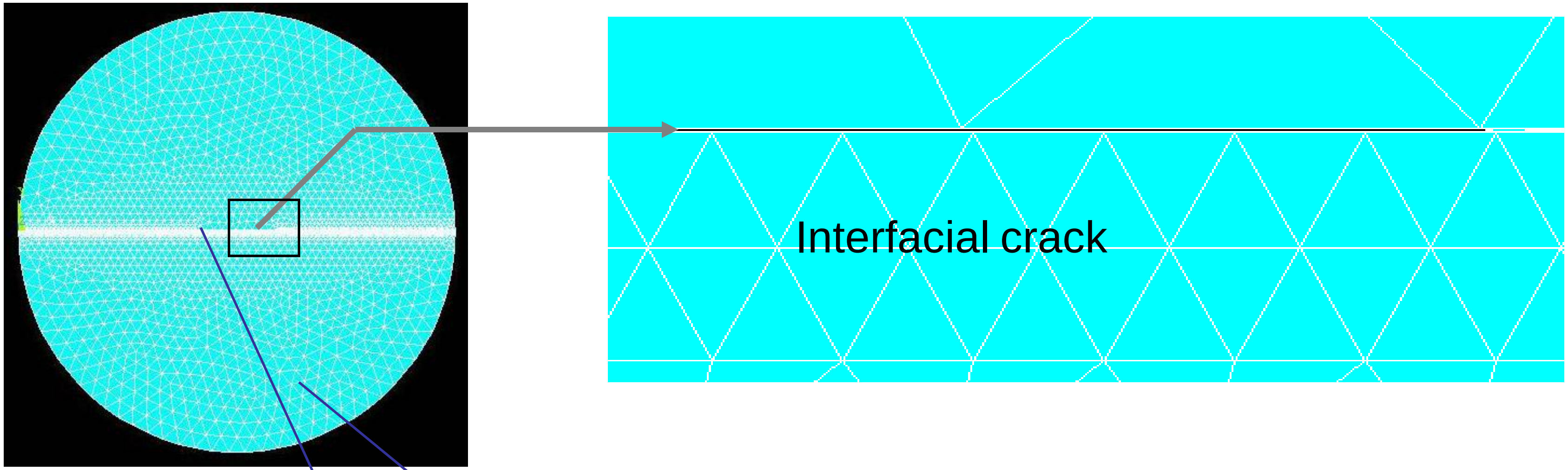
Applied Force







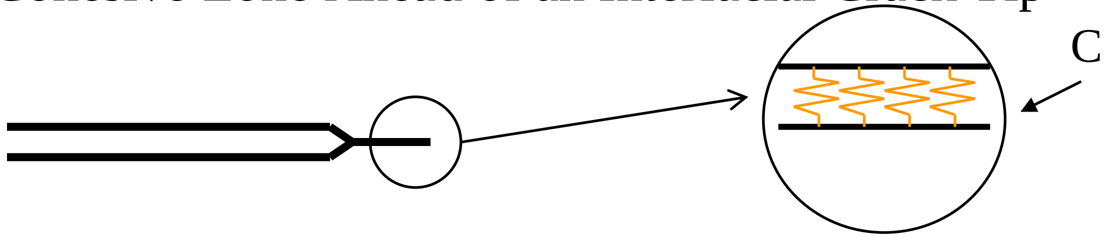
Geometry of Brazil-nut Sandwich Sample in Numerical Simulation



Glass Substrate		
	E (GPa)	ν
	70	0.2
Epoxy Interlayer		
	E (GPa)	ν
	10	0.35

Introduction to Cohesive Zone Models for Interfacial Failure

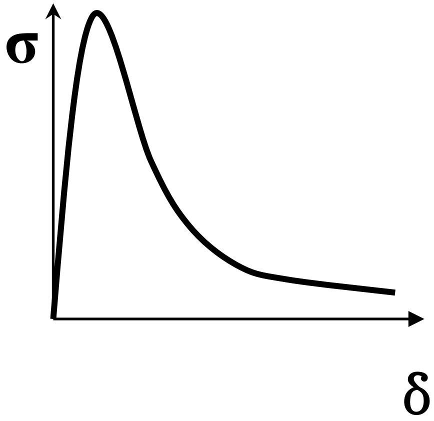
- Cohesive Zone Ahead of an Interfacial Crack Tip



