Micromechanical Modeling of Cortical Bone and Synthetic Biocomposites

Ryan K. Roeder

Department of Aerospace and Mechanical Engineering
Bioengineering Graduate Program
University of Notre Dame, Notre Dame, IN 46556

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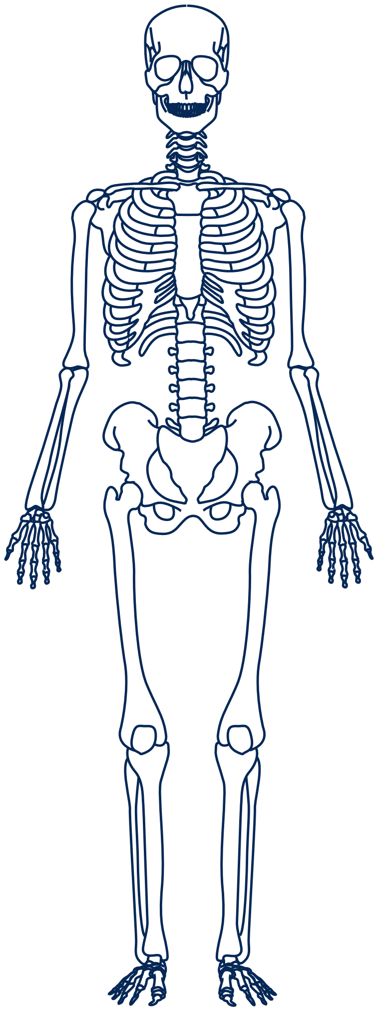
Imagine a Structural Material...

- with high strength to weight ratio.
- with a fatigue life of tens of millions of cycles.
- with microstructure and properties that adapt to the magnitude and direction of loading.
- with the ability to heal cracks and fractures.
- with infinite value added (provided at no ‘cost,’ but ‘priceless’ to replace).

1.5 million osteoporosis-related fractures occur annually.

Osteoporosis costs Americans $38 million each day.

Stress fractures cost the Army $10 million annually.



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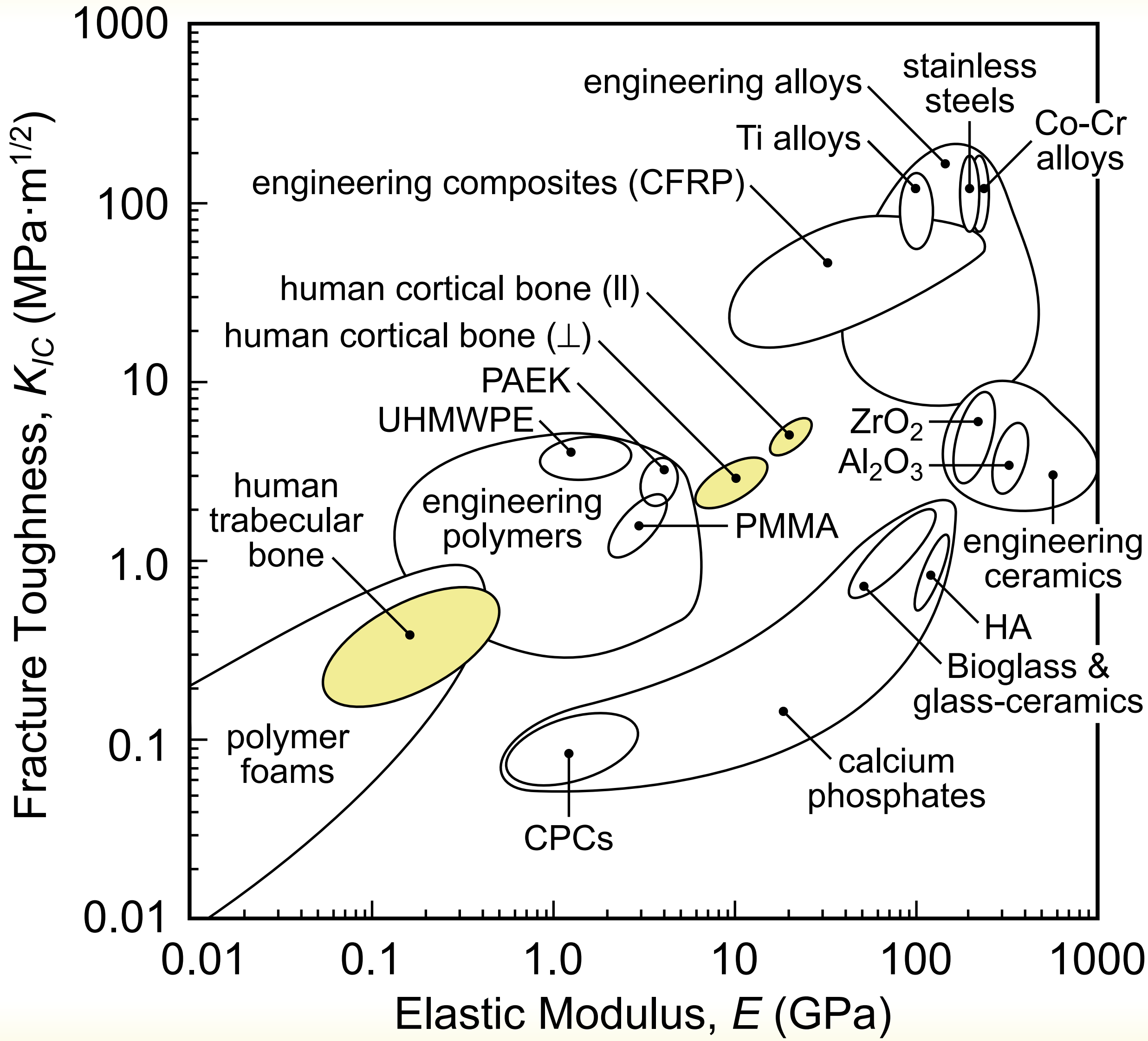
Mechanical Properties of Bone vs. Biomaterials



R.K. Roeder, *et al.*, *JOM*, 2008. Adapted from M.F. Ashby, *Materials Selection in Mechanical Design*,1992, etc.

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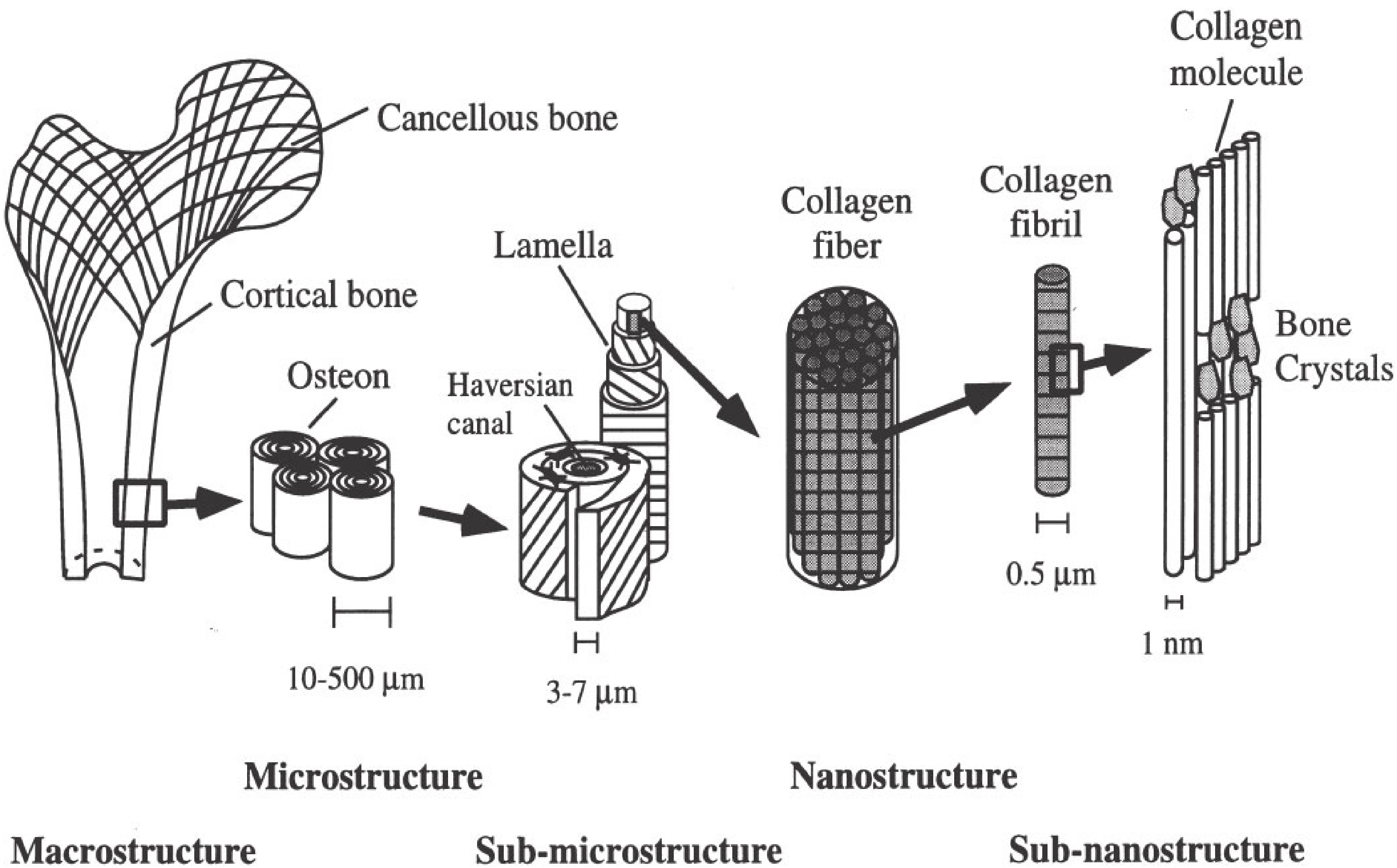
Hierarchical Structure of Bone Tissue

