Mechanical properties of Cementitious Materials Used in Dentistry

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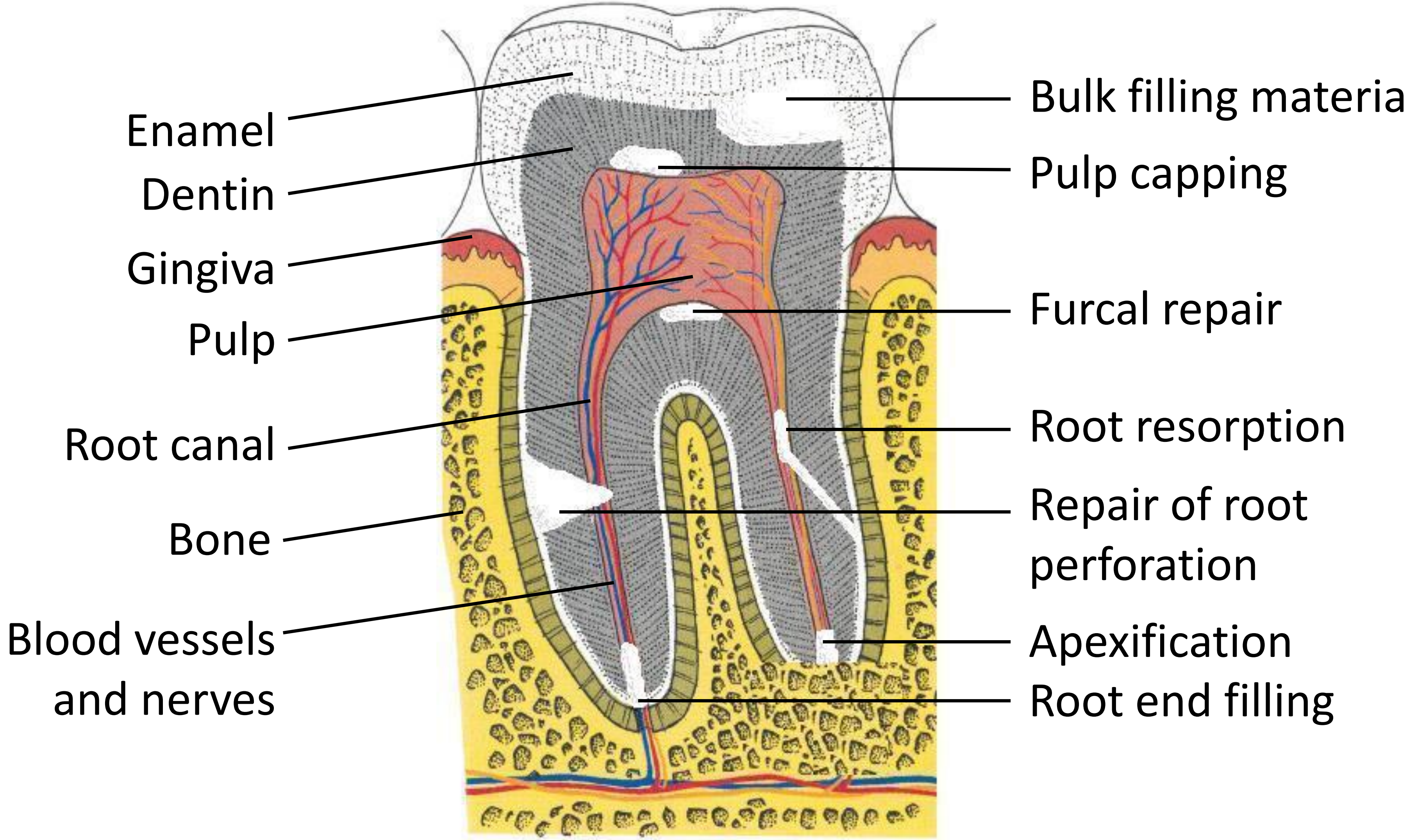
Natural tooth and clinical application of "Bio-Silicates"



Source: https://is.muni.cz/do/fsps/e-learning/zaklady_anatomie/zakl_anatomie_II/pics/2obr-5.jpg