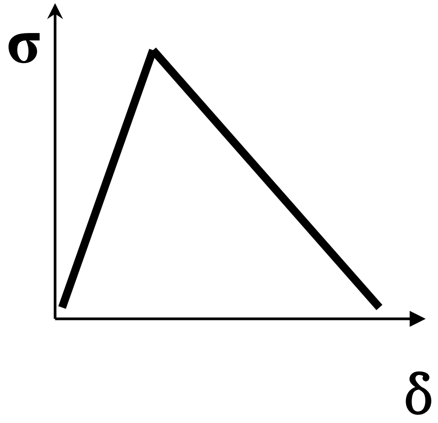
Cohesive Bond Structure

Cohesive Bond Rupture Leads to Physical Crack Growth

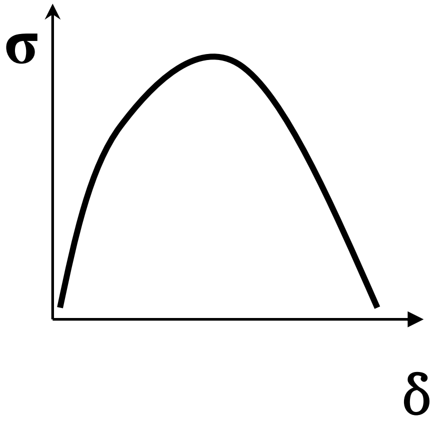
- Various Kinds of Cohesive Zone Laws



(a) Exponential Type



(b) Bilinear Type



(c) Parabolic Type

Interfacial Potential and Tractions

Xu and Needleman (1994) proposed an interfacial potential of the following form

$$\phi(\Delta)=\phi_n+\phi_n\exp\left(-\frac{\Delta_n}{\delta_n}\right)\{[1-r+\frac{\Delta_n}{\delta_n}]\frac{1-q}{r-1}-[q+\left(\frac{r-q}{r-1}\right)\frac{\Delta_n}{\delta_n}]\exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right)$$

to derive the normal and tangential traction as follows

$$T_n=\frac{\partial\phi}{\partial\Delta_n} \qquad \text{and} \qquad T_t=\frac{\partial\phi}{\partial\Delta_t}$$

which gives

$$T_n=-\frac{\phi_n}{\delta_n}\exp\left(-\frac{\Delta_n}{\delta_n}\right)\{\frac{\Delta_n}{\delta_n}\exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right)+\frac{1-q}{r-1}[r-\frac{\Delta_n}{\delta_n}][1-\exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right)]\}$$

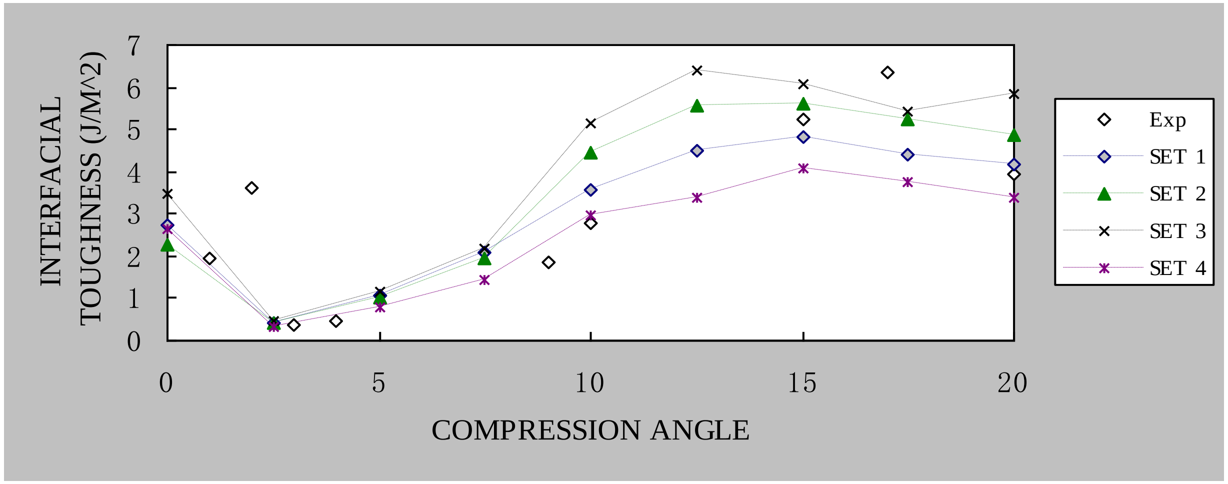
$$T_t=-\frac{\phi_n}{\delta_n}\left(2\frac{\phi_n}{\delta_t}\right)\frac{\Delta_t}{\delta_t}\{q+\left(\frac{1-q}{r-1}\right)\frac{\Delta_n}{\delta_n}\}\exp\left(-\frac{\Delta_n}{\delta_n}\right)\exp\left(-\frac{\Delta_t^2}{\delta_t^2}\right)$$