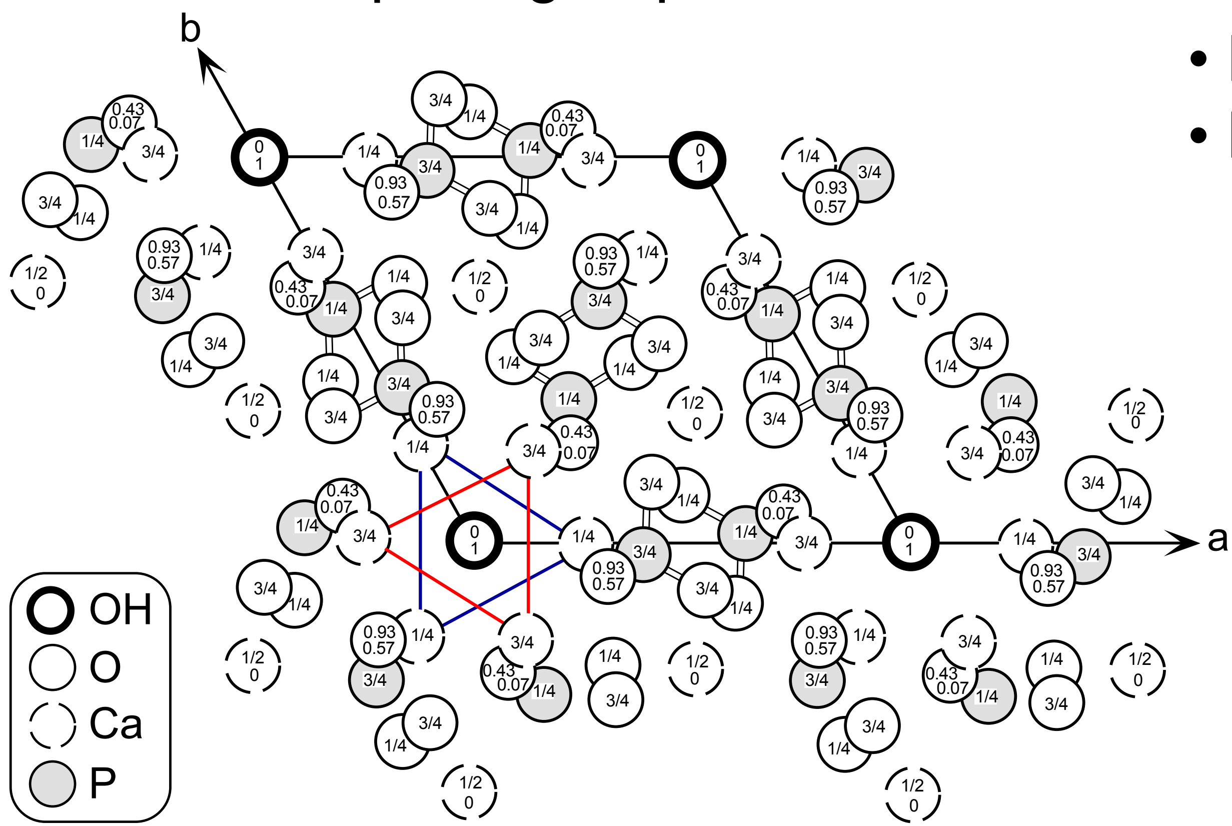


J-Y. Rho, *et al.*, *Med. Eng. Phys.*,1998.

Hydroxyapatite Crystal Structure

$Ca_{10}(PO_4)_6(OH)_2$

space group: $P6_3/m$

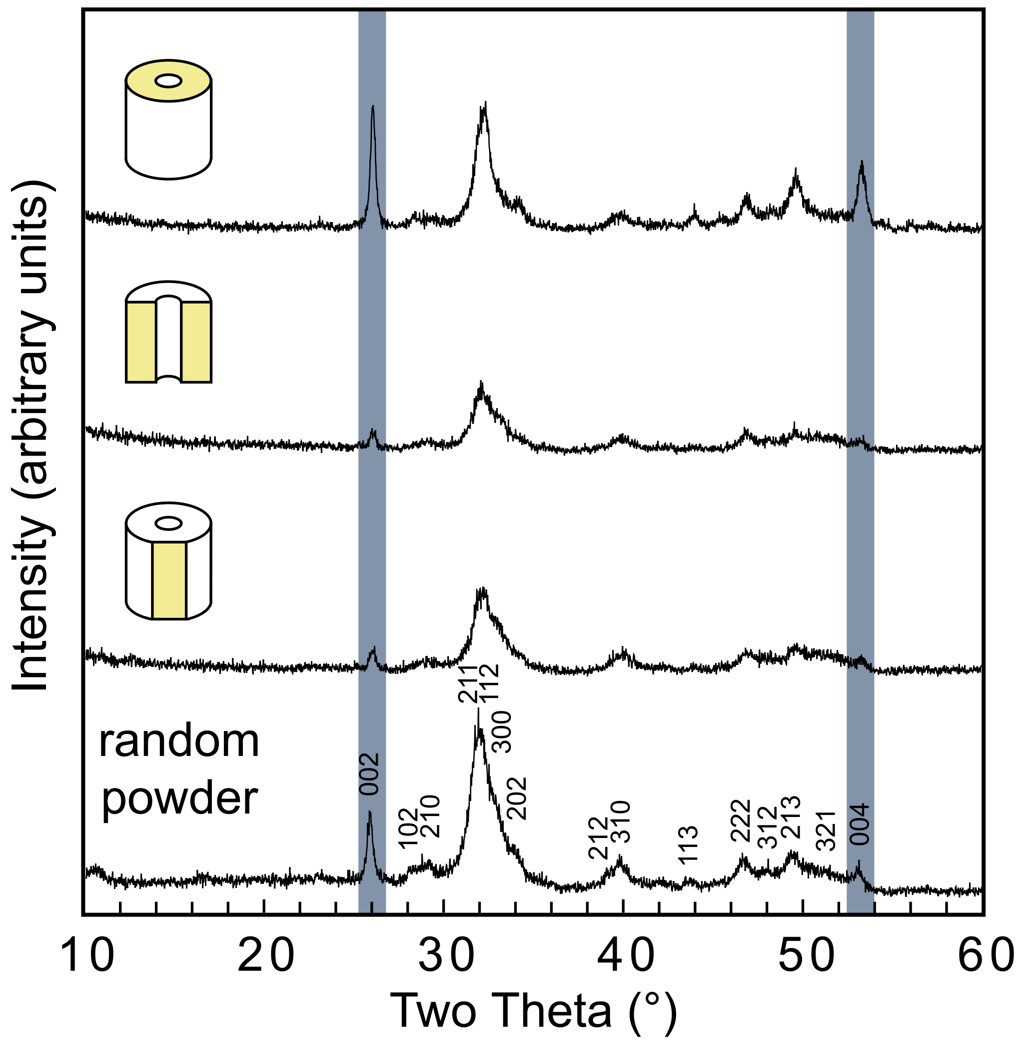


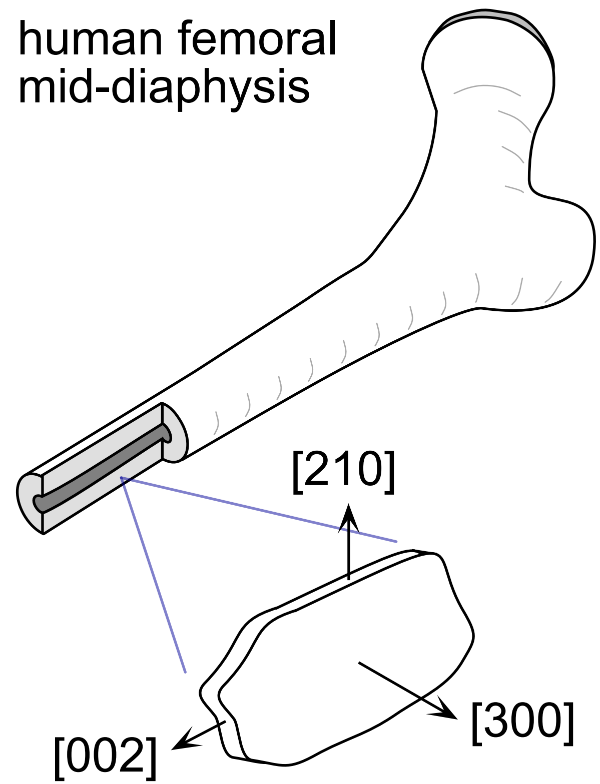
Bone Mineral

- calcium deficient
- highly substituted
- low crystallinity

Adapted from Young and Elliott, *Archs. Oral. Biol.*, 1966.

