Multiscale Strength of Bone and Bone Replacement Materials: An Experimentally Supported Micromechanical Explanation

Christian Hellmich*, Andreas Fritsch
Vienna University of Technology (TU Wien), Austria
Luc Dormieux
Paris Tech Ecole des Ponts, France

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Bone

… is a hierarchically organized **nanocomposite**,

made of

hydroxypatite crystals,

type I collagen molucules, and

water (with mechanically insignificant amount of noncollageneous organic matter)

Our Aim:

- explain **tissue-specific bone strength** from **tissue-specific composition** (hydroxyapatite/collagen/water content),

  based on ‚universal‘ elastic and **strength properties of elementary building blocks** (hydroxyapatite/collagen/water)

2-step strategy

- study hydroxyapatite-water systems („artifical biomaterials“)
- study hydroxyapatite-collagen-water systems („real bone materials“)

Artificial hydroxyaptite

Hydroxyapatite (HA): $Ca_{10}(PO_4)_6(OH)_2$

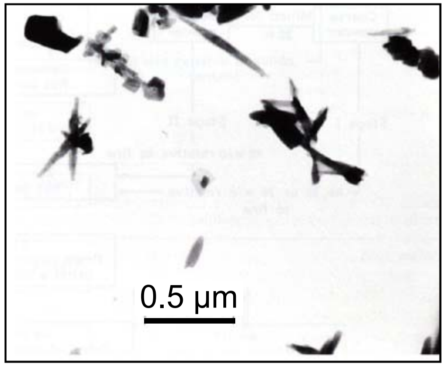
- bone mineral=impure HA

Biomedical applications of pure HA:

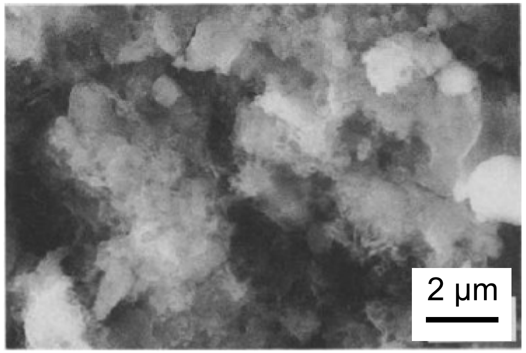
- implant coatings
- reinforcement for ceramic, metallic or polymer composites
- <u>hard tissue replacement implants</u>

macroscopic mechanical properties of entire HA biomaterial family:

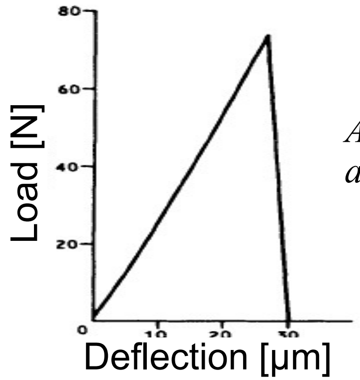
Can they be explained from microstructure?



Shareef et al., 1993



Martin and Brown, 1995



Akao et al., 1981

Theoretical basis: Continuum Micromechanics

e.g. A. Zaoui. Journal of Engineering Mechanics (ASCE), 128(8): 808-816 (2002)

representative volume element (RVE), with *phases 'hydroxyapatite' and 'pores'*

$\Sigma(z)$, $E(z)$, $\Sigma = C(z):E$

Σ^{ult} ?

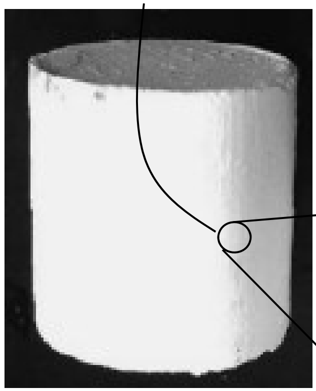
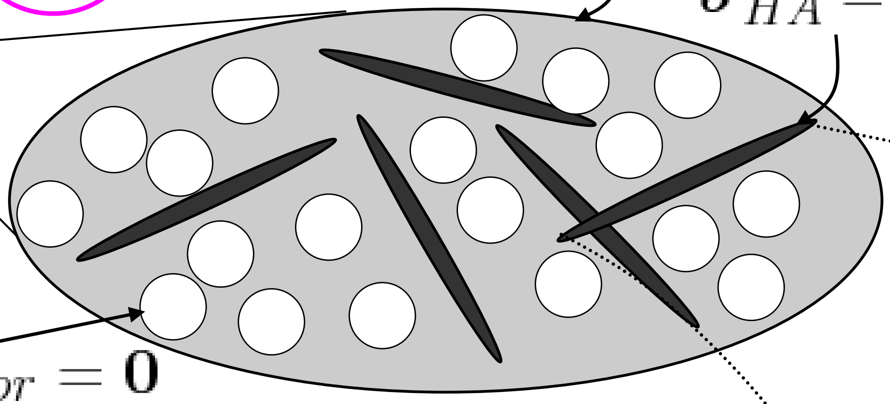


