Macroscopic Through Atomic Characterisations of Bioactive Dental Cements

Dr. Kun V. Tian

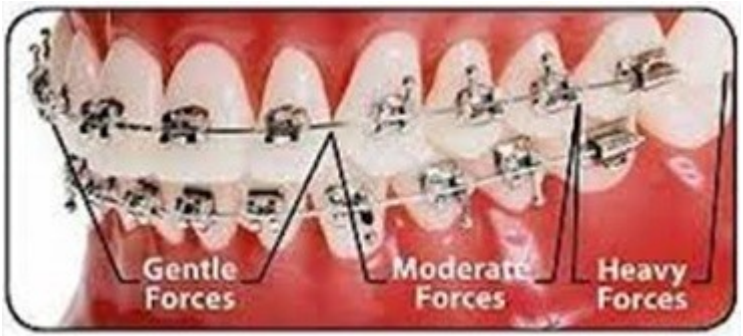
Materials Science Research Institute, Faculty of Dentistry
Semmelweis University, Budapest, Hungary

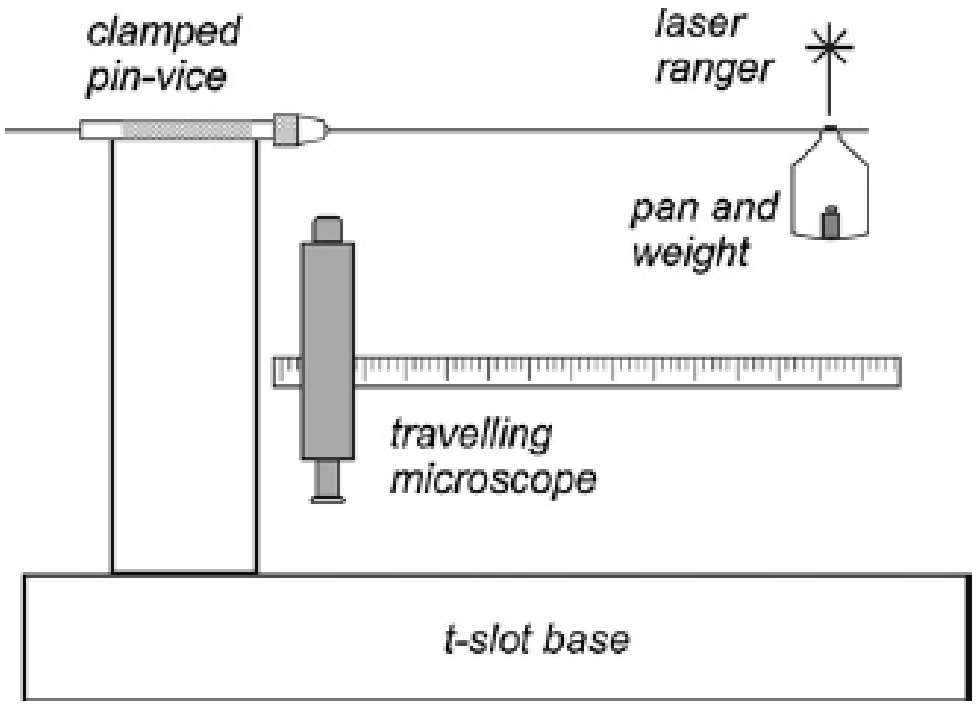
On Yesterday's Show ...