Preferred Orientation of Bone Mineral

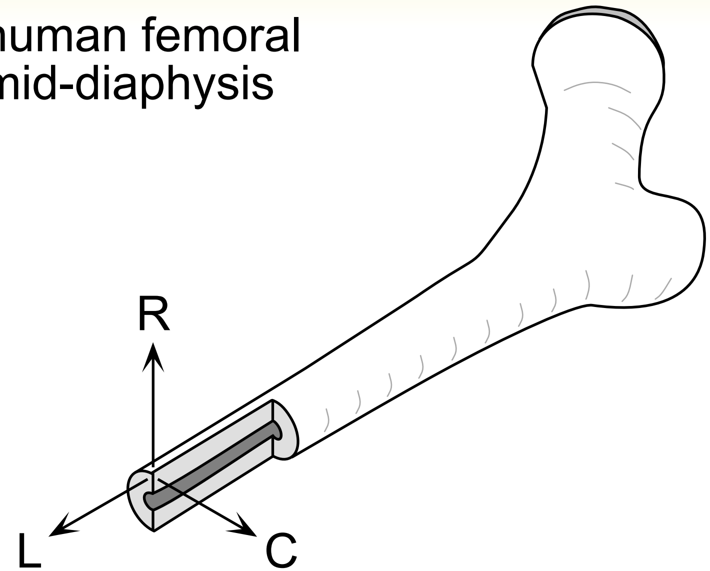




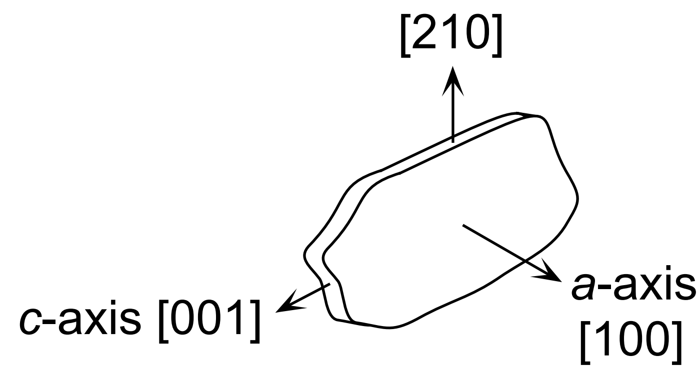
Roeder, *et al.*, *J. Biomed. Mater. Res.*, 2003.

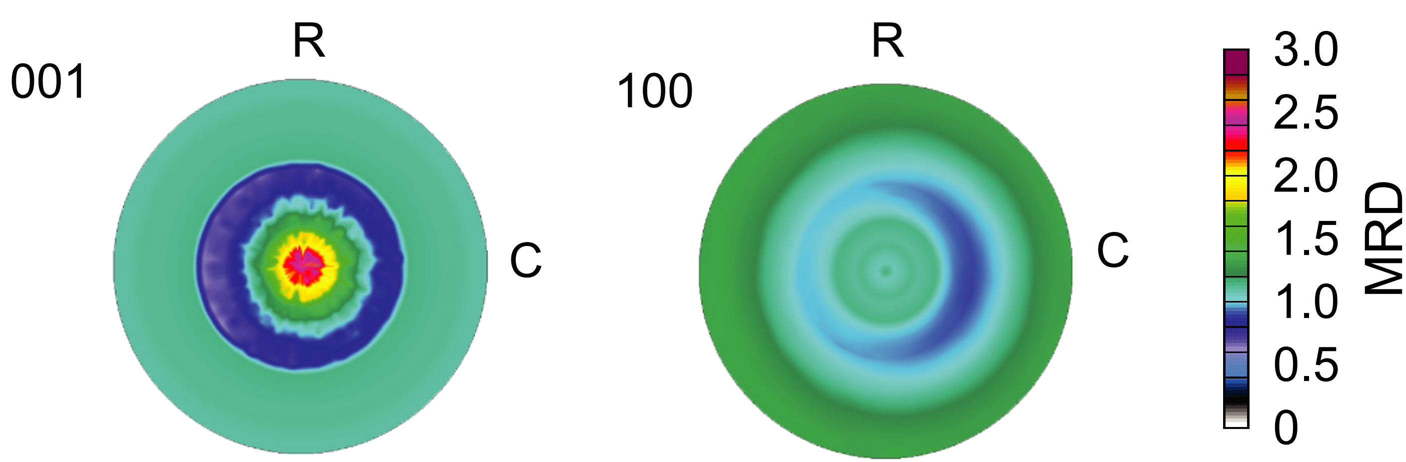
Preferred Orientation of Bone Mineral

human femoral
mid-diaphysis



20-150 x 10-80 x 2-10 nm
average: 50 x 25 x 3 nm





W. Yue and R.K. Roeder, 2006.

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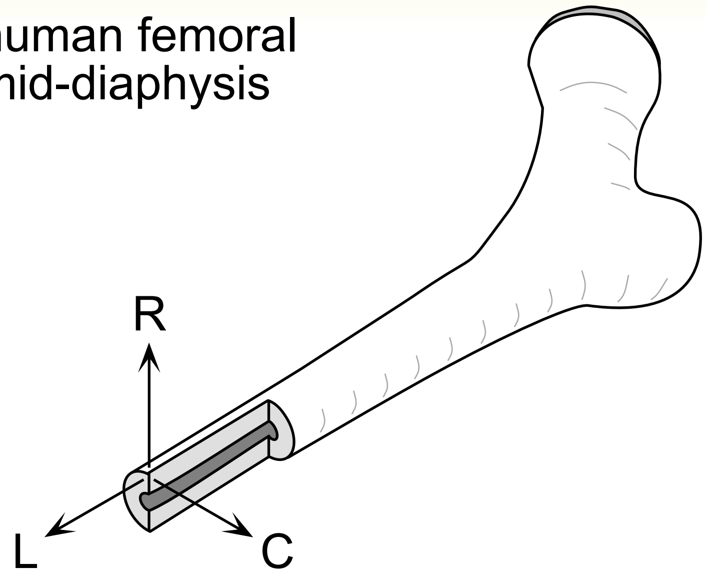
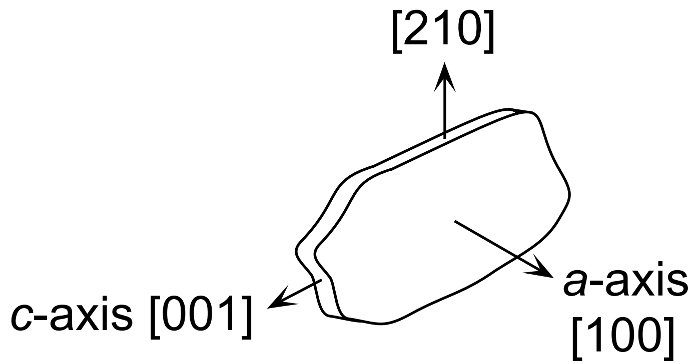
Preferred Orientation of Bone Mineral