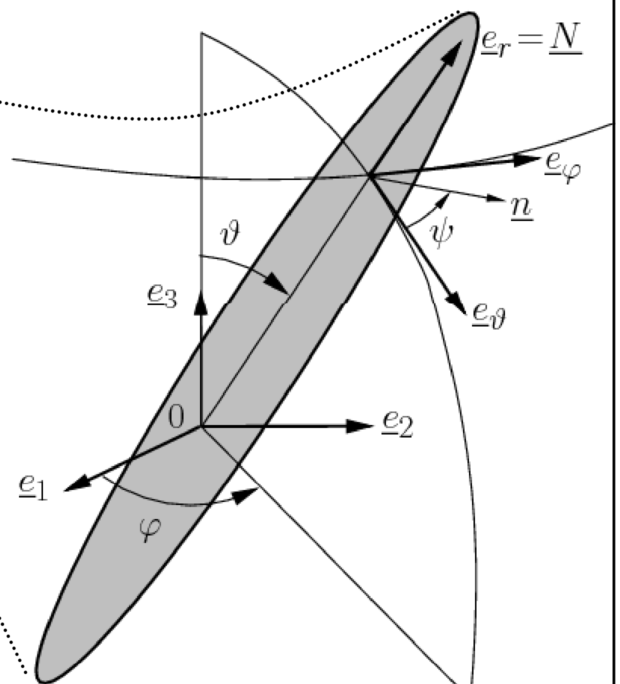
Image Prokopiev and Sevostianov, 2006

$\forall \boldsymbol{x} \in \partial V_{RVE} : \boldsymbol{\xi}(\boldsymbol{x}) = \boldsymbol{E} \cdot \boldsymbol{x}$

$\boldsymbol{\sigma}_{HA} = \mathbb{c}_{HA} : \boldsymbol{\varepsilon}_{HA} \quad f_{HA}(\boldsymbol{\sigma}) = 0$



$\mathbb{c}_{por} = \mathbb{0} \quad \boldsymbol{\sigma}_{por} = \boldsymbol{0}$



brittle failure of single needle („interface"):

$f_{HA}(\sigma) = \max_{\theta,\varphi}[\beta \max_{\psi} |\sigma_{Nn}| + \sigma_{NN})] - \sigma^{ult,t} = 0$

$\sigma_{NN} = \mathbf{N}(\theta,\varphi)\cdot\boldsymbol{\sigma}\cdot\mathbf{N}(\theta,\varphi)$; $\sigma_{Nn} = \mathbf{N}(\theta,\varphi)\cdot\boldsymbol{\sigma}\cdot\mathbf{n}(\theta,\varphi;\psi)$

$\theta = 0,\ldots,\pi$; $\varphi = 0,\ldots,2\pi$; $\psi = 0,\ldots,2\pi$:

Average conditons – concentration problem

$$\mathbf{E} = 1/V \int_V \boldsymbol{\varepsilon}(\mathbf{x})\, dV = (1-\phi) \int_\theta \int_\varphi \boldsymbol{\varepsilon}_{HA}(\theta,\varphi)\, (\sin\theta/4\pi)\, d\varphi d\theta + \phi\, \boldsymbol{\varepsilon}_{por} = \langle\boldsymbol{\varepsilon}\rangle$$

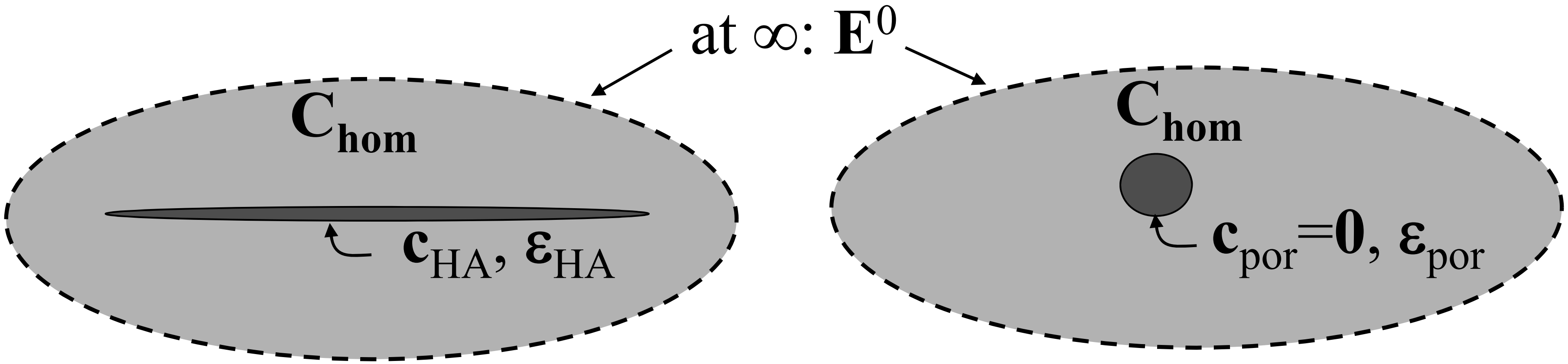
$$\boldsymbol{\Sigma} = 1/V \int_V \boldsymbol{\sigma}(\mathbf{x})\, dV = (1-\phi) \int_\theta \int_\varphi \boldsymbol{\sigma}_{HA}(\theta,\varphi)\, (\sin\theta/4\pi)\, d\varphi d\theta = \langle\boldsymbol{\sigma}\rangle$$