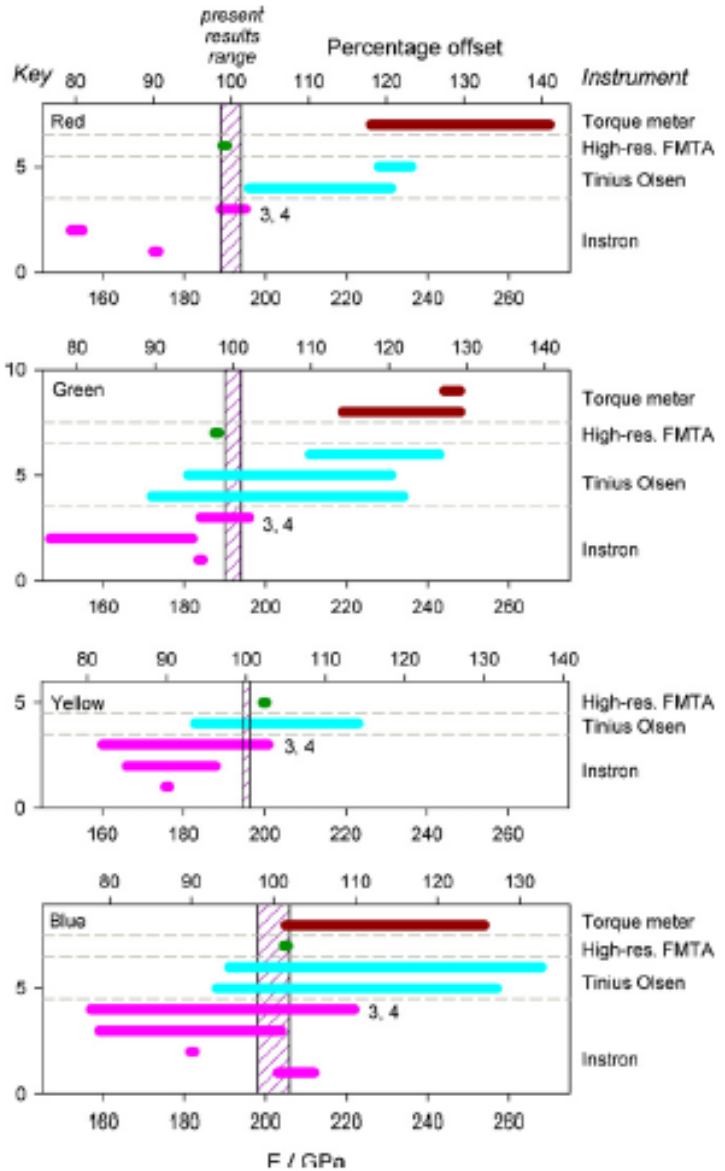
Clinical Material Variability

UNMET CHALLENGES ≈ FUTURE OPPORTUNITY

Elasticity of Orthodontic Archwires

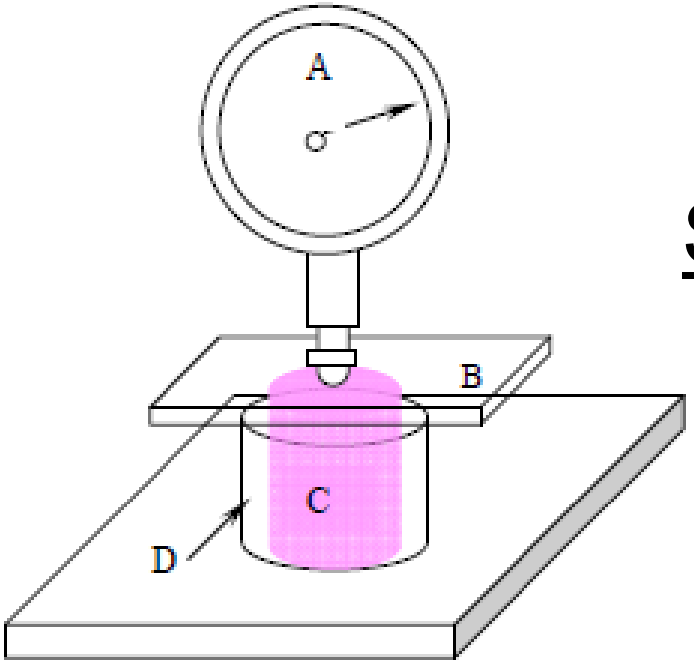




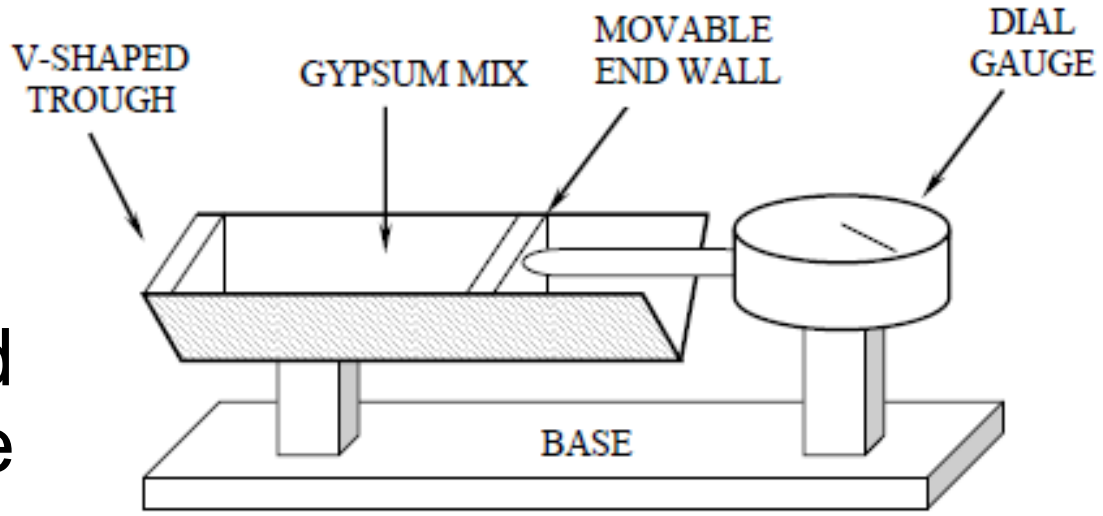


K. Tian, B. W. Darvell, *Dent. Mater*. **26**, 821-829 (2010)

Clinical Variability

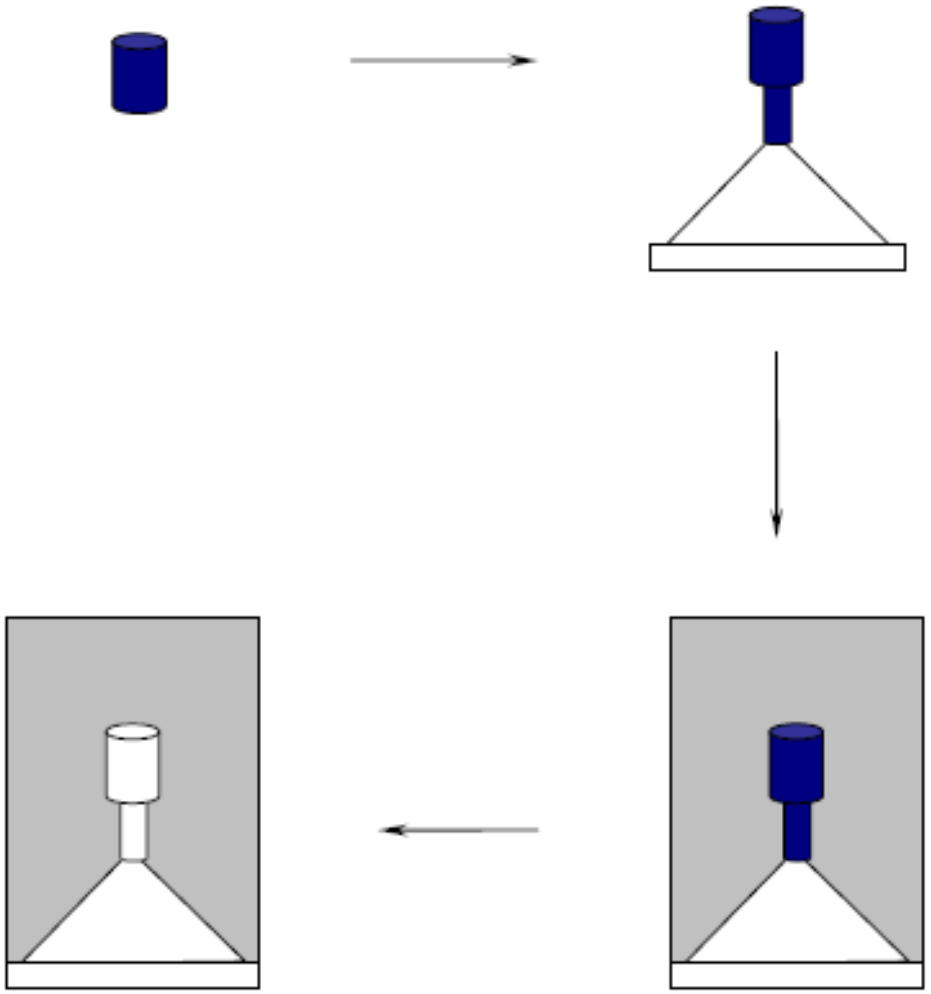


Silicon Impression Moulds
Compression Set



Gypsum
Impression Mould
Setting Shrinkage

Clinical Variability

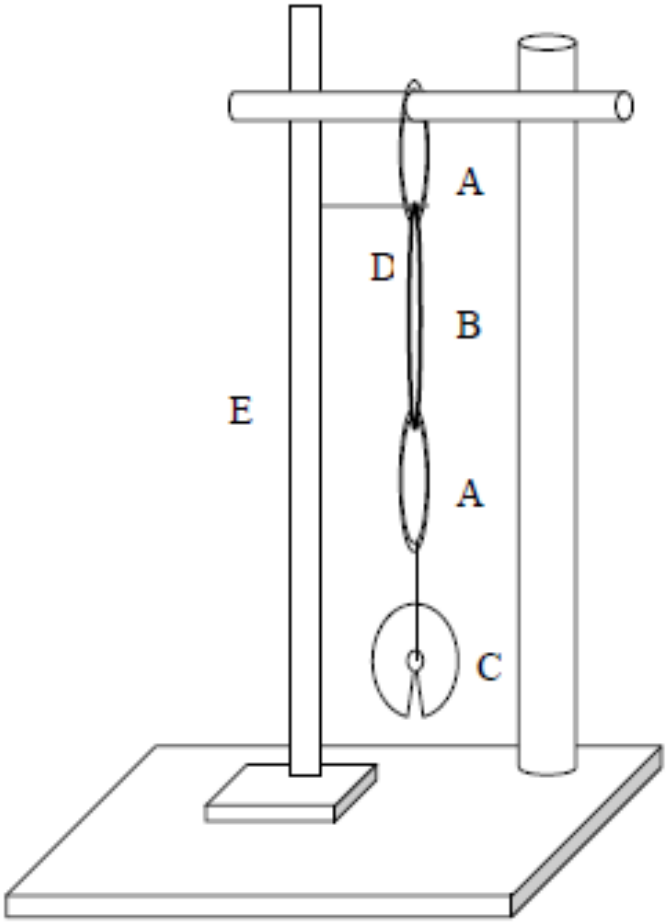


<u>Denture Wax</u>

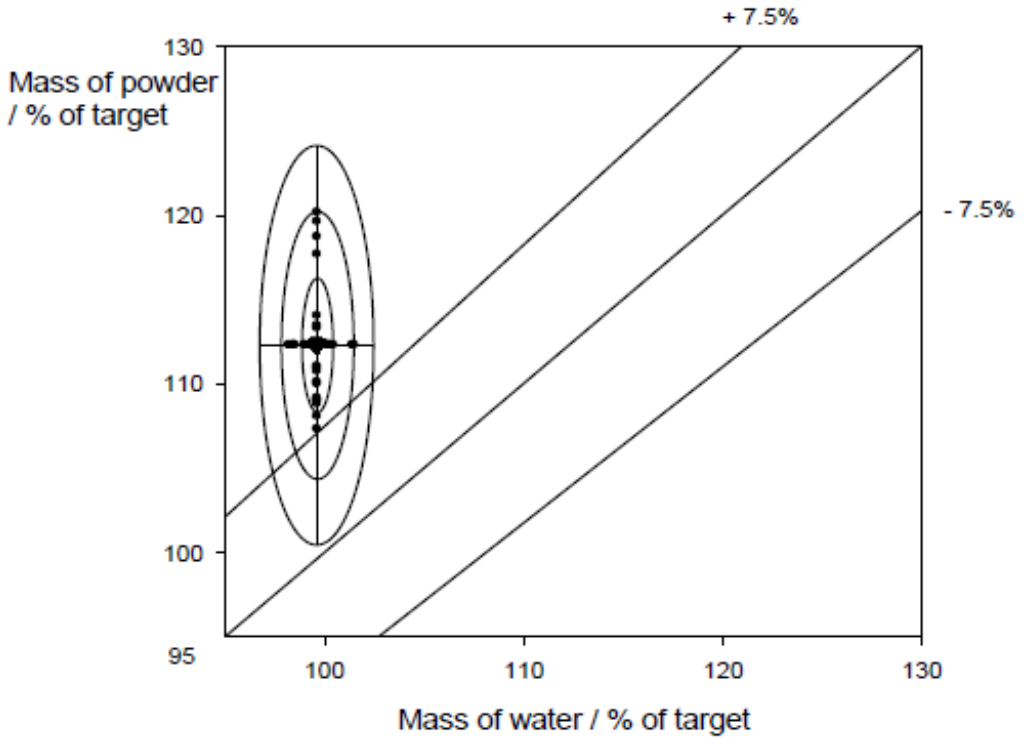
Efficiency of Wax Burn-Out in moulds

Flaws from Carbon-Deposits