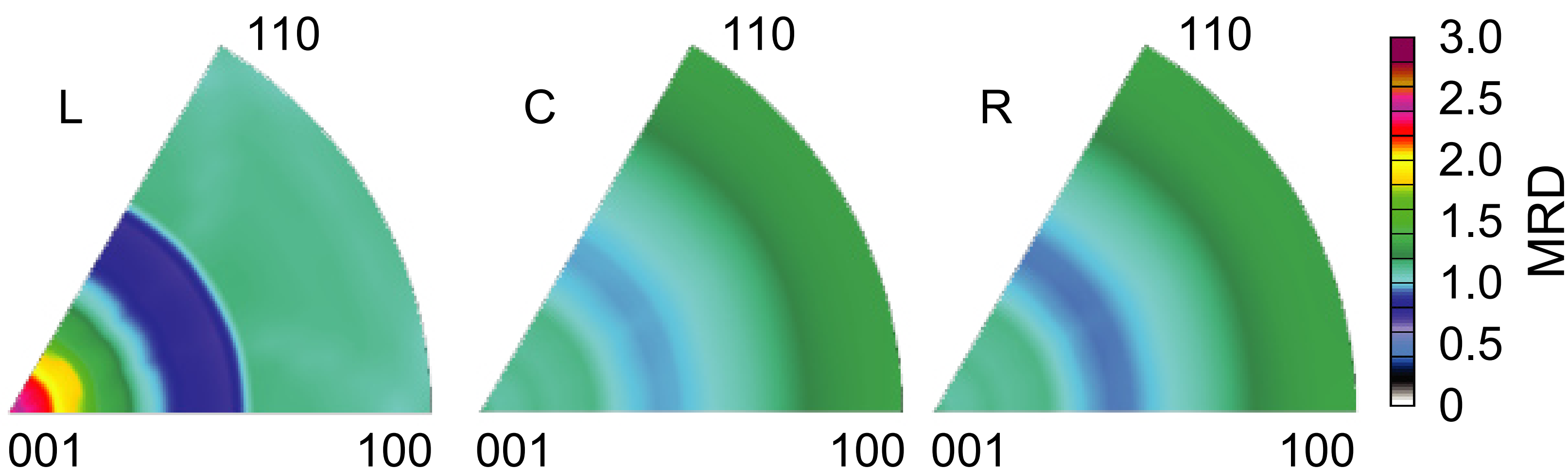
human femoral
mid-diaphysis



20-150 x 10-80 x 2-10 nm

average: 50 x 25 x 3 nm





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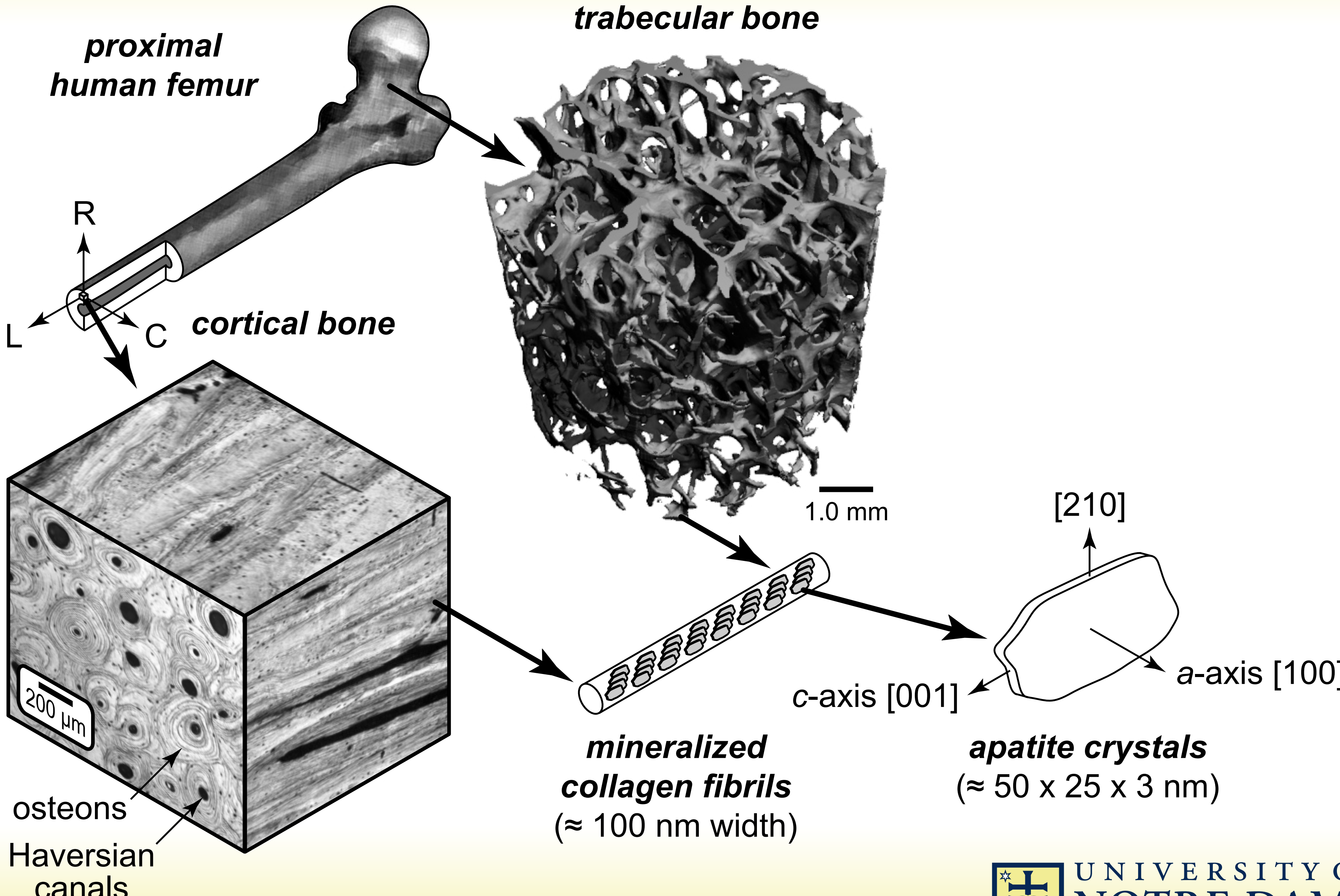
Hierarchical Structure of Bone Tissue



Adapted from R.K. Roeder, *et al.*, *JOM*, 2008.

Micromechanical Model for Whisker or Platelet Reinforced Composites

consider 3 factors:

1) contributions of each phase

HA: $$C_{HA} = \begin{bmatrix} 137 & 42.5 & 54.9 & 0 & 0 & 0 \\ 42.5 & 137 & 54.9 & 0 & 0 & 0 \\ 54.9 & 54.9 & 172 & 0 & 0 & 0 \\ 0 & 0 & 0 & 39.6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 39.6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 47.25 \end{bmatrix} \text{GPa}$$

$E_{HA,L}$ = 138.9 GPa
$E_{HA,T}$ = 113.6 GPa
$G_{HA,LT}$ = 39.5 GPa
$\nu_{HA,LT}$ = 0.25 GPa

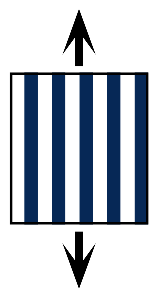
J.L. Katz and K. Ukraincik, *J. Biomechanics*, 1971.

HDPE: E_p = 1.1 GPa G_p = 0.4 GPa ν_p = 0.4
Collagen: E_p = 1.1 GPa G_p = 0.4 GPa ν_p = 0.4

Micromechanical Model for Whisker or Platelet Reinforced Composites

1) contributions of each phase

Voigt (upper bound)



$$\bar{E}_V = \bar{E}_{HA,L} \cdot V_{HA} + E_p \cdot (1 - V_{HA})$$

$$\bar{E}_{HA,L} = \left[\left[\frac{\sum_\theta \left(T_\sigma \cdot C \cdot T_\sigma^T \right) \cdot f(\theta)}{\sum_\theta f(\theta)} \right]^{-1}_{33} \right]^{-1}$$

Reuss (lower bound)

$$\bar{E}_R = \frac{\bar{E}_{HA,T} \cdot E_p}{\bar{E}_{HA,T} \cdot (1 - V_{HA}) + E_p \cdot V_{HA}}$$

$$\bar{E}_{HA,T} = \left[\frac{\sum_\theta \left(T_\varepsilon \cdot S \cdot T_\varepsilon^T \right)_{11} \cdot f(\theta)}{\sum_\theta f(\theta)} \right]^{-1}$$

where,

$$T_\sigma = \begin{bmatrix} a_{11}^2 & a_{12}^2 & a_{13}^2 & 2a_{12}a_{13} & 2a_{11}a_{13} & 2a_{11}a_{12} \\ a_{21}^2 & a_{22}^2 & a_{23}^2 & 2a_{22}a_{23} & 2a_{21}a_{23} & 2a_{21}a_{22} \\ a_{31}^2 & a_{32}^2 & a_{33}^2 & 2a_{32}a_{33} & 2a_{31}a_{33} & 2a_{31}a_{32} \\ a_{21}a_{31} & a_{22}a_{32} & a_{23}a_{33} & a_{22}a_{33} + a_{23}a_{32} & a_{23}a_{31} + a_{21}a_{33} & a_{31}a_{22} + a_{21}a_{32} \\ a_{11}a_{31} & a_{12}a_{32} & a_{13}a_{33} & a_{13}a_{32} + a_{12}a_{33} & a_{11}a_{33} + a_{13}a_{31} & a_{11}a_{32} + a_{12}a_{31} \\ a_{11}a_{21} & a_{12}a_{22} & a_{13}a_{23} & a_{12}a_{23} + a_{13}a_{22} & a_{11}a_{23} + a_{13}a_{21} & a_{11}a_{22} + a_{12}a_{21} \end{bmatrix}$$