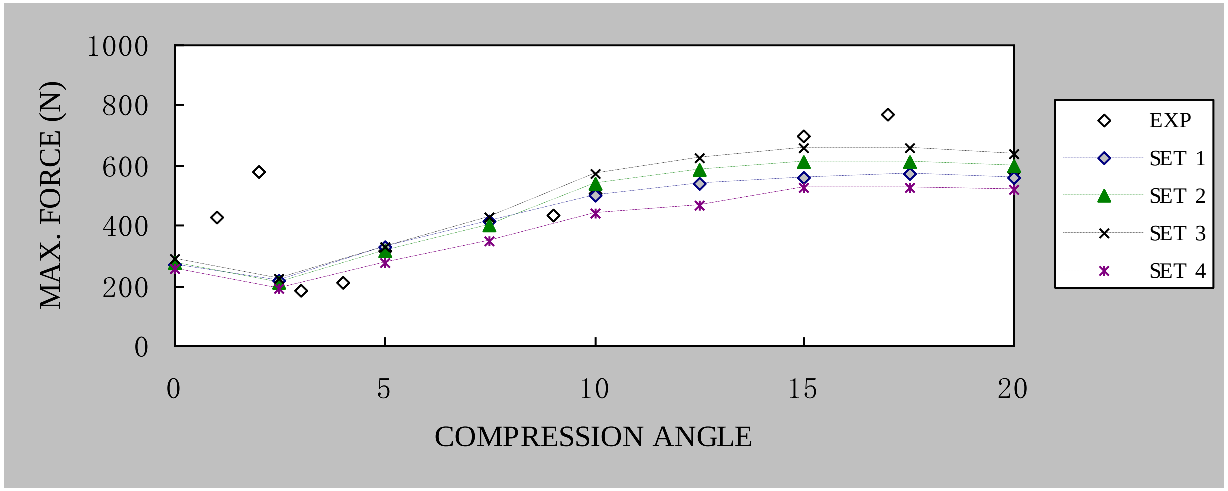
Interfacial Properties Employed in Simulation

	COHESIVE ENERGY (J/M/M)	NORMAL COHESIVE STRENGTH (MPA)	TANGENTIAL COHESIVE STREGNTH (MPA)	CRITICAL INTERFACIAL SEPARATION (micron)
SET 1	16.3	6	7	1
SET 2	17.6	6.5	7.6	1
SET 3	19	7	8.2	1
SET 4	15	5.5	6.4	1