- linear elasticity and linearized strain
- → superposition principle
- → linear concentration relations:
- $\boldsymbol{\varepsilon}_{HA}(\theta,\varphi)=\mathbf{A}_{HA}(\theta,\varphi):\mathbf{E}$, $\boldsymbol{\varepsilon}_{por}=\mathbf{A}_{por}:\mathbf{E}$

- with strain concentration tensor
  $\mathbf{A}(\mathbf{x})$; $\langle\mathbf{A}(\mathbf{x})\rangle=\mathbf{I}$

Eshelby problem

The matrix-(ellipsoidal) inclusion problem



$\varepsilon_{\mathrm{HA}}(\theta,\varphi)=[\mathbf{I}+\mathbf{P}_{\mathrm{cyl}}(\theta,\varphi):(\mathbf{c}_{\mathrm{HA}}-\mathbf{C}_{\mathrm{hom}})]^{-1}:\mathbf{E}^0$

$\varepsilon_{\mathrm{por}}=[\mathbf{I}+\mathbf{P}_{\mathrm{sph}}:(-\mathbf{C}_{\mathrm{hom}}]^{-1}:\mathbf{E}^0$

$\mathbf{P}_{\mathrm{cyl}}$ and $\mathbf{P}_{\mathrm{sph}}$ depend on shape of inclusion (needle/sphere) and stiffness of matrix ($\mathbf{C}_{\mathrm{hom}}$)

Analytical and semianalytical expressions:

Eshelby, 1957: for isotropic matrices

Eshelby-based Concentration Tensors

Use of inclusion strains ε_{HA} and ε_{por} in strain average rule →
$\mathbf{E}^0 = f(\mathbf{E})$,
use in matrix-inclusion problem →
concentration tensors for needles and pores:

$$\mathbf{A}_{HA}(\theta,\varphi)=[\mathbf{I}+\mathbf{P}_{cyl}(\theta,\varphi):(\mathbf{c}_{HA}-\mathbf{C}_{hom})]^{-1}:$$
$$\{(1-\phi)\int_\theta\int_\varphi [\mathbf{I}+\mathbf{P}_{cyl}(\theta,\varphi):(\mathbf{c}_{HA}-\mathbf{C}_{hom})]^{-1}\sin\theta\, d\theta\, d\varphi/4\pi + \phi[\mathbf{I}-\mathbf{S}_{sph}]^{-1}\}^{-1}$$

$$\mathbf{A}_{por}=[\mathbf{I}-\mathbf{S}_{sph}]^{-1}:$$
$$\{(1-\phi)\int_\theta\int_\varphi [\mathbf{I}+\mathbf{P}_{cyl}(\theta,\varphi):(\mathbf{c}_{HA}-\mathbf{C}_{hom})]^{-1}\sin\theta\, d\theta\, d\varphi/4\pi + \phi[\mathbf{I}-\mathbf{S}_{sph}]^{-1}\}^{-1}$$

Stiffness and strength estimates

- combination of concentration tensors $\mathbf{A}_{HA}(\theta,\varphi)$ and $\mathbf{A}_{por}$ with stress averaging rule and microscopic linear elastic law → **macroscopic stiffness**:

$$\mathbf{C}_{hom}=\sum f_r\, \mathbf{c}_r:\mathbf{A}_r=$$

$$= (1-\phi)\, \mathbf{c}_{HA:} \int_\theta \int_\varphi [\mathbf{I}+\mathbf{P}_{cyl}(\theta,\varphi):(\mathbf{c}_{HA}-\mathbf{C}_{hom})]^{-1} \sin\theta\, d\theta\, d\varphi/4\pi :$$

$$\{(1-\phi) \int_\theta \int_\varphi [\mathbf{I}+\mathbf{P}_{cyl}(\theta,\varphi):(\mathbf{c}_{HA}-\mathbf{C}_{hom})]^{-1}\sin\theta\, d\theta\, d\varphi/4\pi + \phi[\mathbf{I}-\mathbf{S}_{sph}]^{-1}\}^{-1}$$