Clinical Variability



Clinical mixing ratios vs. Properties



<u>Orthodontic Elastics</u>

Influence of Environment and T°

So …
WHY CEMENTS?
WHY NOW?

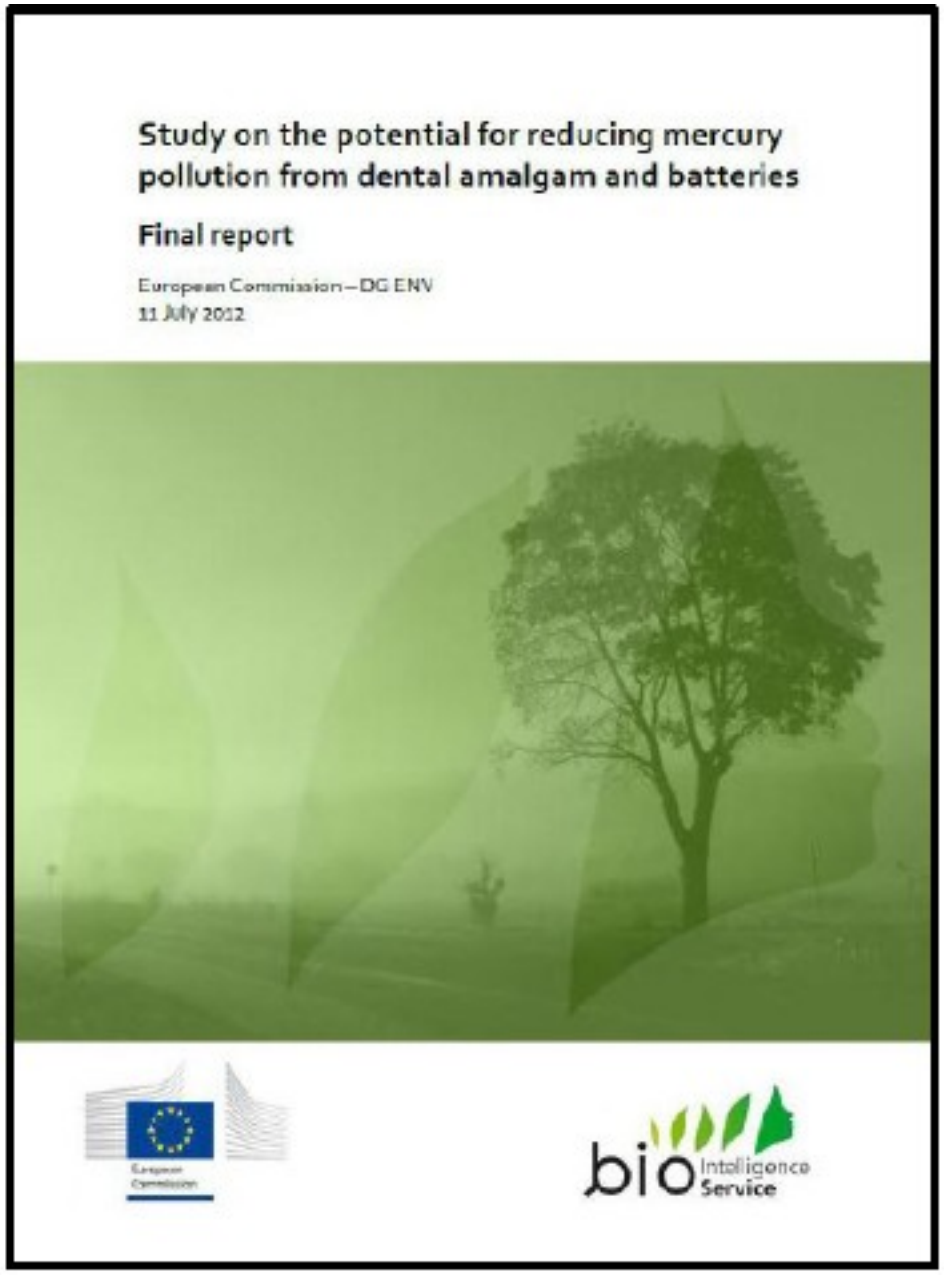
Phasing-out Hg-Usage in the EU

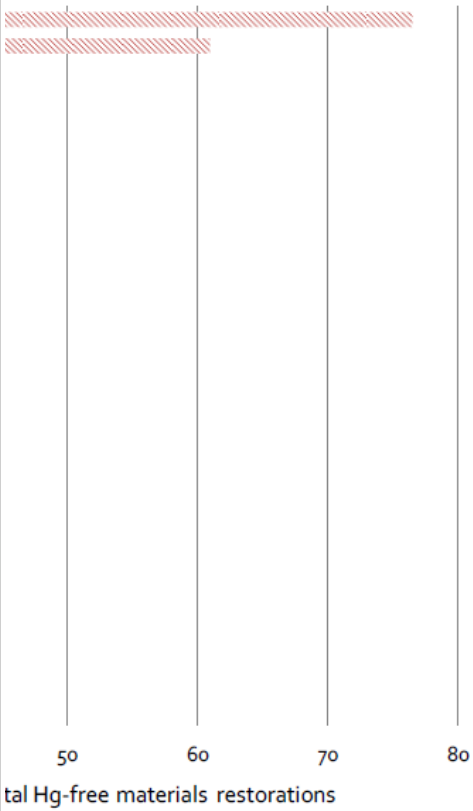
• more wealthy EU-st
ones lagging the furth
in phasing-out Hg-am

• most promising alte
are unknown by a lar
of dental practitioners
~44% in UK)

• Italy is among 5 cou
(DK,EE,SE,IT,FI) exp
have 0% share of Hg
in 2025
• FR, PL, RO, UK, CZ
users of dental-Hg (0
tonnes)

• Main reasons for co
of Hg-amalgams = cc
knowledge on GICs !!





Tooth/Bone Implants & Restorations

Highly Invasive / Hg!