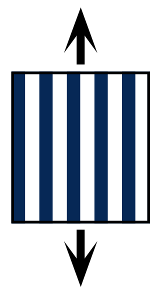
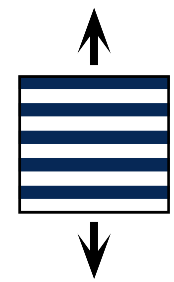
$$a_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & \sin(\theta) \\ 0 & -\sin(\theta) & \cos(\theta) \end{bmatrix}$$

$$T_\varepsilon = \left[T_\sigma^T \right]^{-1}$$

Micromechanical Model for Whisker or Platelet Reinforced Composites

consider 3 factors:

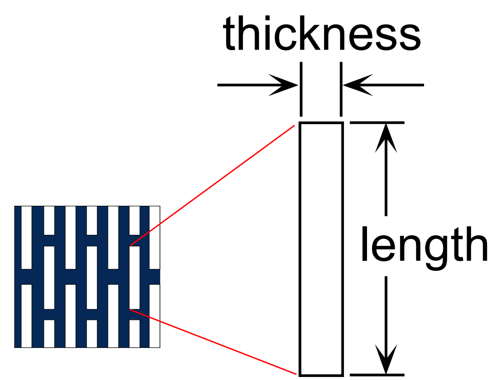
1) contributions of each phase (HA and polymer or collagen)

Voigt (upper bound)  Reuss (lower bound) 

2) morphology of reinforcements

using the Halpin-Tsai Equations

representative volume element (RVE)



aspect ratio, $R = \dfrac{\text{length}}{\text{thickness}}$

Micromechanical Model for Whisker or Platelet Reinforced Composites

2) morphology of reinforcements (Halpin-Tsai Equations)

$$E_L = E_p \frac{1+\zeta \cdot \eta \cdot V_{HA}}{1-\eta \cdot V_{HA}} \quad \text{where} \quad \eta = \frac{E_{HA,L}}{E_p} - 1 \bigg/ \frac{E_{HA,L}}{E_p} + \zeta \qquad \zeta = 2 \cdot R + 40 \cdot V_{HA}^{10}$$

$$E_T = E_p \frac{1+\zeta \cdot \eta \cdot V_{HA}}{1-\eta \cdot V_{HA}} \quad \text{where} \quad \eta = \frac{E_{HA,T}}{E_p} - 1 \bigg/ \frac{E_{HA,T}}{E_p} + \zeta \qquad \zeta = 2 + 40 \cdot V_{HA}^{10}$$

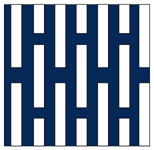
$$G_{LT} = G_p \frac{1+\zeta \cdot \eta \cdot V_{HA}}{1-\eta \cdot V_{HA}} \quad \text{where} \quad \eta = \frac{G_{HA,LT}}{G_p} - 1 \bigg/ \frac{G_{HA,LT}}{G_p} + \zeta \qquad \zeta = 1 + 40 \cdot V_{HA}^{10}$$

$$\nu_{LT} = \nu_{HA,LT} \cdot V_{HA} + \nu_p \cdot (1 - V_{HA}) \qquad \nu_T \approx 1 - (E_T / G_T)$$

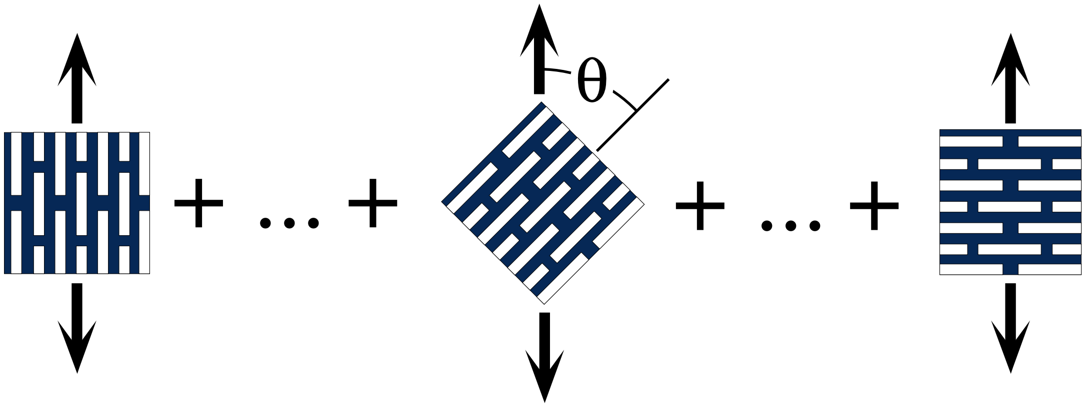
J.C. Halpin, *Primer on Composite Materials Analysis*, 2nd Ed., 1992.

Micromechanical Model for Whisker or Platelet Reinforced Composites

3) preferred orientation of the reinforcements

representative volume element (RVE) 

weight the contribution of each misorientation by an ODF, $g(\theta)$

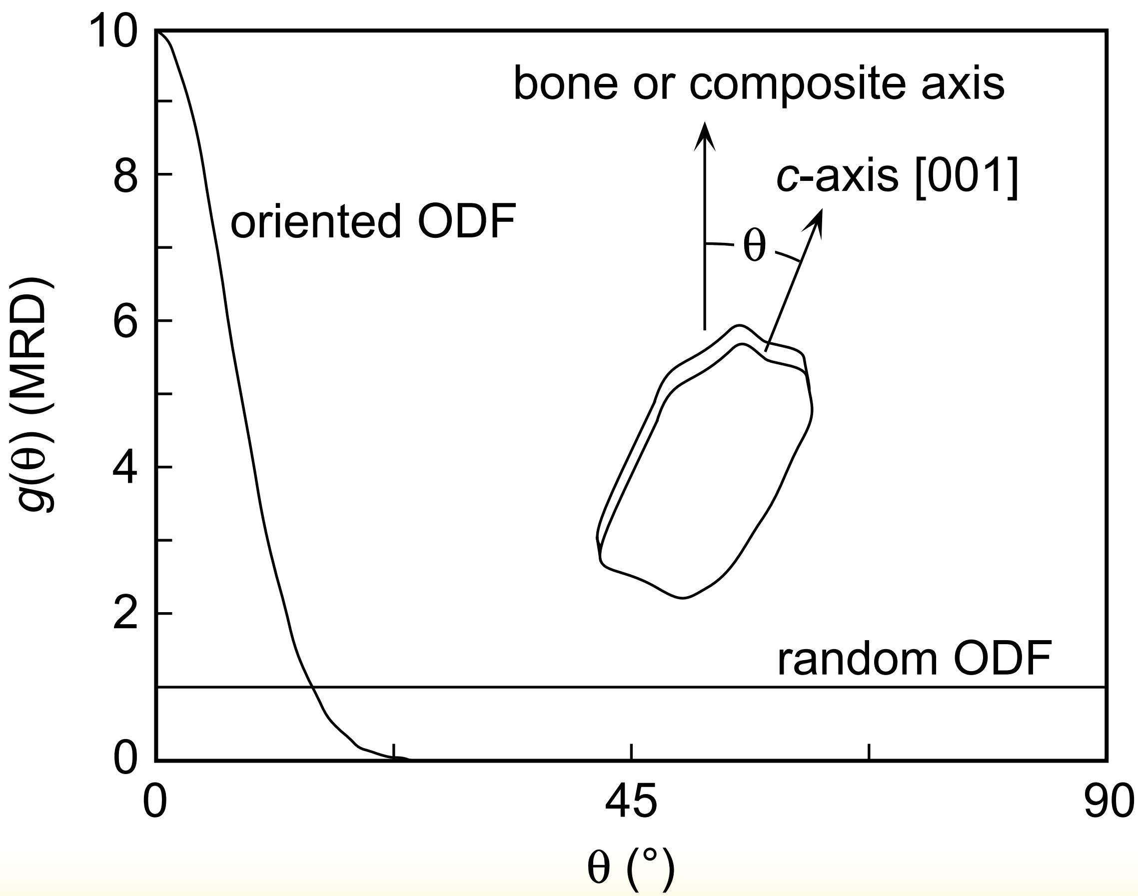


$\theta = 0°$ θ $\theta = 90°$

$$\bar{E}_L = \frac{\int_\theta g(\theta)\cdot E_L(\theta)\cdot d\theta}{\int_\theta g(\theta)\cdot d\theta}$$