- combination of concentration tensor with averaging rules, micro/macroscopic linear elastic law, and microscopic failure criterion → **macroscopic brittle failure criterion**:

$$F(\boldsymbol{\Sigma}) = \max_{\theta,\varphi}\{\beta \max_{\psi}|\mathbf{N}\cdot(\mathbf{c}_{HA}:\mathbf{A}_{HA}(\theta,\varphi):\mathbf{C}_{hom}{}^{-1}):\boldsymbol{\Sigma}\cdot\mathbf{n}|+$$

$$+\mathbf{N}\cdot (\mathbf{c}_{HA}:\mathbf{A}_{HA}(\theta,\varphi):\mathbf{C}_{hom}{}^{-1}):\boldsymbol{\Sigma}\cdot\mathbf{N}\}-\boldsymbol{\sigma}^{ult,t}=0$$

Mechanical properties of single needle

Exp. set I: ´Universal´ properties of HA

- **Stiffness** of **dense** hydroxyapatite from ultrasonic tests on powder

  (Gilmore and Katz, 1982):

  k_{HA}=82.6 GPa, μ_{HA}=44.9 GPa

- **Tensile/Shear Strength** of **dense** (*polycrystalline*) hydroxyapatite derived from mechanical tests

  (Shareef et al., 1993; Akao et al., 1981):

  $\sigma^{ult,t}$=52.2 MPa, $\sigma^{ult,s}$=80.3 MPa

- Density: ρ_{HA}=3.16 g/cm^3

NOTE: **tensile strength of SINGLE hydroxyapatite crystals:**

~ 500 – 1000 MPa

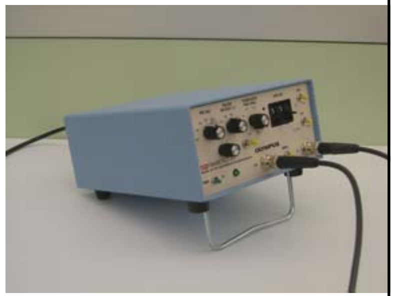
Teraoka, Ito, Maekawa, Onuma, Tateishi, Tsutsumi, J Dent Res 77(7), 1560-1568, 1998

Model validation

Experimental set II – Model test

A: biomaterial-specific porosity
calculated from mass and volume

$\phi = 1 - M/(V\ \rho_{HA})$



B-1: corresponding biomaterial-specific stiffnesses C from

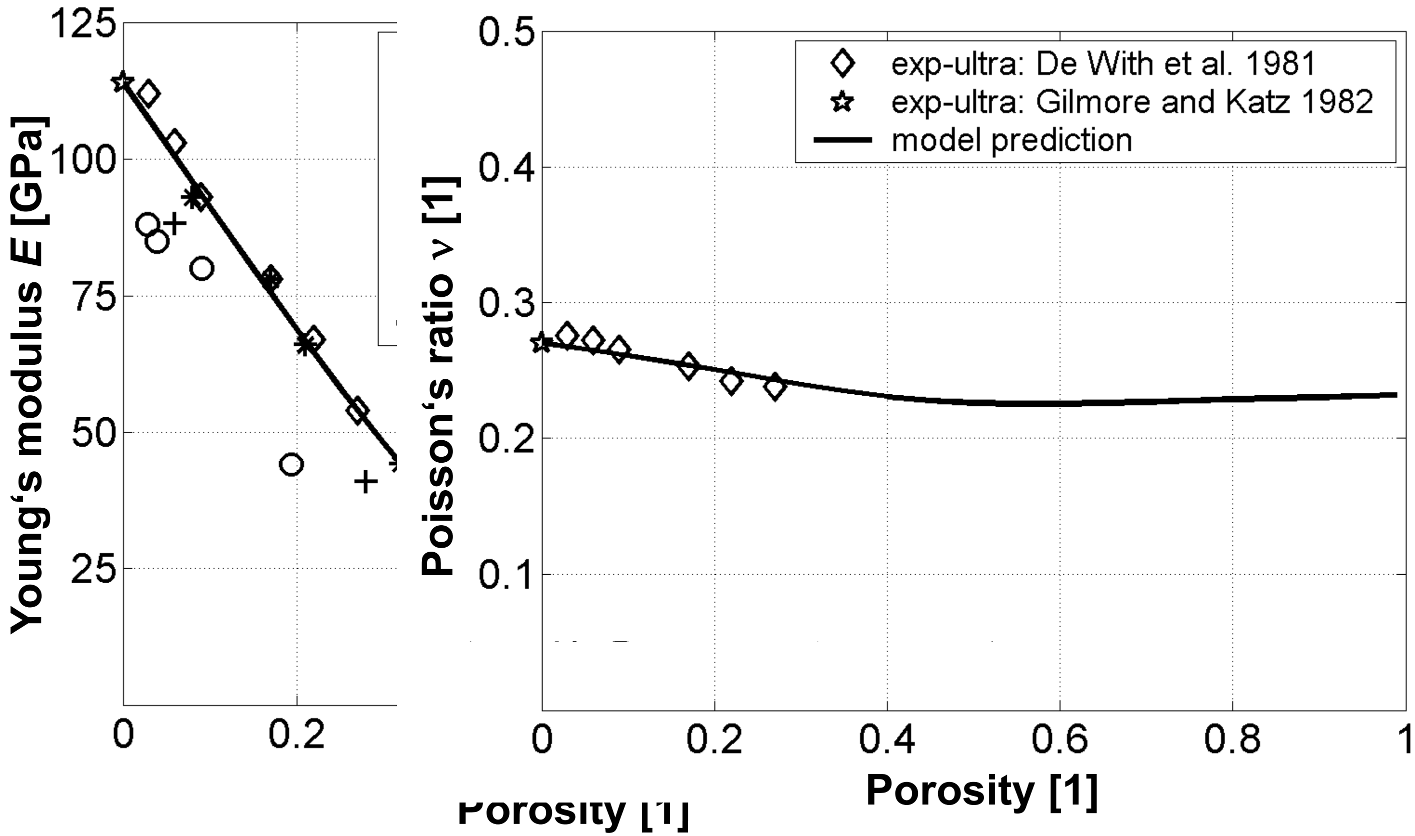
- Ultrasonic (acoustical) testing
- Resonance frequency testing
- Quasi-static mechanical testing