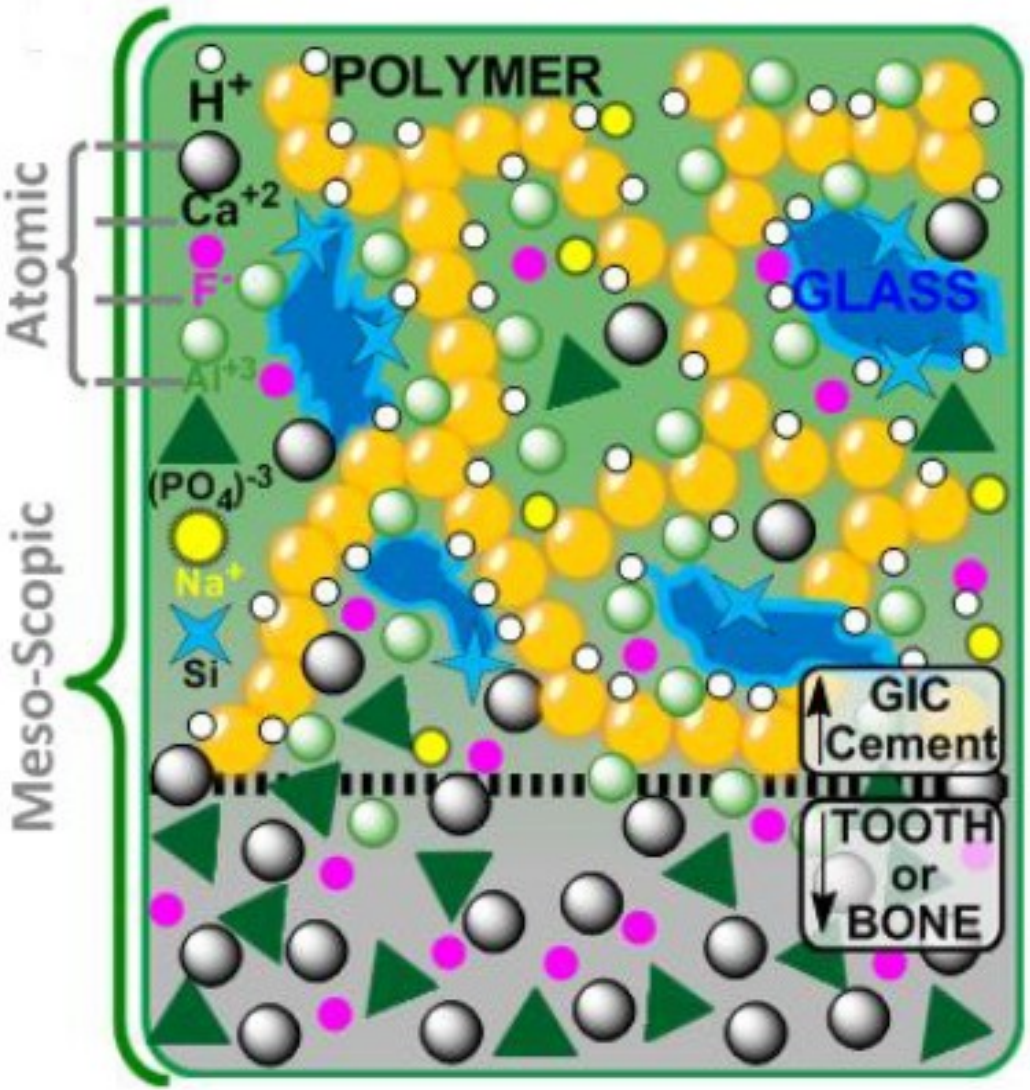
Amalgams

Composite Restorations

Poor Adhesion / Toxic

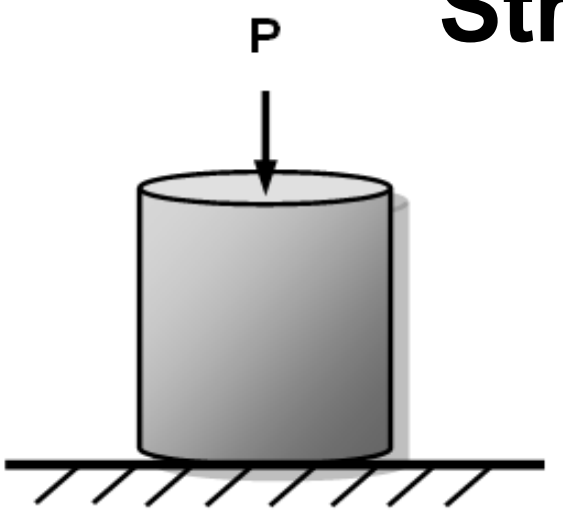
€ € € £££ $$$

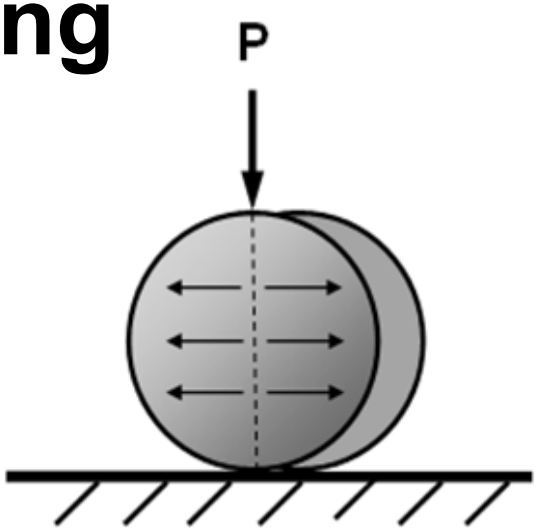
Bioactive Glass Ionomer Cements (GIC)