Micromechanical Model for Whisker or Platelet Reinforced Composites

3) preferred orientation of reinforcements (simulated ODFs)



Micromechanical Model for Whisker or Platelet Reinforced Composites

3) preferred orientation of reinforcements

$$\bar{E}_L = \frac{\int_\theta g(\theta)\cdot E_L(\theta)\cdot d\theta}{\int_\theta g(\theta)\cdot d\theta}$$

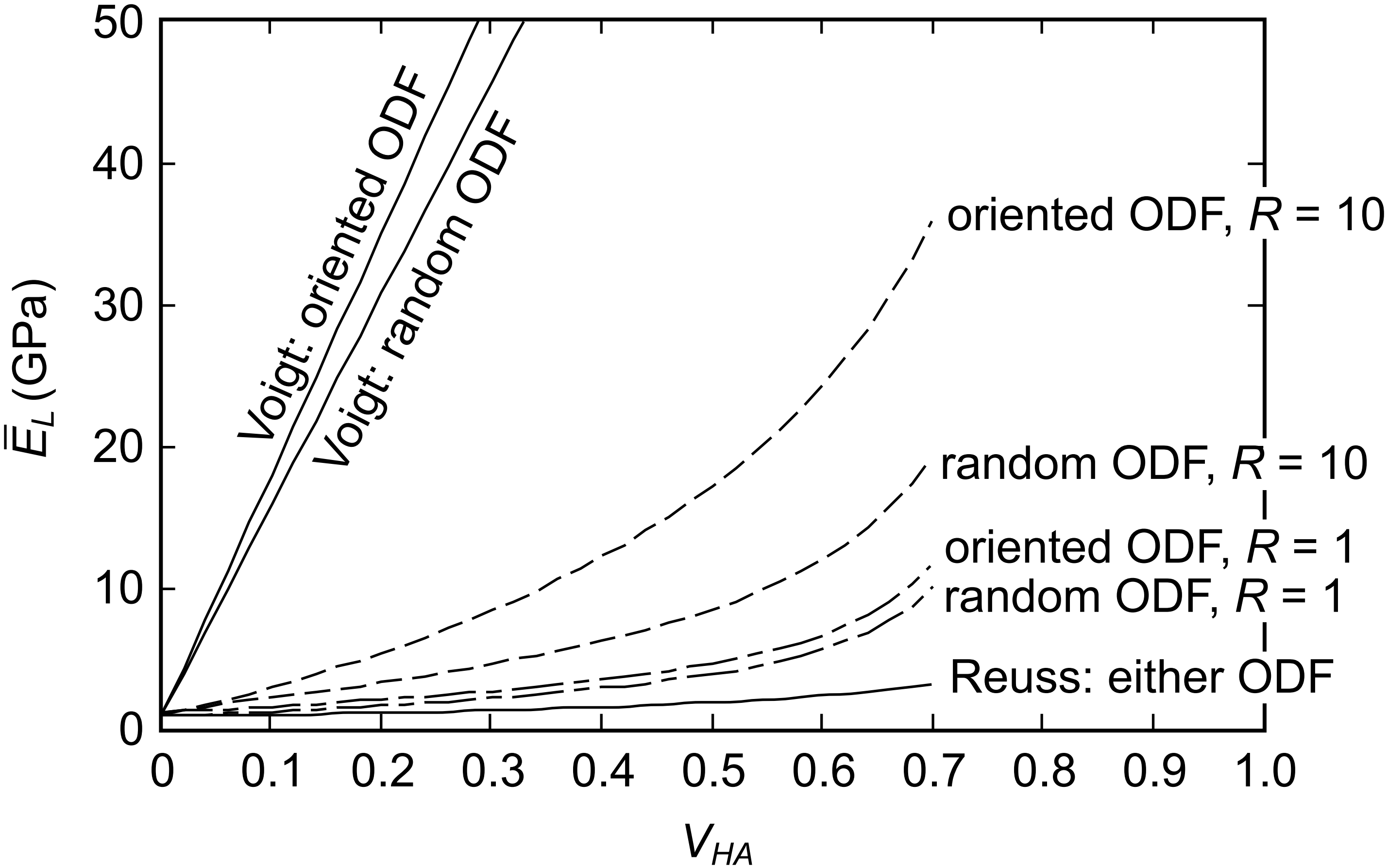
$$E_L(\theta) = \left[T_\varepsilon \cdot S_{RVE} \cdot T_\varepsilon^T\right]_{33}^{-1}$$

$$S_{RVE} = \begin{bmatrix} \frac{1}{E_T} & \frac{-\nu_T}{E_T} & \frac{-\nu_{LT}}{E_L} & 0 & 0 & 0 \\ \frac{-\nu_T}{E_T} & \frac{1}{E_T} & \frac{-\nu_{LT}}{E_L} & 0 & 0 & 0 \\ \frac{-\nu_{LT}}{E_L} & \frac{-\nu_{LT}}{E_L} & \frac{1}{E_L} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{LT}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{LT}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2\cdot(1+\nu_T)}{E_T} \end{bmatrix}$$

or

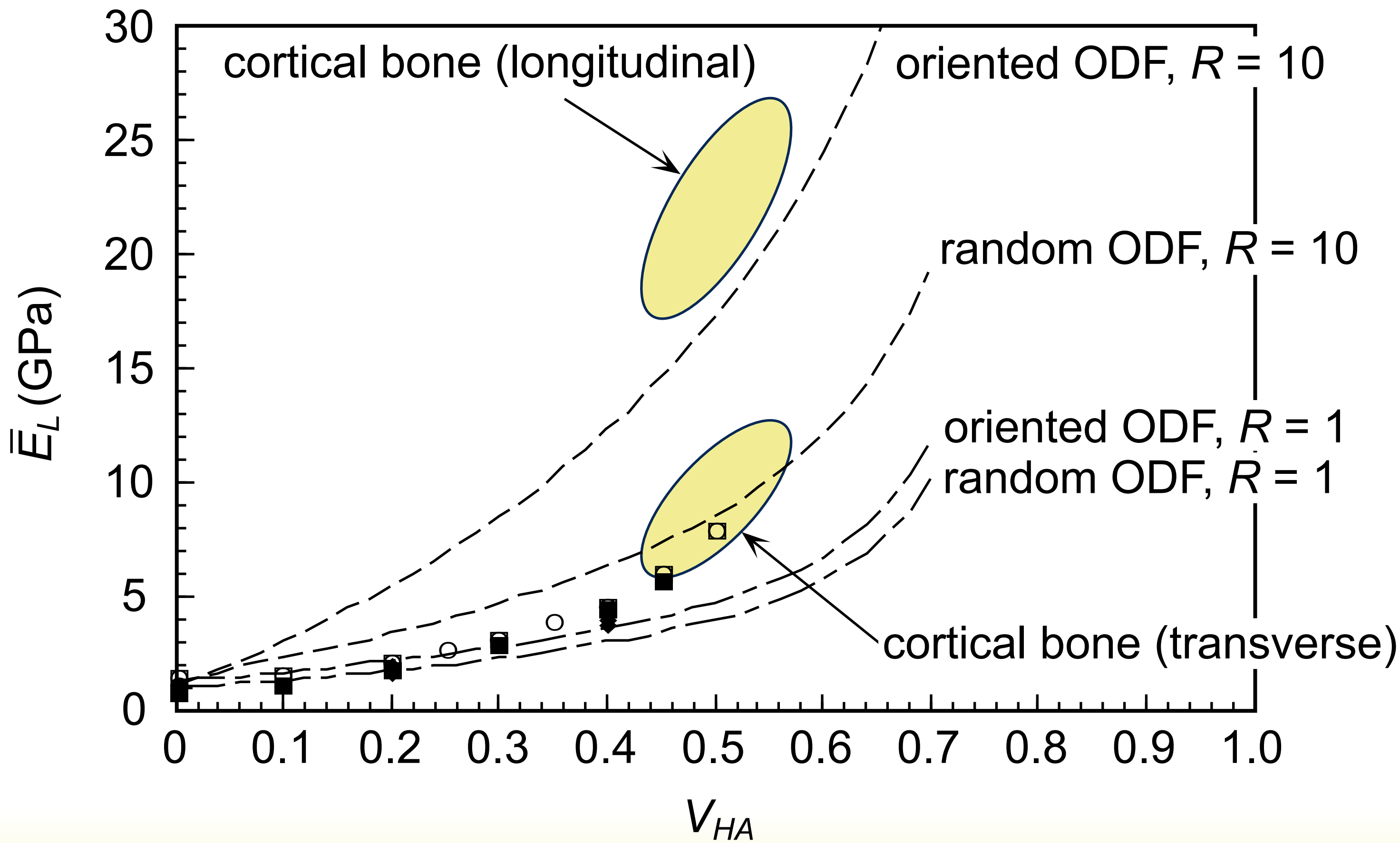
$$E_L(\theta) = \left[\frac{\cos^4(\theta)}{E_L} + \frac{\sin^4(\theta)}{E_T} + \sin^2(\theta)\cdot\cos^2(\theta)\cdot\left(\frac{1}{G_{LT}} - \frac{2\cdot\nu_{LT}}{E_L}\right)\right]^{-1}$$