Biodenine©

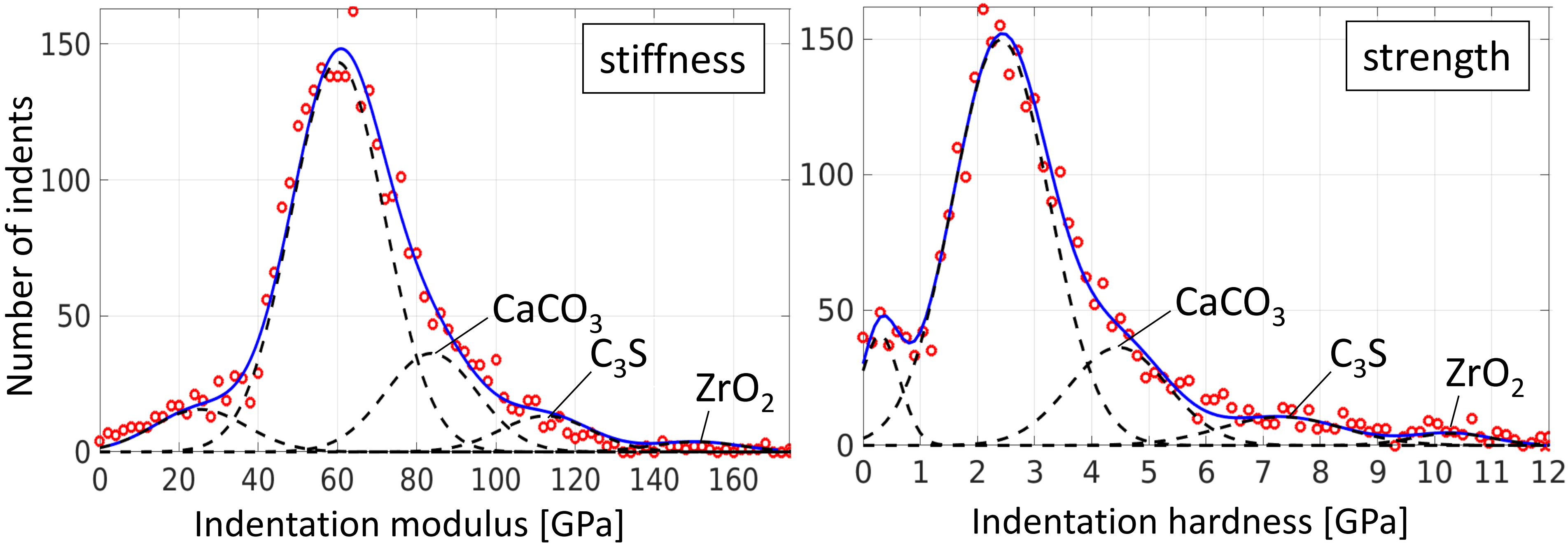
- Dry binder powder:
  - $3CaO\ SiO_2$ = main hydraulic phase
  - $CaCO_3$ = finely ground filler
  - ZrO_2 = radiopacifier
- Mixing liquid:
  - Water
  - Superplasticizer
  - Accelerator

Source: https://www.septodont.com/

- Setting in 12 minutes; close-to-final properties after 24 hours
- **Aim of the project:** Upscaling of mechanical properties from scale of grid nanoindentation to the application scale

Grid nanoindentation into mature Biodentine©

- 5748 indents, maximum force = 1 mN



- Modal analysis: five material phases identified.
- Upscaling: methods from continuum micromechanics

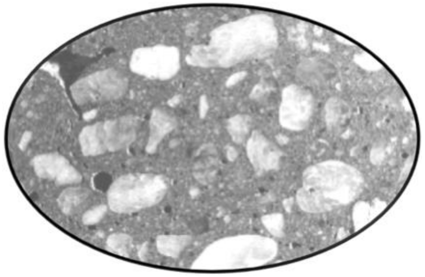
Scale transitions in heterogeneous materials

Loading: uniform strain boundary conditions:

$\underline{\xi}(\underline{x}) = \boldsymbol{E} \cdot \underline{x}$

$\underline{\xi}$ … prescribed displacements
$\boldsymbol{E}$ … strain imposed on RVE
$\underline{x}$ … position vector

Example: concrete
RVE = representative volume element



2 material phases:
$i = 1$ … cement paste
$i = 2$ … aggregates

micro-to-MACRO stiffness homogenization

$\varepsilon_i = \mathbb{A}_i : \boldsymbol{E}$

ε_i … average microscopic phase strain
$\mathbb{A}_i$ … phase strain concentration tensor

MACRO-to-micro strain concentration

$$\mathbb{C}_{\mathrm{hom}} = \sum_{i=1}^{2} f_i \, \mathbb{C}_i : \mathbb{A}_i$$

$\mathbb{C}_{\mathrm{hom}}$ … homogenized stiffness tensor
f_i … phase volume fraction
$\mathbb{C}_i$ … phase stiffness tensor

Strain concentration tensors $\mathbb{A}_i$ allow for scale transitions!