THE PROBLEM - Brittleness

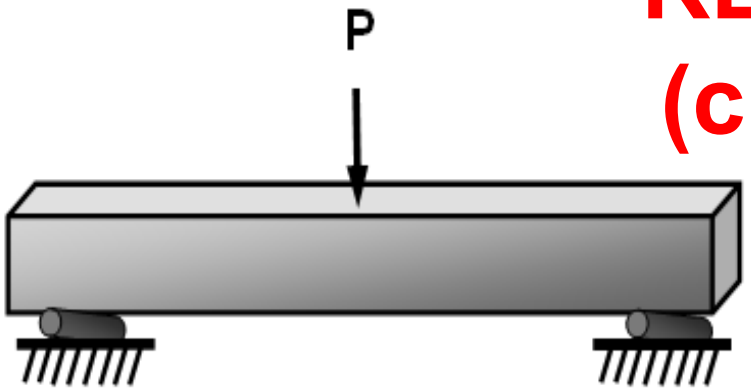
Strength Testing

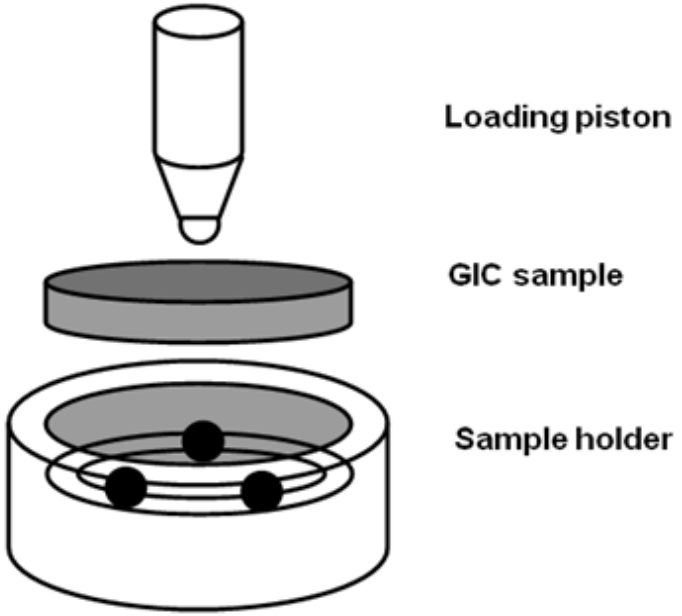




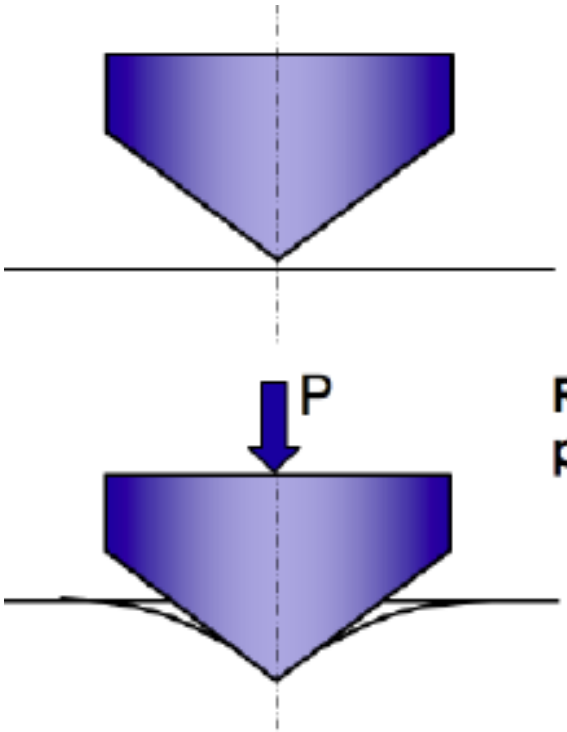
SAMPLE IDENTITY SPECIFIC

NON REALISTIC (clinically)