Micromechanical Model for Whisker or Platelet Reinforced Composites

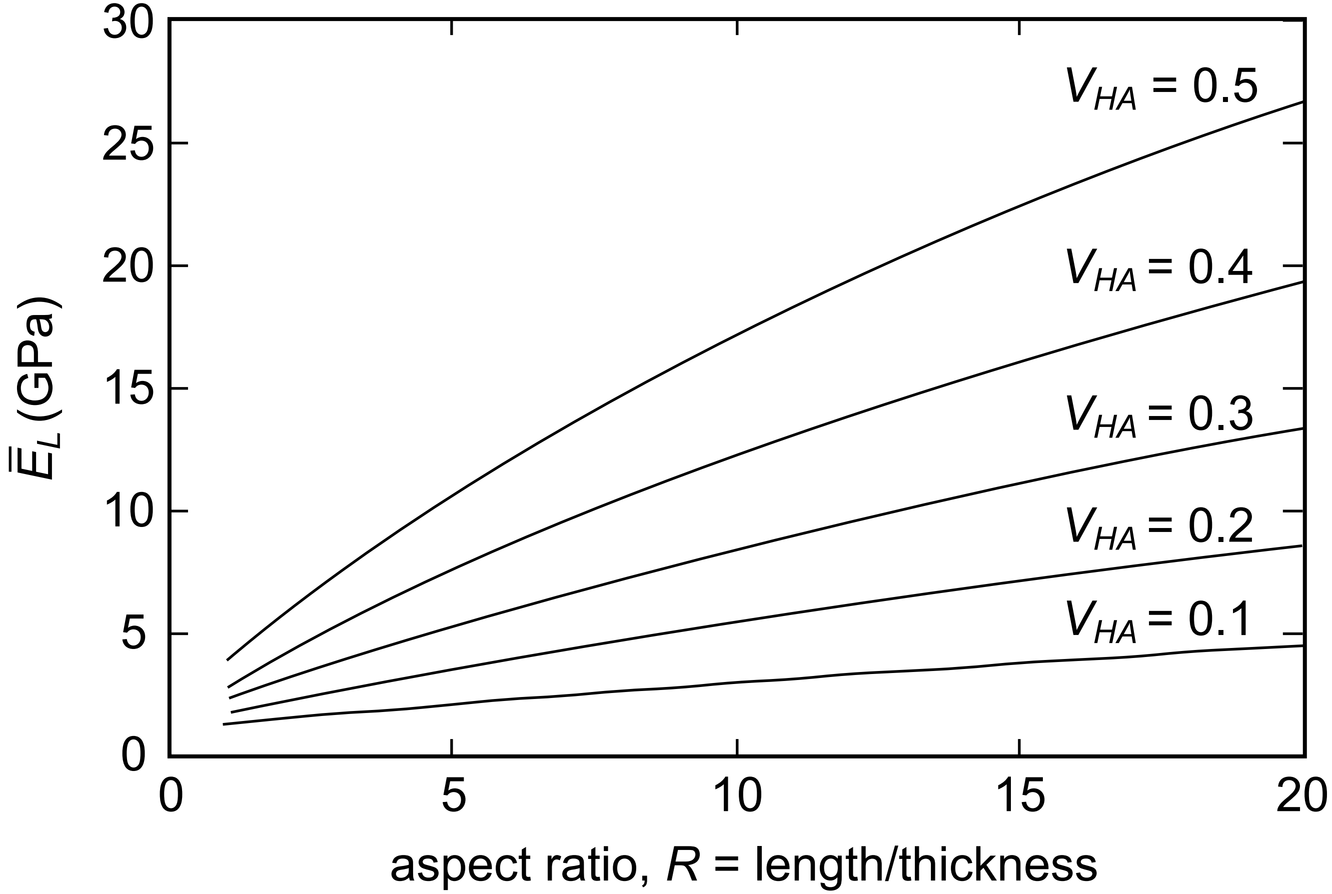


Micromechanical Model for Whisker or Platelet Reinforced Composites

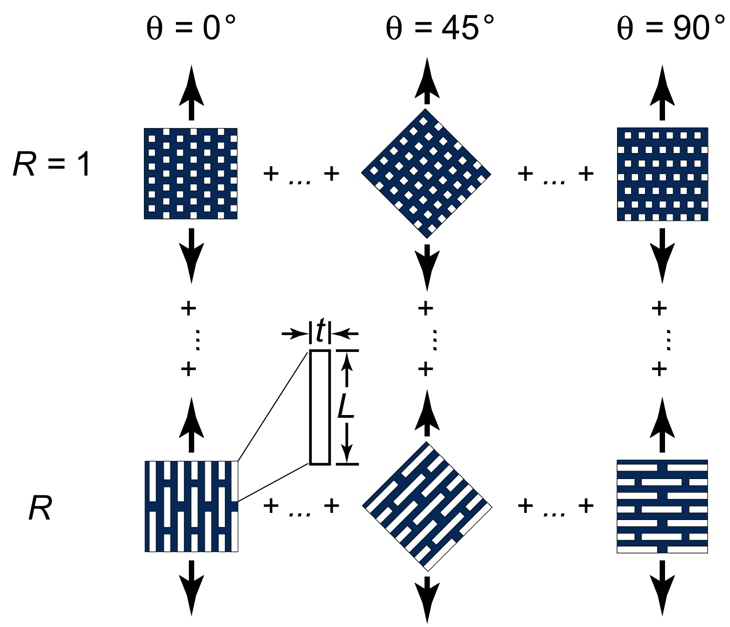
Comparison to data for cortical bone and HA-PE composites.



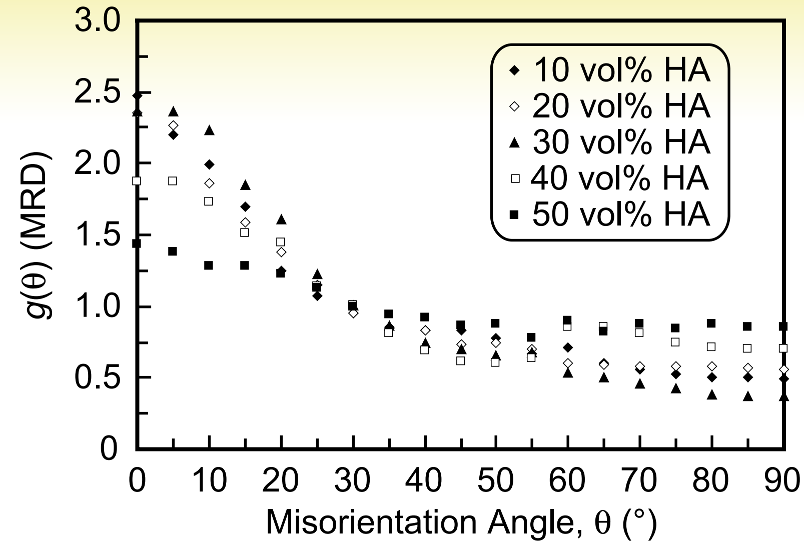
Micromechanical Model for Whisker or Platelet Reinforced Composites

