Multiscale structure-functional modeling of musculoskeletal mineralized tissues

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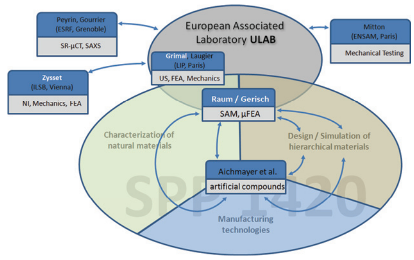
Summary

Musculoskeletal mineralized tissues (MMTs) achieve a unique combination & variability of stiffness and strength with one common building block & structural hierarchy.

Material properties + hierarchical structure = macroscopic elastic function

Hypothesis: multiscale experimental elastic data & numerical homogenization allow to decouple structural & material properties and their respective impacts on the elastic functional behavior of the compound.



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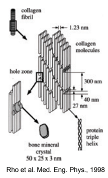
ULAB: ULtrasound bases Assessment of Bone

Nanoscale - mineralized collagen fibril

- well known structure and elastic properties of major components (hydroxyapatite, collagen, water)
- variable mineral deposition & platelet size
- self assembly mechanisms lead to dense regular structures [1]

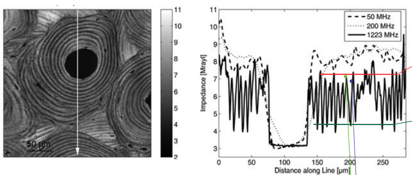


Rho et al. Med. Eng. Phys., 1998

nm

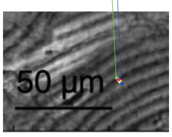
SAXS, SR-µCT

Validation: $C_{exp} \approx C_{eff}$



µm

- *1 - 1.5 GHz SAM* [5]
  lamellar unit size & transverse isotropic stiffness of fibril bundles



1 GHz SAM, NI

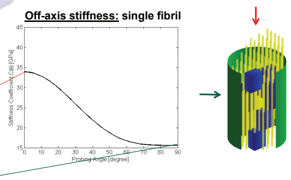
- *Nanoindentation* (small indentation depth) [6]
  Goal: anisotropic elastic modulus & Poisson ratios

Numerical "Bottom-Up" Model

M-I Mineralized Fibril

Goal: time-dependent intra- & interfibrillar mineral deposition and mineral growth[2]

transverse isotropic stiffness tensor $C_{eff}^{nano} = f(t)$

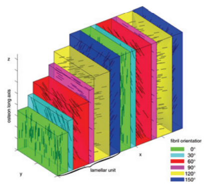


Comparison with exp. data

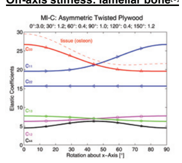
c_{ij} \ [GPa]	SAM [3]	NI [4]
c_{33}	33.9	40.6
c_{11}	15.6	32.8
c_{12}	5.2	15.1
c_{13}	8.8	17.5
c_{44}	3.4	9.1

M-II Lamellar Bone [3]

$$C_{eff}^{micro} = f\left(C_{exp}^{nano}(\vec{x})\right)$$



structure + fibril properties



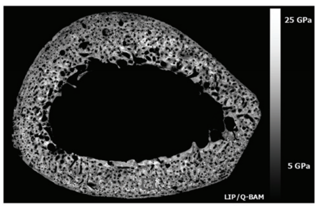
orthotropic stiffness tensor

Validation: $C_{exp} \approx C_{eff}$

Microscale

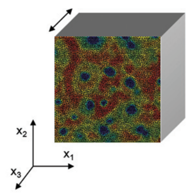
- *50 - 200 MHz SAM* [7]
  heterogeneous tissue elasticity & porous microstructure
- *Nanoindentation* (large indentation depth) [6]
  Goal: anisotropic elastic modulus & Poisson ratios

mm



M-III Mesoscale Model [7]

$$C_{eff}^{meso} = f\left(C_{exp}^{micro}(\vec{x})\right)$$



50 - 200 MHz SAM, NI

porous structure + heterogeneous tissue properties at 1-mm length scale

orthotropic stiffness tensor

Validation: $C_{exp} \approx C_{eff}$

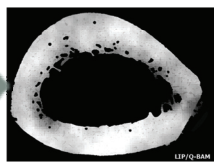
Mesoscale / Macroscale

- Low frequency ultrasound (1 - 10 mm)
  orthotropic tissue elasticity

- *Mechanical testing* (> 5 mm)
  anisotropic elastic modulus

$$C_{exp}^{macro} = C_{eff}^{macro}$$

Macroscale Simulation



Goal:
suitable & realistic input for standard FE analysis

Homogenization

Input inhomogeneous material tensor $C(\vec{x})$ with small scale variations in Representative Volume Element (RVE).

Objective find effective material tensor C_{eff} for RVE, such that mechanical responses of RVE with $C(\vec{x})$ and C_{eff} are similar.

Method Numerical homogenization, i.e. compute C_{eff} from spatially averaged results of the solution of the equations of linear elasticity in the RVE subjected to specific loading conditions and using $C(\vec{x})$.

Implementation Finite Element Method (FEM) using Comsol Multiphysics and high resolution experimentally derived elastic input data.

Application use C_{eff} as input for the FE simulations on larger scales.

Mathematical challenges choice of loading conditions; accuracy control and speed-up of the FE solution; sensitivity investigations.

Samples

Tissue type	Origin	Mineral content	Fiber Orientation	Periodic Size
Mineralized tendon	Turkey	< 50 wt%	parallel	up to 1mm
Parallel-fibered bone	Young cattle	~ 65 wt%	parallel	~ 100 µm
Plexiform bone	Cattle		parallel + lamellar	~ 100 µm
Plywood structure	Mature Cattle, Human	30-70 wt%	orthogonal twisted (osteons, interstitial tissue)	< 5 µm
Artificial compound	MPI Golm Aichmayer	n.a.	parallel	< 1 cm

Definition of Length Scales

Length scale	Composition	Compound	Nomenclature
1 - 200 nm	hydroxyapatite, collagen, water, other	mineralized collagen fibril	nanoscale
0.2 - 10 µm	mineralized collagen fibrils, pores	mineralized tissue matrix (variable structures)	microscale
0.01 - 1 mm	mineralized tissue matrix, pores	MMTs	mesoscale
> 1 mm	MMTs, macrostructure	organs	macroscale

Outcomes

1. Linked experimental assessment / numerical modeling of mechanical function of MMTs at several length scales.
2. Validation of the results by cross-validation at all scales.
3. Tool to simulate mechanical outcome of compositional /structural alterations (e.g. maturation, pathologies)
4. Application to biomimetic hierarchically structured materials (Aichmayer).

References

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[7] Raum et al. Phys Med Biol, 2006
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