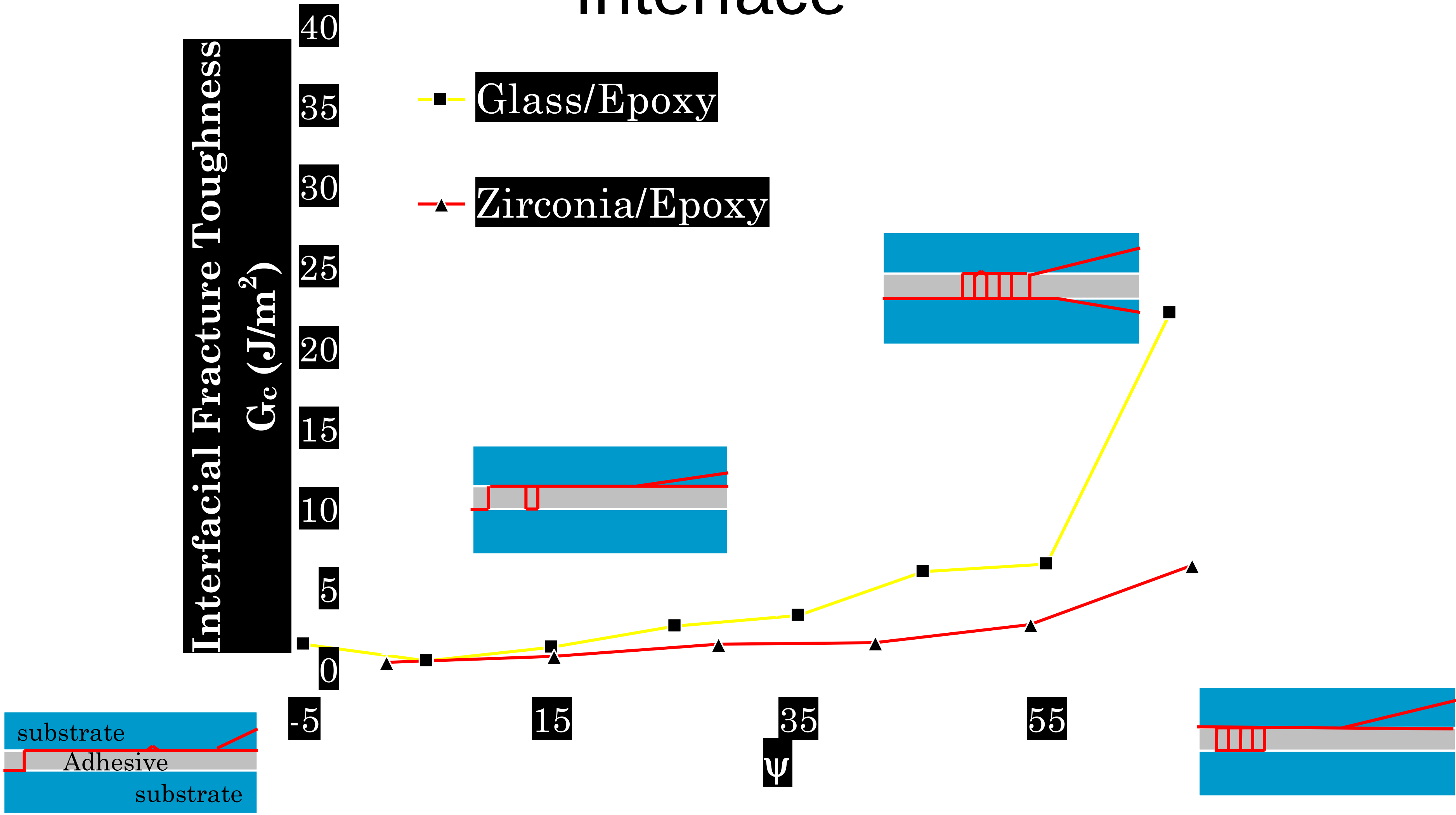
For simplicity, the cohesive energy and critical interfacial separation are assumed to be equal in both normal and tangential direction