B-2: corresponding biomaterial-specific strength values Σ^{ult} from

- uniaxial compressive testing
- three-point bending testing
- ring bursting test

Validation of stiffness model

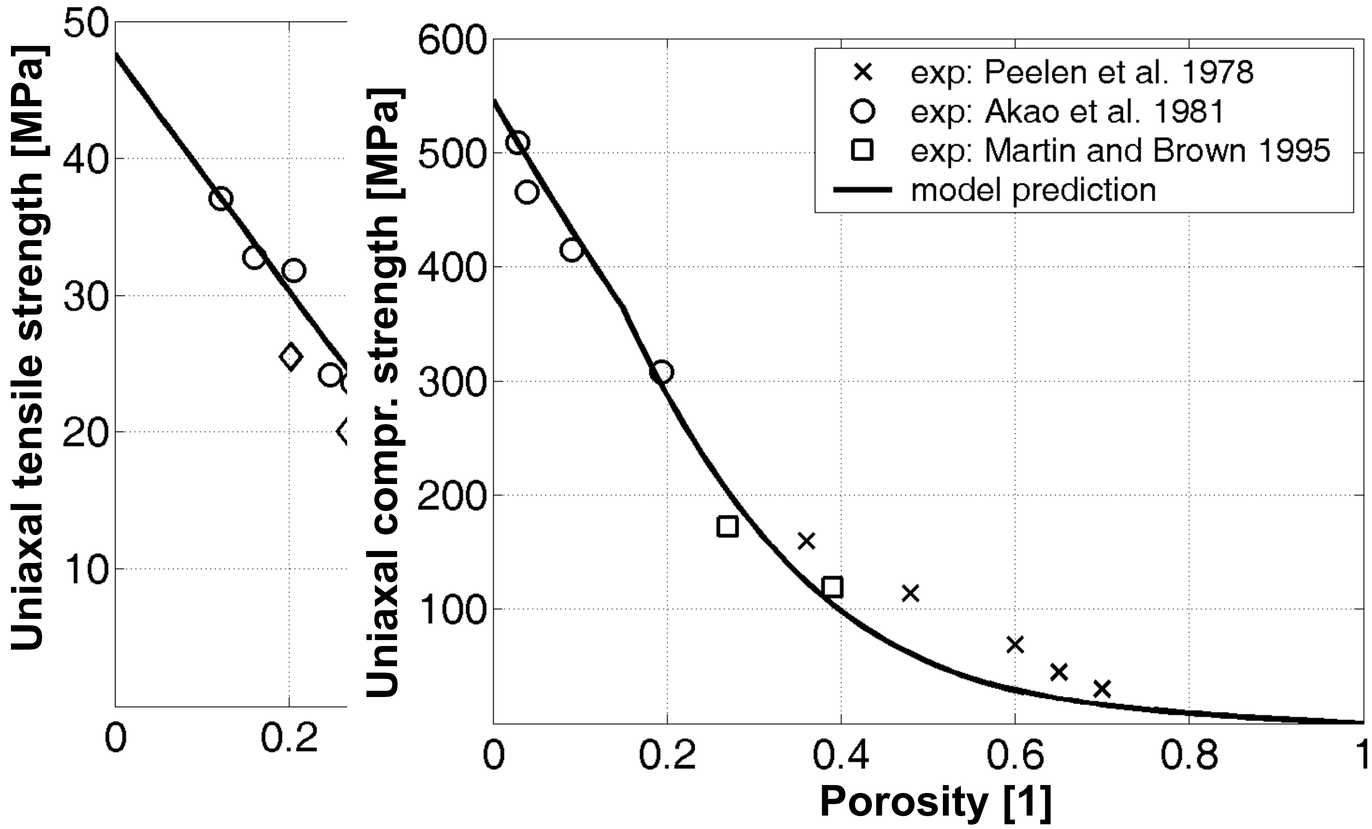
- *sample-specific* model predictions for stiffnesses, based on (sample-independent) universal properties of HA [exp. set I] and on sample-specific porosity [exp. set IIA]