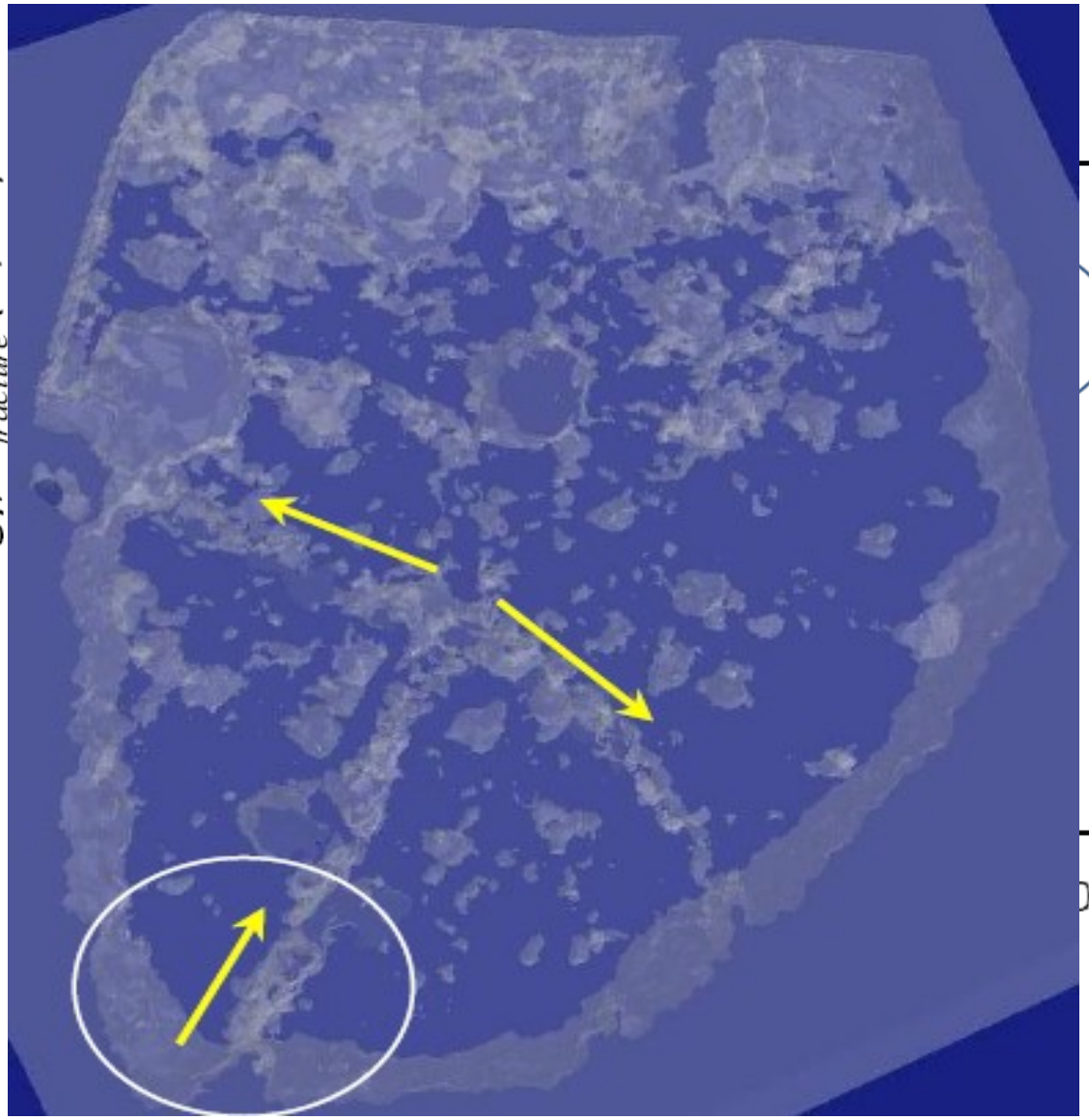


Hardness & Poisson's Ratio



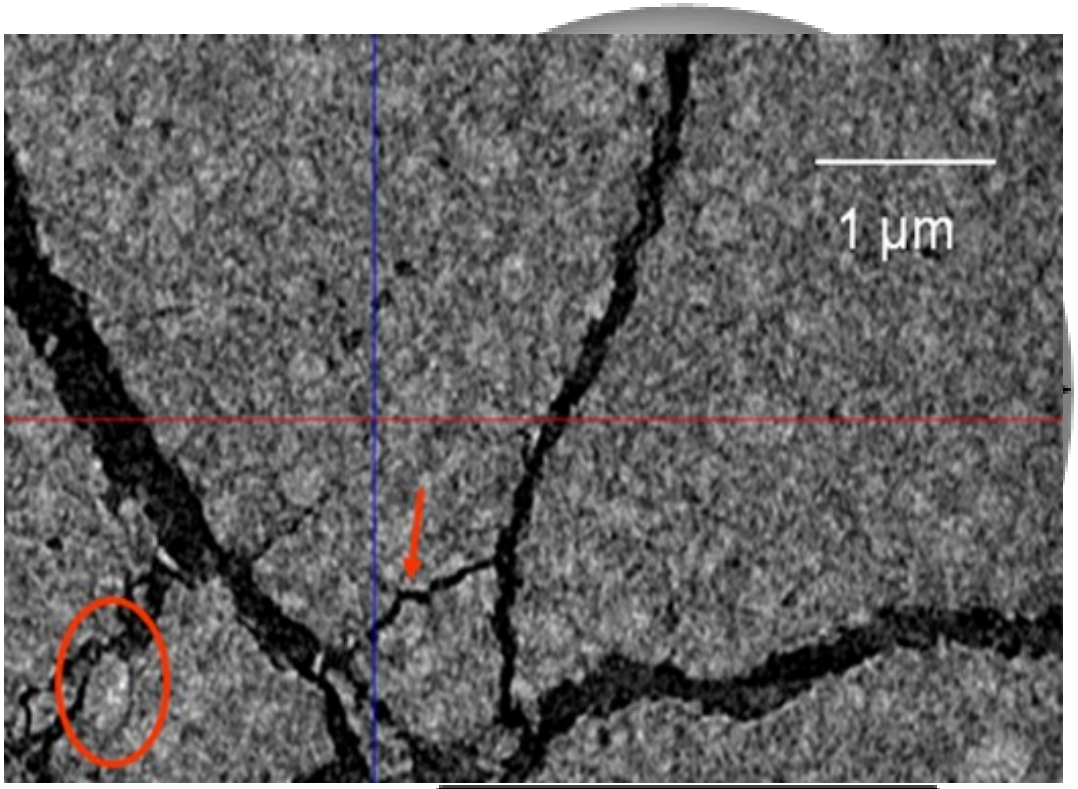
Instantaneous elasticity

$\sigma = H_{el} \propto E/(1-\nu^2) >> H$

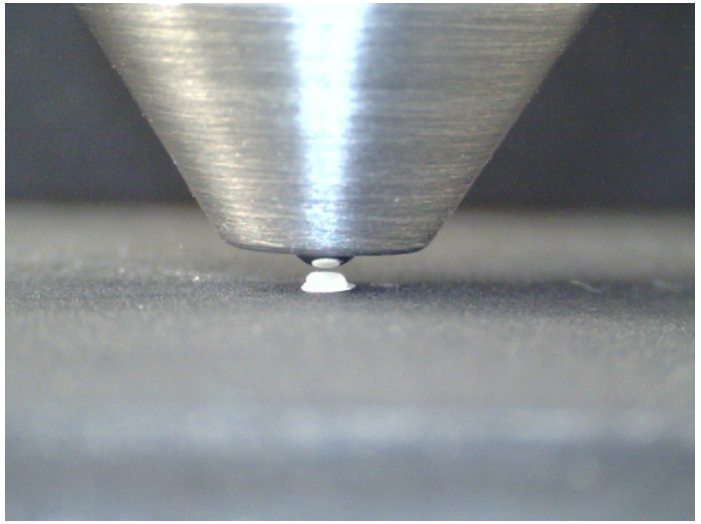


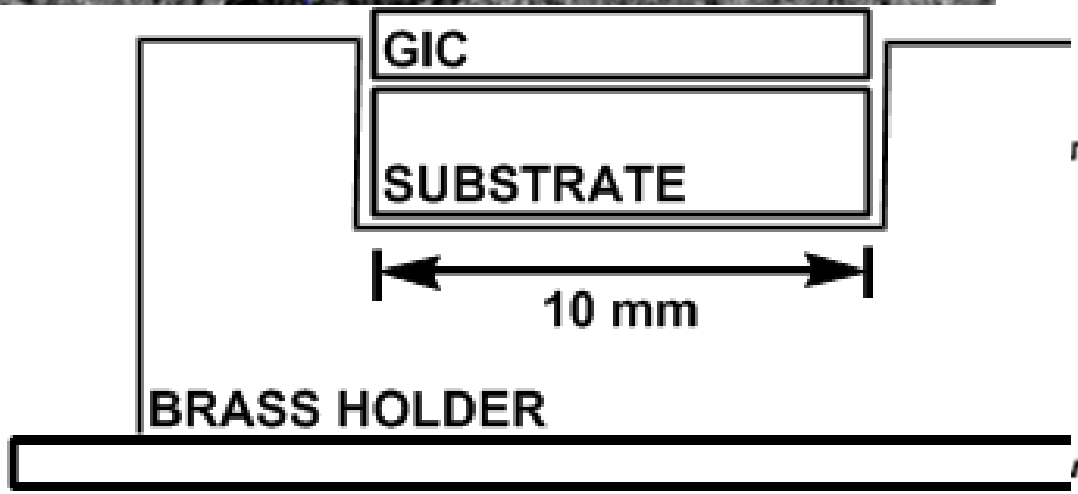
Tian KV *et al*, J Mater Sci Mater Med 2012;**23**:677-85.

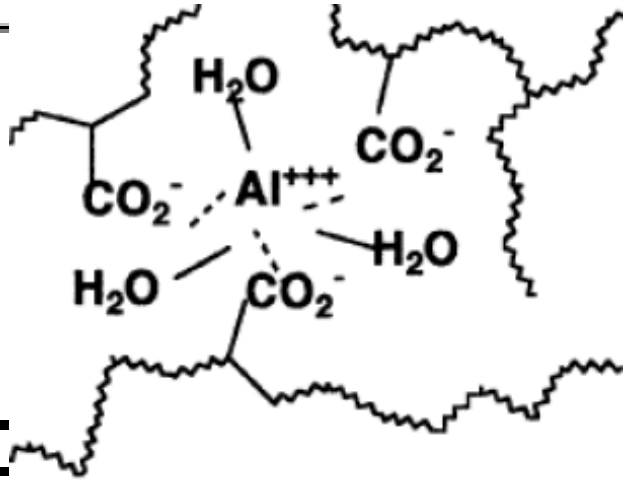
Failure at Glass-Polymer Interface...?