Comparison between Simulation and Experimental Results

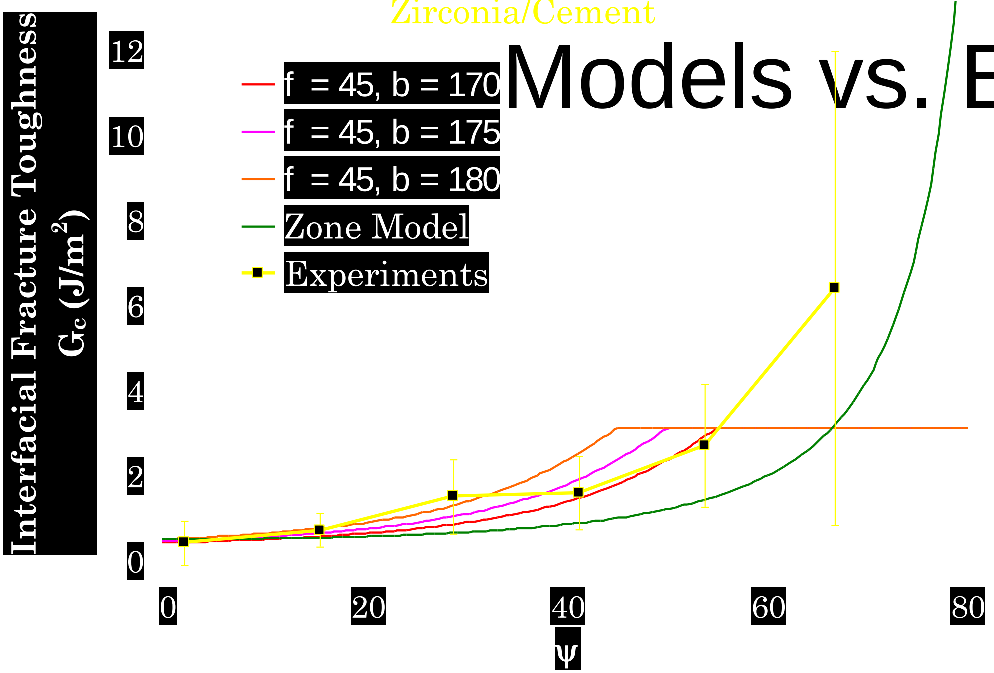


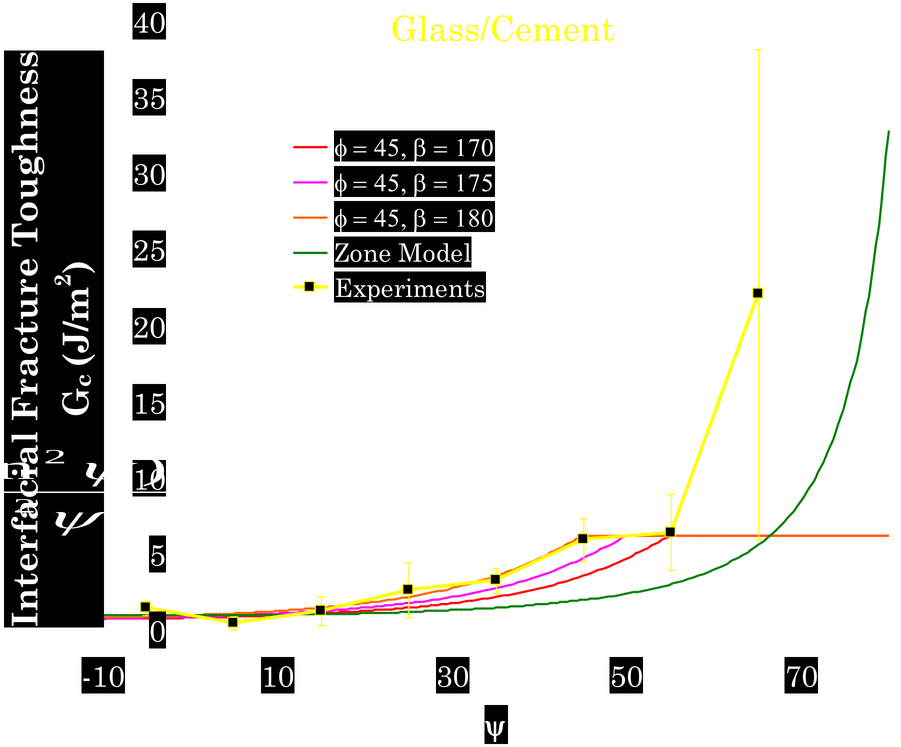


Fracture Toughness of Glass/Cement and Zirconia/Cement Interface

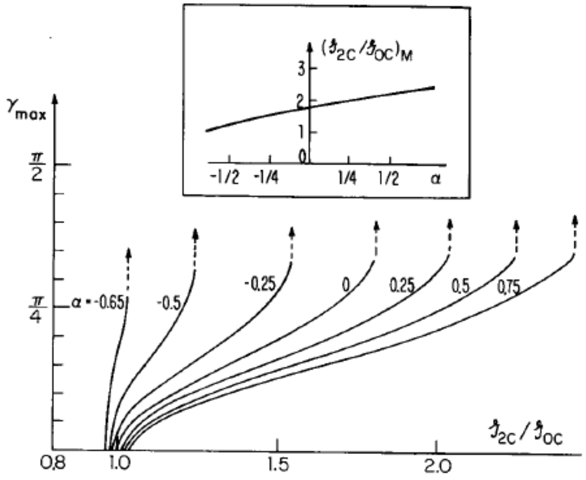


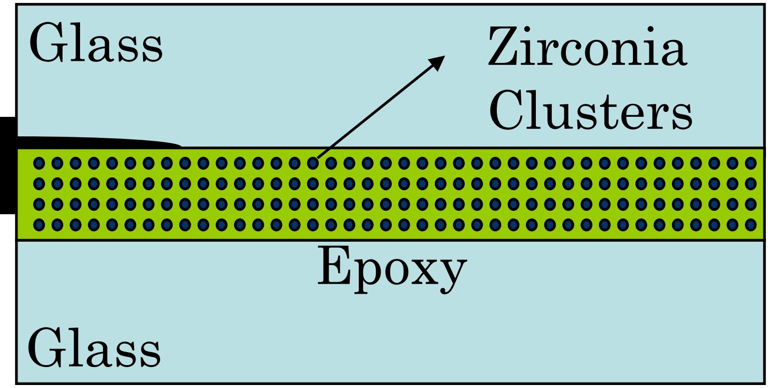
Glass/Epoxy Interface Fracture Resistance: Models vs. Experiment