- *sample-specific* experimental stiffnesses [exp. set IIB-1]

Validation of strength model

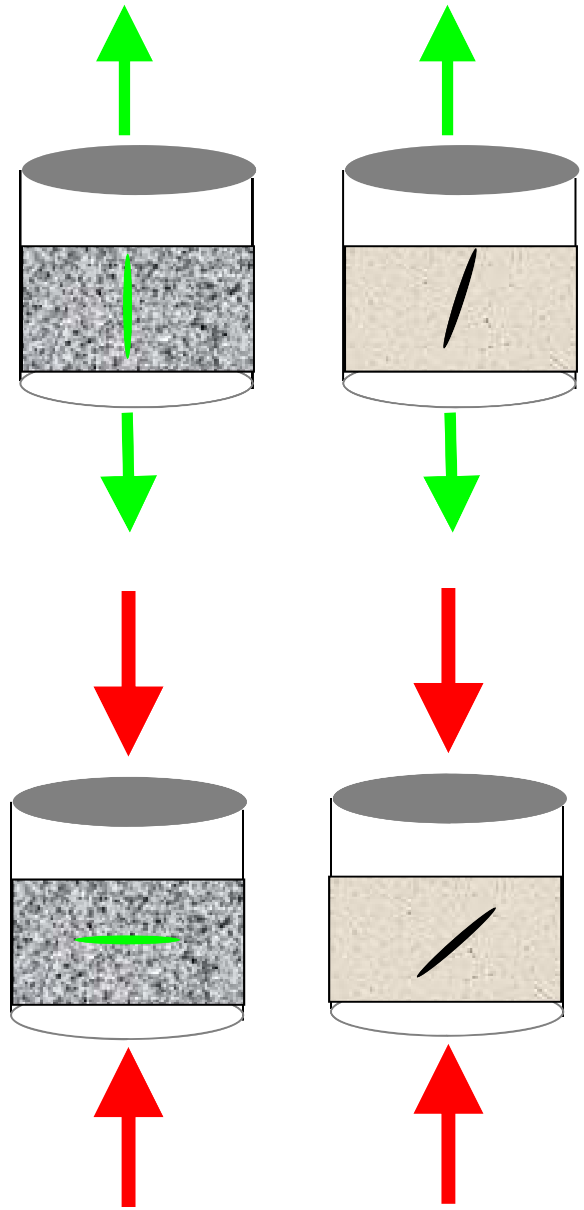
• *sample-specific* model predictions for uniaxial strength, based on (sample-independent) universal properties of HA [exp. set I] and on sample-specific porosity [exp. set IIA]



• *sample-specific* experimental strength values [exp. set IIB-2]

Model characteristics

- Overall tensile failure of high porosity materials: tensile **rupture of vertical needle**
- Overall tensile failure of low porosity materials: **rupture of needle with θ→20°** (shear stress reduces tensile strength of needle/needle interface)
- Overall compressive failure of high porosity materials: tensile **rupture of horizontal needle** (θ→90°)
- Overall compressive failure of low porosity materials: shear **rupture of needle with θ→70°** (compressive stress increases shear strength of needle/needle interface)