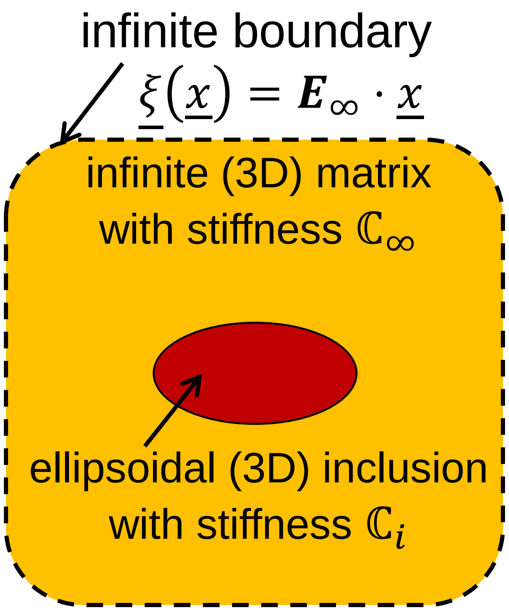
Lit: Hill: J. Mechanics and Physics of Solids, 1963, **http://doi.org/czddmm**

Eshelby-problem = basis for homogenization methods

Non-trivial three-dimensional strain concentration problem …

with *analytical* solution

$$\varepsilon_i = [\mathbb{I} + \mathbb{P}_i^{\infty} : (\mathbb{C}_i - \mathbb{C}_\infty)]^{-1} : \boldsymbol{E}_\infty$$



2D sketch of 3D problem!

ε_i … uniform deformation of the inclusion

$\mathbb{I}$ … identity matrix

$\mathbb{P}_i^{\infty}$ … morphology tensor (accounting for shape and orientation of inclusion)

$\mathbb{C}_i$ … stiffness of inclusion

$\mathbb{C}_\infty$ … stiffness of infinite matrix

$\boldsymbol{E}_\infty$ … remotely imposed uniform deformation

Link Eshelby problem to heterogeneous materials

- One Eshelby-problem for each constituent -> inclusion
- Strain in inclusion := average strain of constituents
- Link between $\boldsymbol{E}_\infty$ and $\boldsymbol{E}$ by enforcing strain-average-rule

Estimated phase strain concentration tensors:

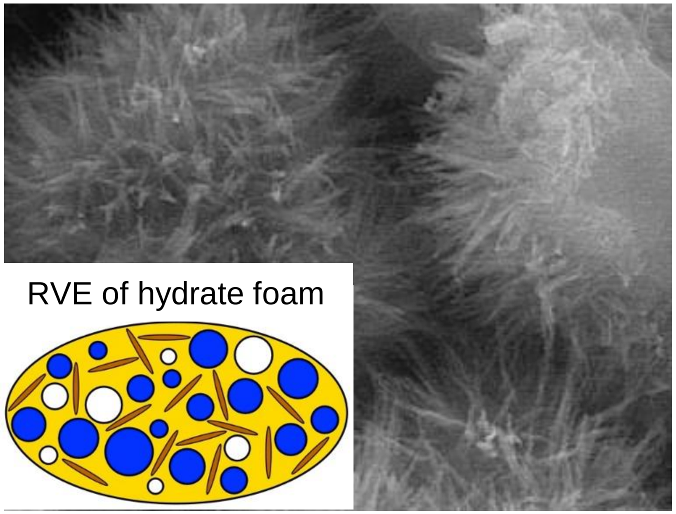
$$\mathbb{A}_i = [\mathbb{I} + \mathbb{P}_i^\infty : (\mathbb{C}_i - \mathbb{C}_\infty)]^{-1} \left[\sum_{j=1}^{n} f_j [\mathbb{I} + \mathbb{P}_j^\infty : (\mathbb{C}_j - \mathbb{C}_\infty)]^{-1}\right]^{-1}$$

(grey) phase volume fractions
(green) elastic stiffness tensors of phases
(red) characteristic phase shapes
(blue) phase interaction

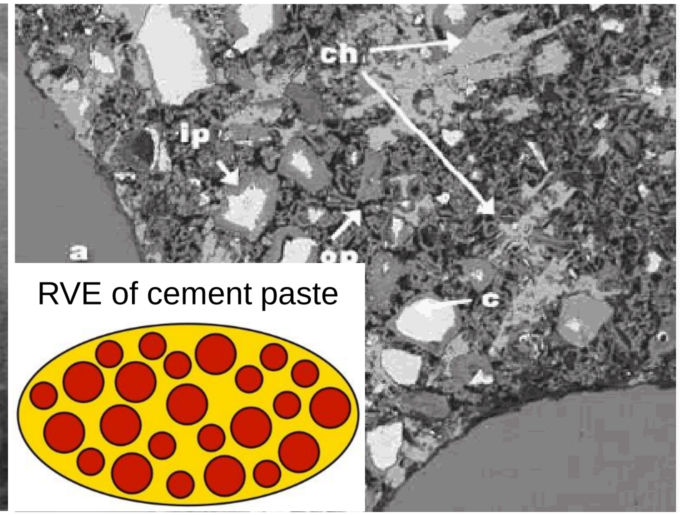
- Matrix-inclusion composite $\mathbb{C}_\infty = \mathbb{C}_m$ … Mori-Tanaka scheme
- Polycrystalline composite $\mathbb{C}_\infty = \mathbb{C}_{hom}$ … Self-consistent scheme