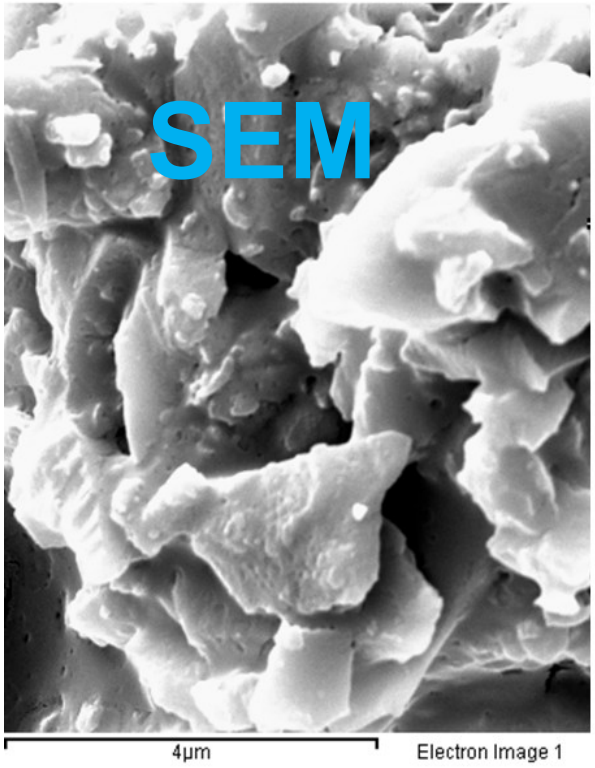
P

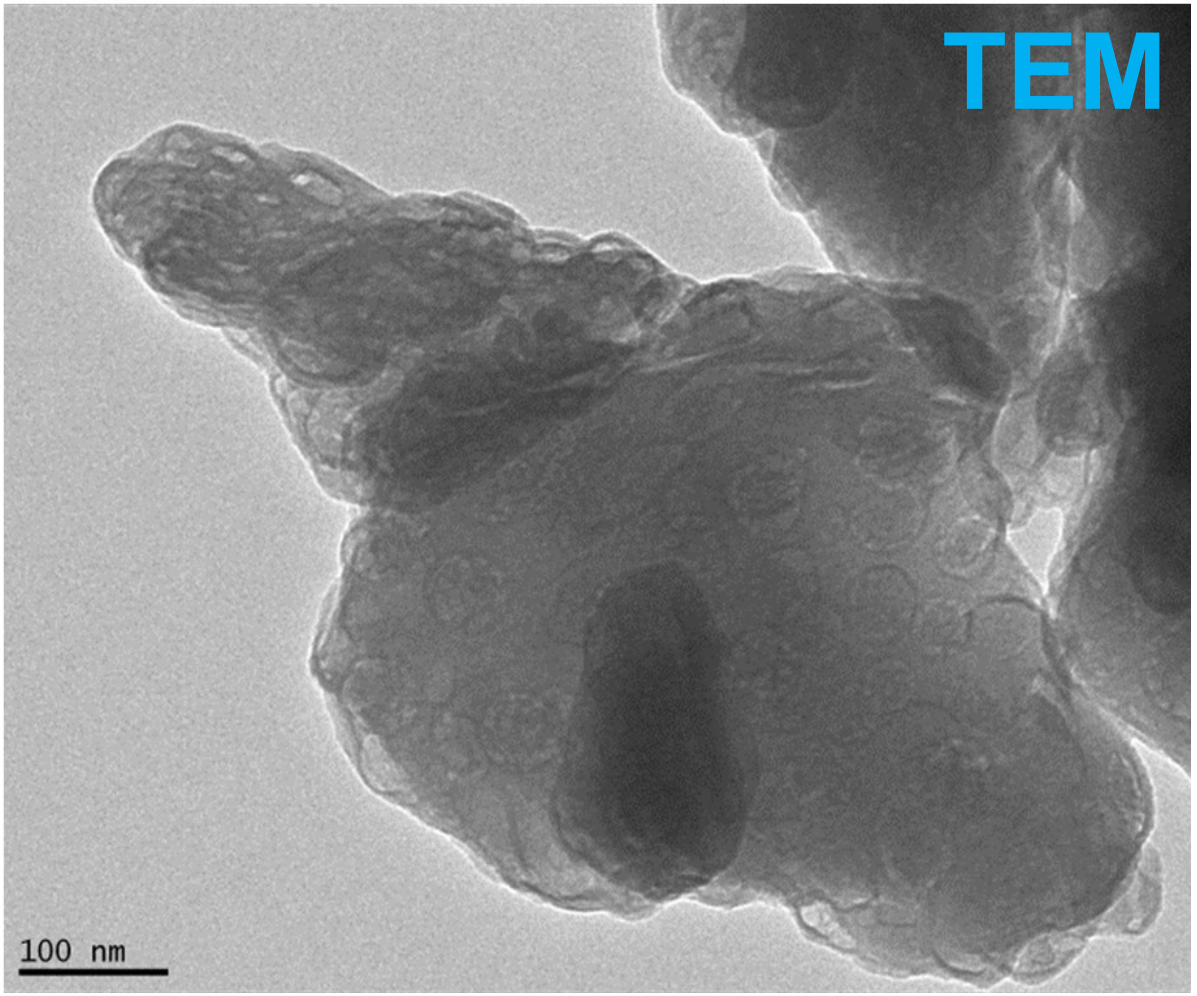






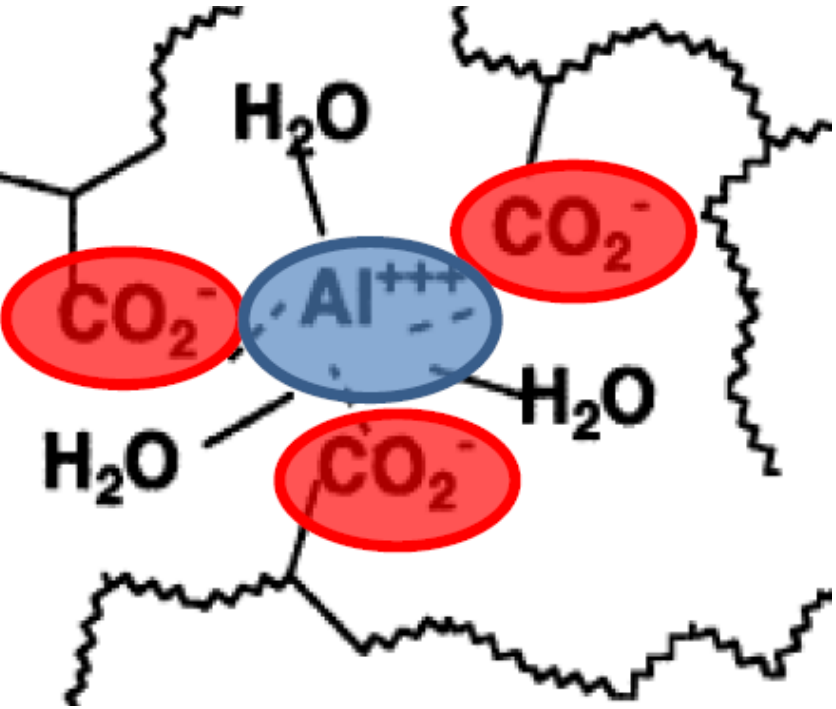
SEM & TEM Imaging

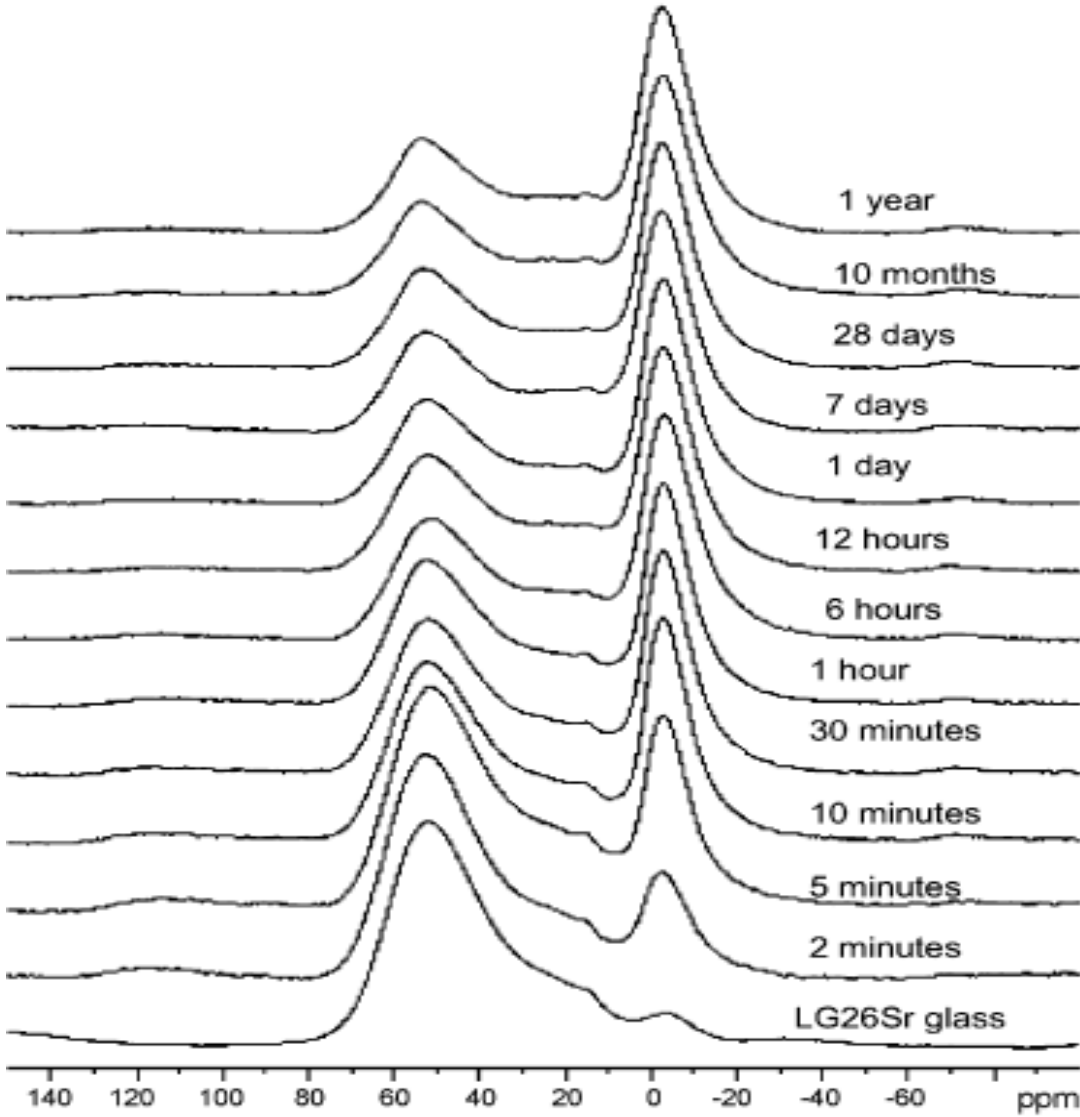




2 (3?) phases

^{27}Al-NMR - Tracking Al-Coordination





NMR Standard = $AlCl_3$•6(H_2O)

Zainuddin N *et al*, Dent. Mater. 2009;**25**:290-5.