… and now: natural bone

6-step scheme

Hellmich, Ulm; *J Eng Mech 128(8):* 898 (2002)
Hellmich, Barthelemy, Dormieux, *Eur.J.Mech A 23:* 783 (2004)
Fritsch, Hellmich, *J Theor Biol, 244:* 597 (2007)
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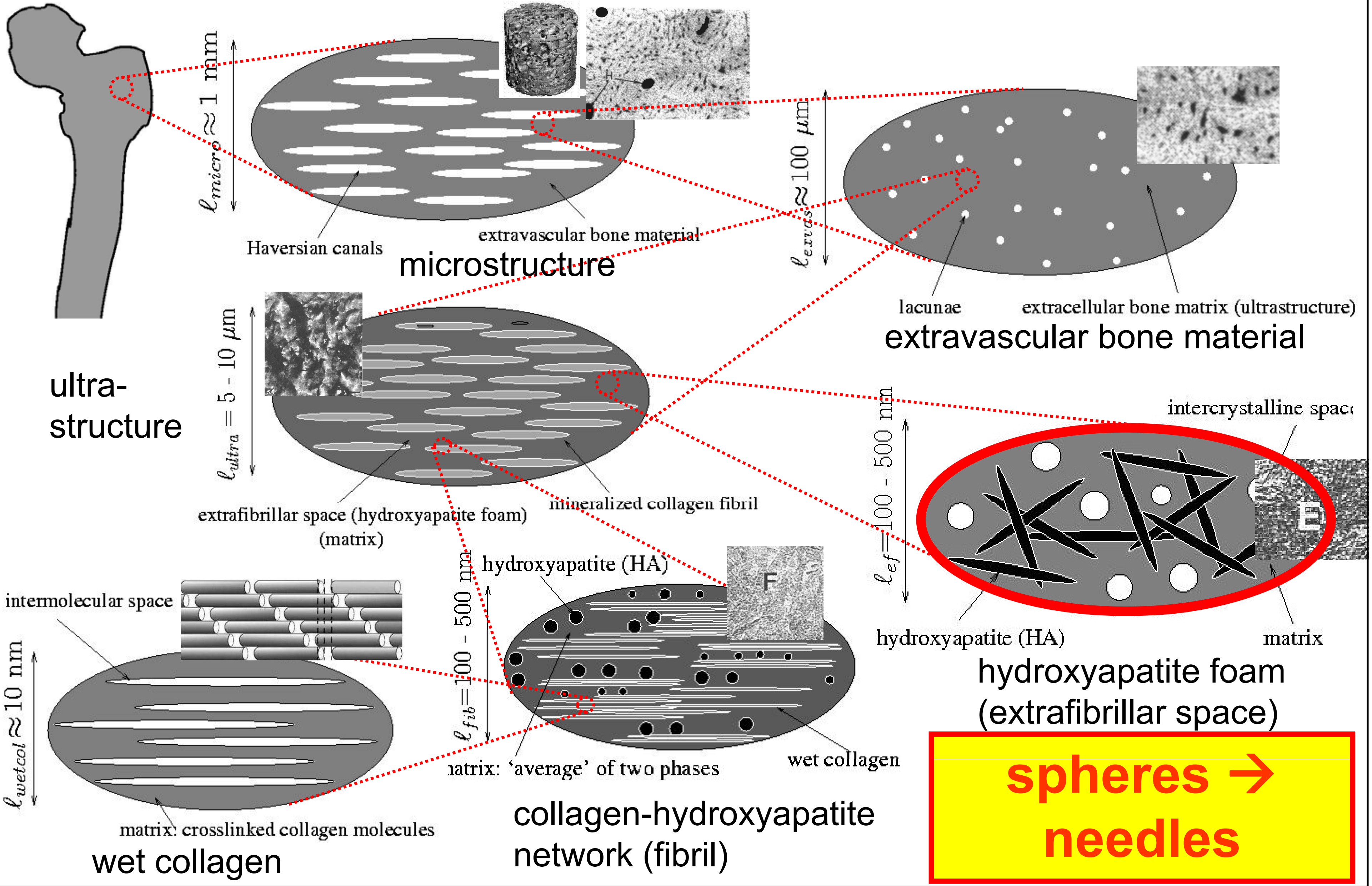
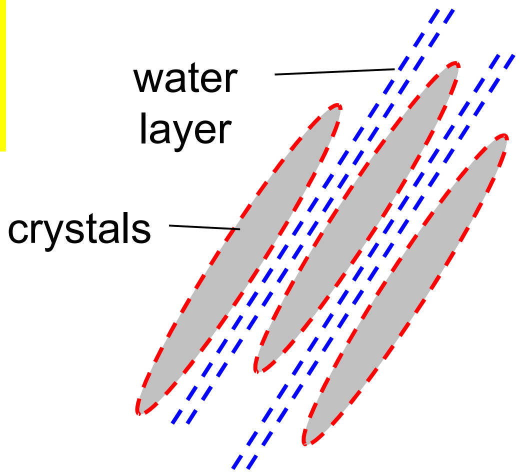


New vision on bone strength

„ductile sliding of hydroxyapatite crystals, prior to failure of collagen cross links“



Ideal elastoplasticity at level of hydroxyapatite phase

$$\boldsymbol{\sigma}_r = \mathbb{c}_r : \left(\boldsymbol{\varepsilon}_r - \boldsymbol{\varepsilon}_r^p\right) \qquad \dot{\boldsymbol{\varepsilon}}_r^p = \dot{\lambda}_r \frac{\partial \mathfrak{f}_r}{\partial \boldsymbol{\sigma}_r}, \quad \dot{\lambda}_r \mathfrak{f}_r(\boldsymbol{\sigma}_r) = 0 \quad \dot{\lambda}_r \geq 0, \quad \mathfrak{f}_r(\boldsymbol{\sigma}_r) \leq 0$$