Microstructure Effect : FIB



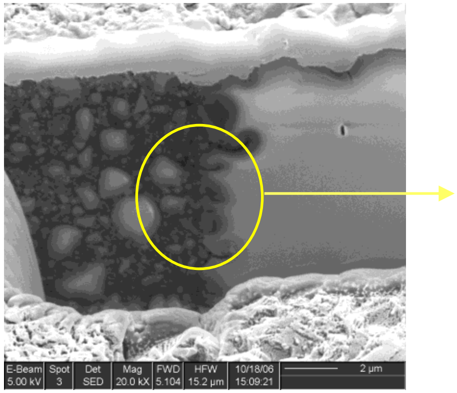


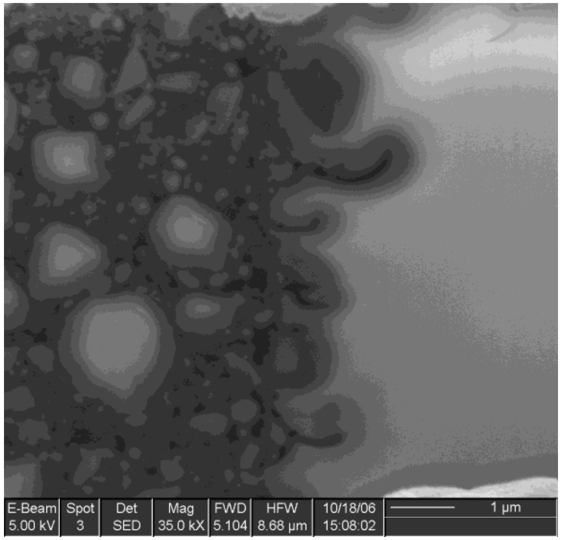
Glass

Zirconia Clusters

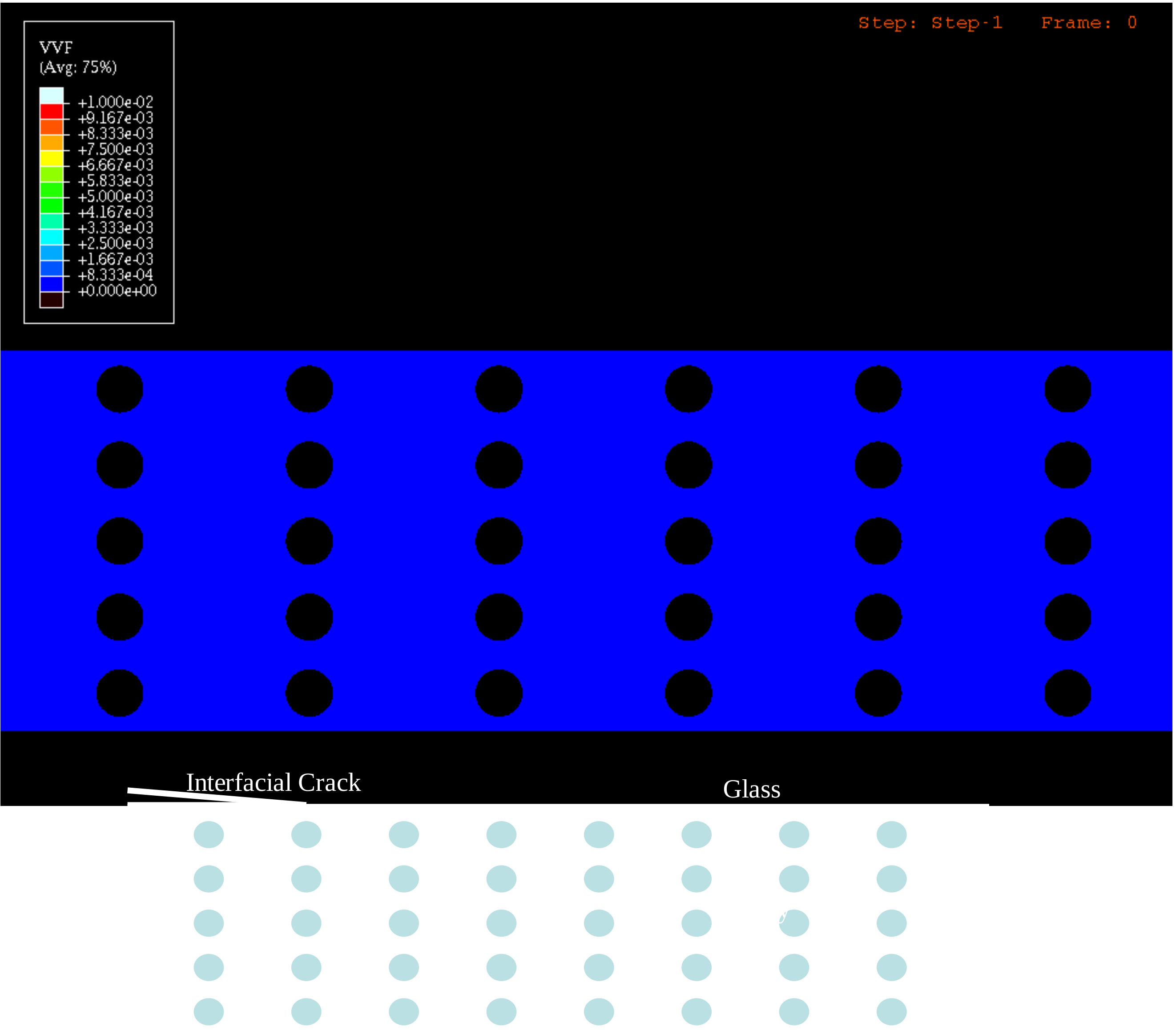
Epoxy

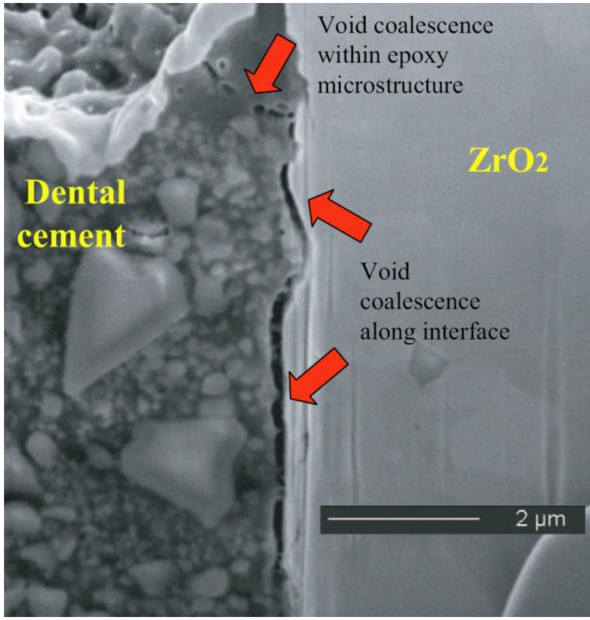
Glass





Focused Ion Beam Images of Interfacial Cracks in Ceramic/Cement Interface





Concluding Remarks

- This class presents an introduction to contact damage in dental multilayers
- Complex loading and geometry idealized to provide insights into mechanisms
- Rate-dependent slow crack growth model used to describe underlying physics
- Bio-inspired design concept presented for the design of robust interfaces
- Interfacial fracture mechanisms explored using a combination of models and experiments