Lit: Zaoui: J. Engineering Mechanics (ASCE), 2002, **http://doi.org/fg26cd**

Cement pastes: two-scale materials



source: B. Möser, FIB Weimar, 1999



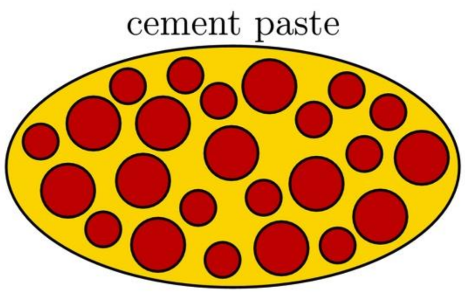
source: https://www.fhwa.dot.gov

2D sketches showing *qualitative* properties of 3D RVEs!

Qualitative / quantitative key properties of material phases

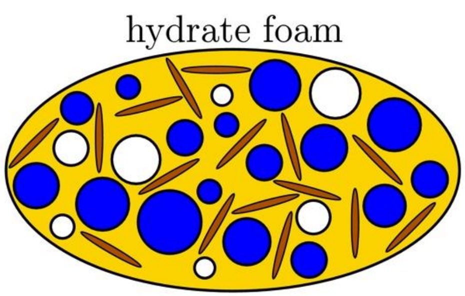
Characteristic shape	Volume fractions (*evolving* with hydration!)
Interaction	Mechanical properties (material *constants*!)

Evolving volume fractions of microscopic material phases



$$f_{clin} = \frac{20\,(1-\xi)}{20+63\,(w/c)}$$

$$f_{hf} = \frac{20\,\xi+63\,(w/c)}{20+63\,(w/c)}$$

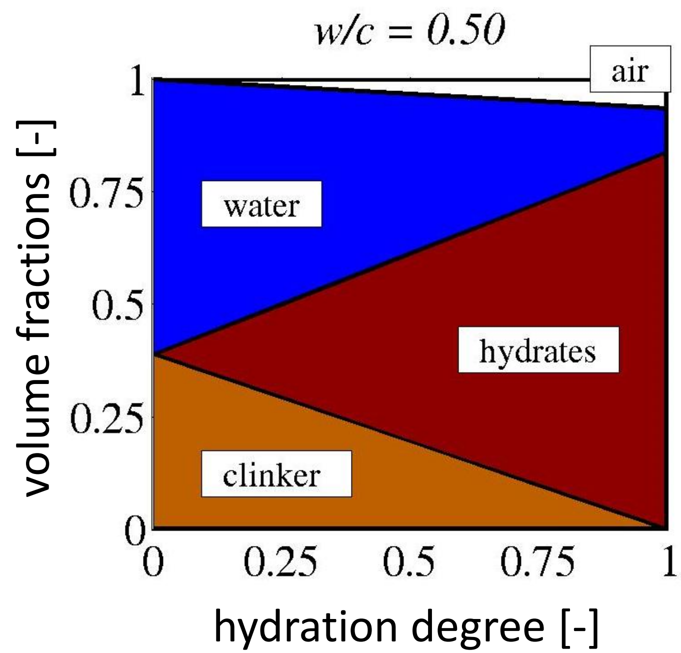


$$\tilde{f}_{hyd} = \frac{43.15\,\xi}{20\,\xi+63\,(w/c)}$$

$$\tilde{f}_{H_2O} = \frac{63\,(w/c)-26.46\,\xi}{20\,\xi+63\,(w/c)}$$

$$\tilde{f}_{air} = \frac{3.31\,\xi}{20\,\xi+63\,(w/c)}$$

Powers' hydration model



Functions of composition: w/c … initial water-to-cement mass ratio
and maturity: ξ … degree of hydration

Isotropic phase elasticity + strength *constants*

	hydrate gel needles	cement grains
bulk modulus	18.7 GPa	116.7 GPa
shear modulus	11.8 GPa	53.8 GPa
cohesion	50 MPa	
angle of internal friction	12°	

Outlook

- Demonstrate similarities and differences between cement pastes used in dentistry and in construction
- Indicate directions for further improving the mechanical properties of cement paste used in the construction sector

Outreach: Sep 18, 2019, SPŠE Olomouc, Czech Republic

Industrial secondments: Septodont, short visit in April 2018
Septodont, start in March 2020

Thank you for your attention

Appendix

Public outreach evaluation