Extension of strain concentration concept

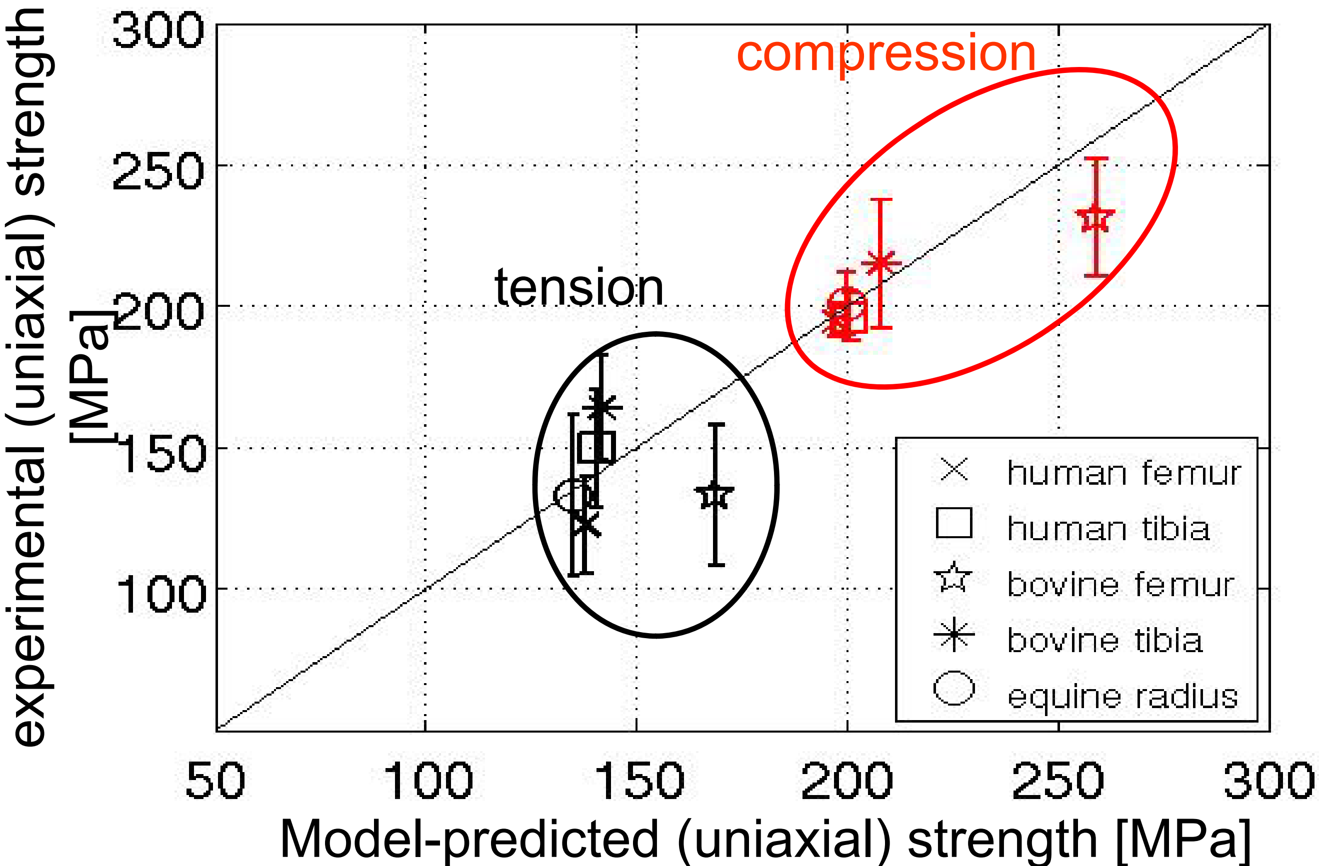
$$\boldsymbol{\varepsilon}_r = \mathbb{A}_r : \boldsymbol{E} + \sum_s \mathbb{D}_{rs} : \boldsymbol{\varepsilon}_s^p$$

influence tensors
estimated from matrix-inclusion problems with plastic strains in inclusion and matrix

Universal material properties concerning „bone strength“

from experiments on **HA minerals**: $\sigma^{ult,t}$=52.2 MPa, $\sigma^{ult,s}$= 80.3 MPa
from experiments on **collagen** – uniaxial strength: $\sigma^{ult,COLL}$= 144.7 MPa

Validation of multiscale elastoPLASTIC bone model



based on universal elastic and strength properties of hydroxyapate and colllagen and on sample-specific composition

Conclusions and Perspectives

- **continuum micromechanics** is suitable for **predicting the mechanical properties** **(elasticity and brittle/ductile failure)** of porous HA biomaterials and real bone, from their **microstructure and composition**
- **design tool for** hydroxyapatite-based **biomaterials and tissue-engineering scaffolds**
- enables **patient-specific bone failure risk assessment** based on micromechanics-supported Finite Element analyses at organ scale

References:

A. Fritsch, L. Dormieux, Ch. Hellmich, J. Sanahuja, *Journal of Biomedical Materials Research 88A: 149-161, 2009*

A. Fritsch, Ch. Hellmich, L. Dormieux, *Journal of Theoretical Biology, DOI:10.1016/j.jtbi.2009.05.021, 2009*