IV→V→VI

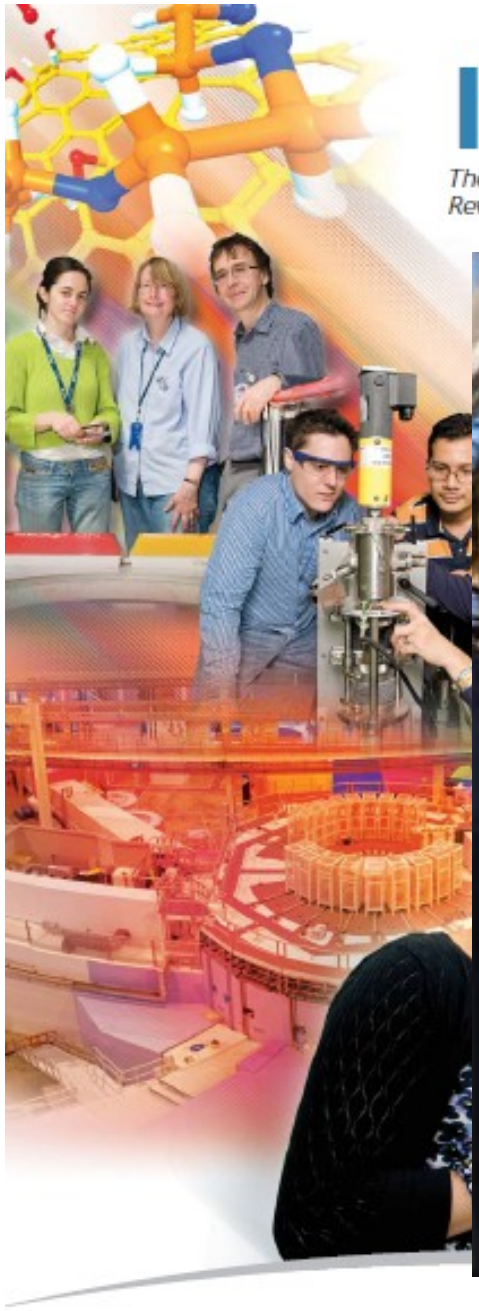
Work Ongoing

The glass and polymer components of GICs, in addition to the GIC cement and its setting profile are currently under investigation using the following techniques:

- Differential scanning calorimetry (DSC)
- Coherent THz Spectroscopy (CTHz)
- Neutron Comptom Scattering (NCS)
- Small / Wide Angle Neutron Scattering (SANS/WANS)
- Quasi-Elastic Neutron Scattering (QENS)
- Computational modeling

ISIS 2011

The ISIS Pulsed Neutron and Muon Source
Review of the Year



Science & Technology Facilities Council

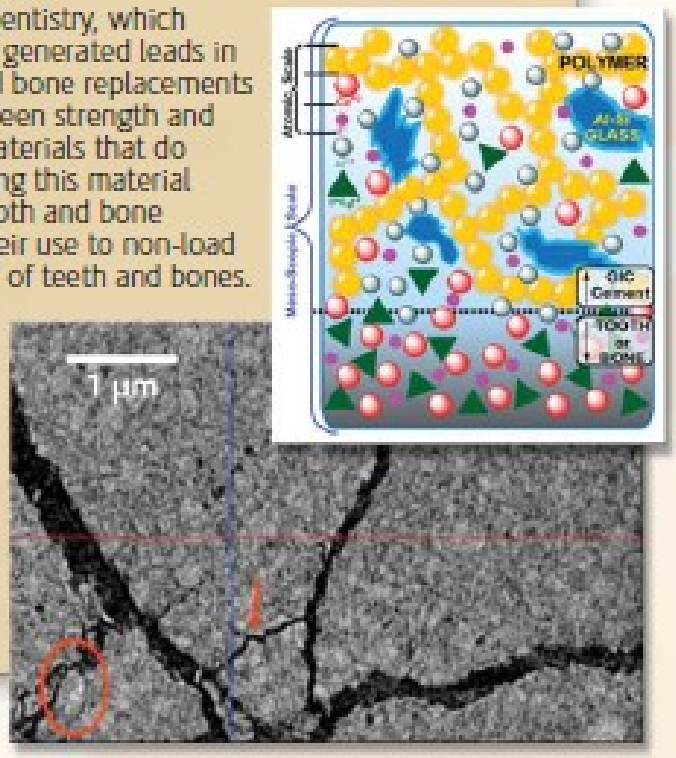
Gold teeth are passé –
glassy teeth (and bones!) are now 'in'

KV Tian, C Dobo-Nagy (Semmelweis University, Budapest), DT Bowron, J Mayers, F Fernandez-Alonso (ISIS), JW Nicholson (St. Mary's University), GA Chass (Queen Mary, University of London), GN Greaves (University of Cambridge)
Support for research: EPSRC-funded project equipment (EP/H030077/1 and EP/H030077/2).

The historic implantation of foreign materials into the human body is epitomised by dentistry, which continues to be by far its most pervasive example. Successes in dental materials have generated leads in orthopaedics and beyond. However, the rational optimisation and design of tooth and bone replacements remains an unmet challenge. Problems stem from the as-yet unresolved conflict between strength and toughness. Problems of adhesion, biocompatibility, appearance and cost beleaguer materials that do satisfy mechanical thresholds. Glass Ionomer Cements (GICs) show promise of resolving this material dichotomy in filling and adhesion applications, complemented by ideal bonding to tooth and bone surfaces. Although the brittleness of these biocompatible composites has confined their use to non-load bearing applications, new evidence signals their potential to match the high toughness of teeth and bones.

Neutron diffraction on Nimrod and scattering on Vesuvio have provided valuable clues as to the factors controlling toughness and strength, through quantitative tracking of changes in structure and dynamics at the atomic and microscopic scales during cementation of GICs.

Contact: *GA Chass, g.chass@qmul.ac.uk*
Further reading: *KV Tian et al., J. Mater. Sci. Mater. Med. 23 (2012) 677; Adv. Mater. (submitted)*



***Top**: Structure of ion exchange layer between GIC and tooth/bone; polymer (orange), glass (blue) and interface are shown. **Bottom**: Tomographic image of fractured GIC.*

Summary & Future Prospects

- GICs have been made overly strong (thus brittle) at the expense of toughness

- DSC, Neutron and THz spectroscopies provide effective means for characterising GICs and their setting reactions

- Strong potential for similarly characterising setting and mechanical properties in other cementitous materials

Acknowledgements

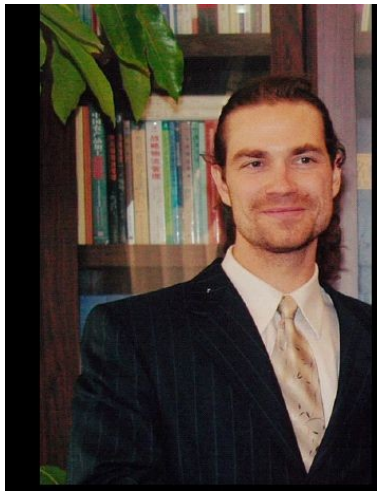
Imre G. Csizmadia
U. Toronto, CA

Csaba Dobó-Nagy
Semmelweis U., HU

A. Lindsay Greer
U. Cambridge, UK

John W. Nicholson
Nat. Phys. Labs, UK

Dominique Massiot
CNRS, Director, FR



Gregory A. Chass
U. London, UK

G. Neville Greavs
U. Cambridge, UK

Yuanzheng Yue
Aalborg U., DK