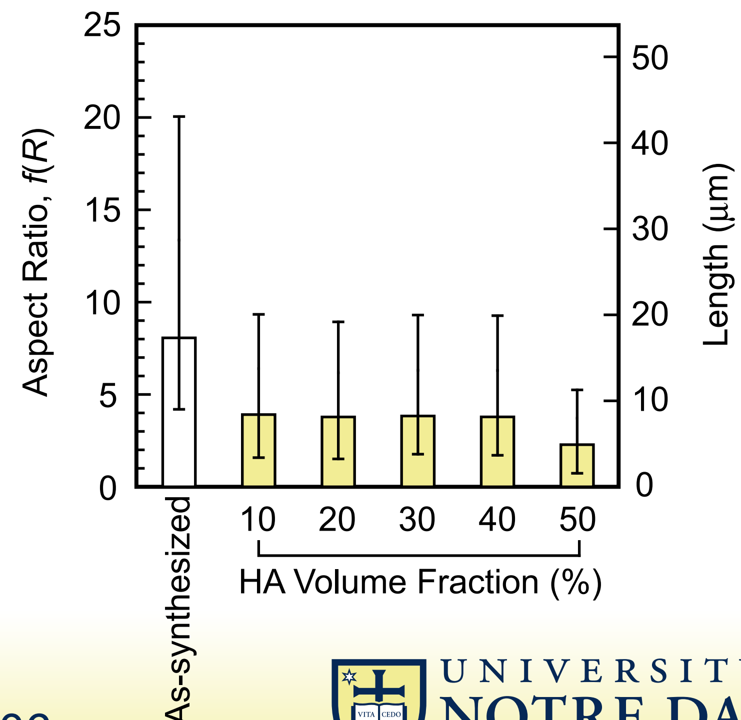


HA Whisker Reinforced HDPE



$$\bar{E}_{ij}(R,\theta) = \frac{\int_\theta \int_R g(\theta)\cdot f(R)\cdot E_{ij}(R,\theta)\cdot dR\cdot d\theta}{\int_\theta \int_R g(\theta)\cdot f(R)\cdot dR\cdot d\theta}$$





Yue and Roeder, *J. Mater. Res.*, 2006.

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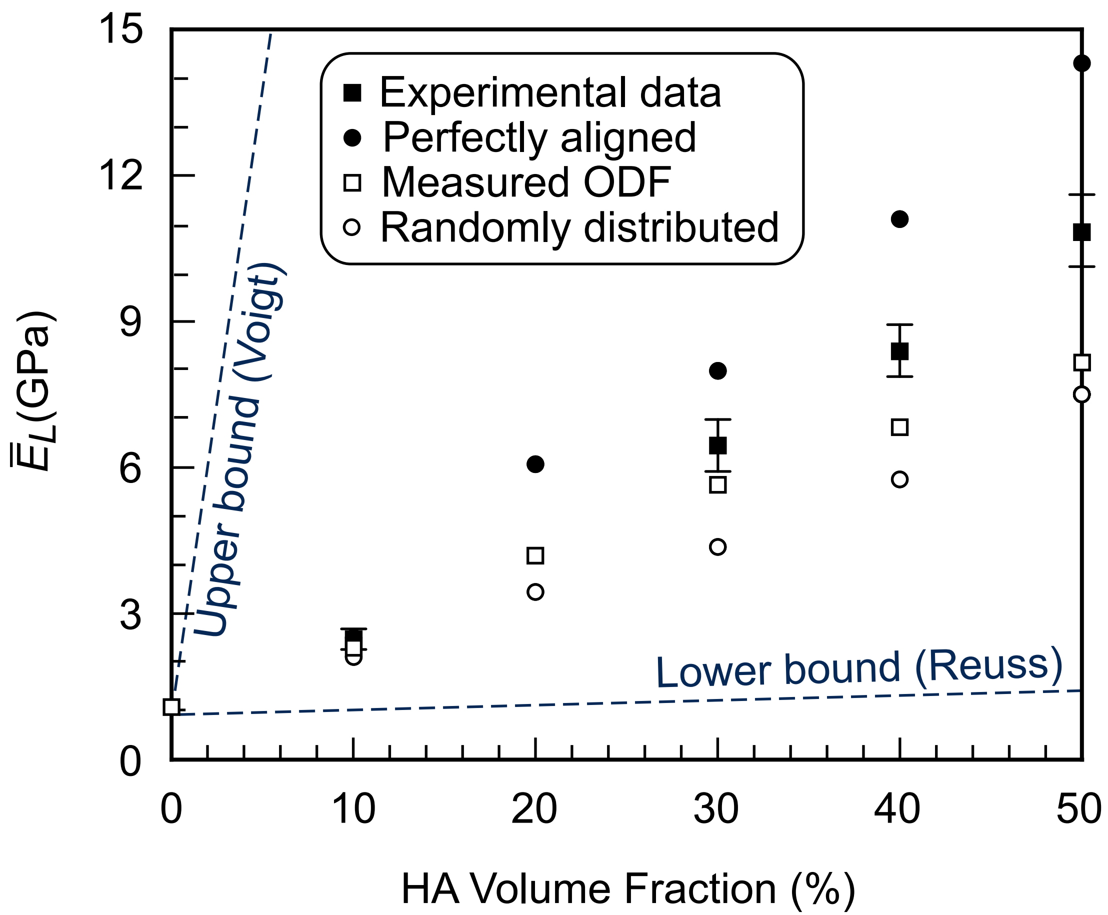
HA Whisker Reinforced HDPE

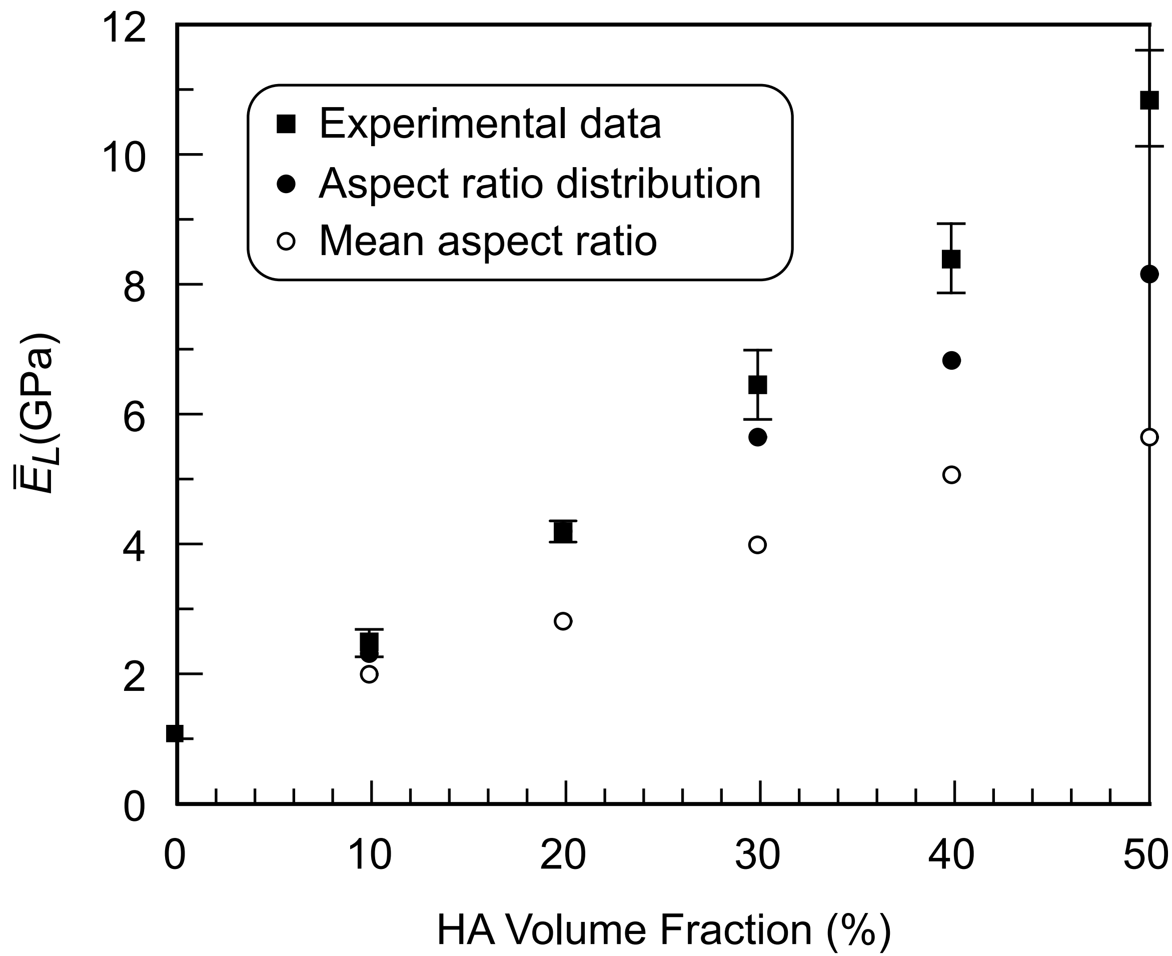
using the aspect ratio distribution



Yue and Roeder, *J. Mater. Res.*, 2006.

HA Whisker Reinforced HDPE

using the measured ODFs



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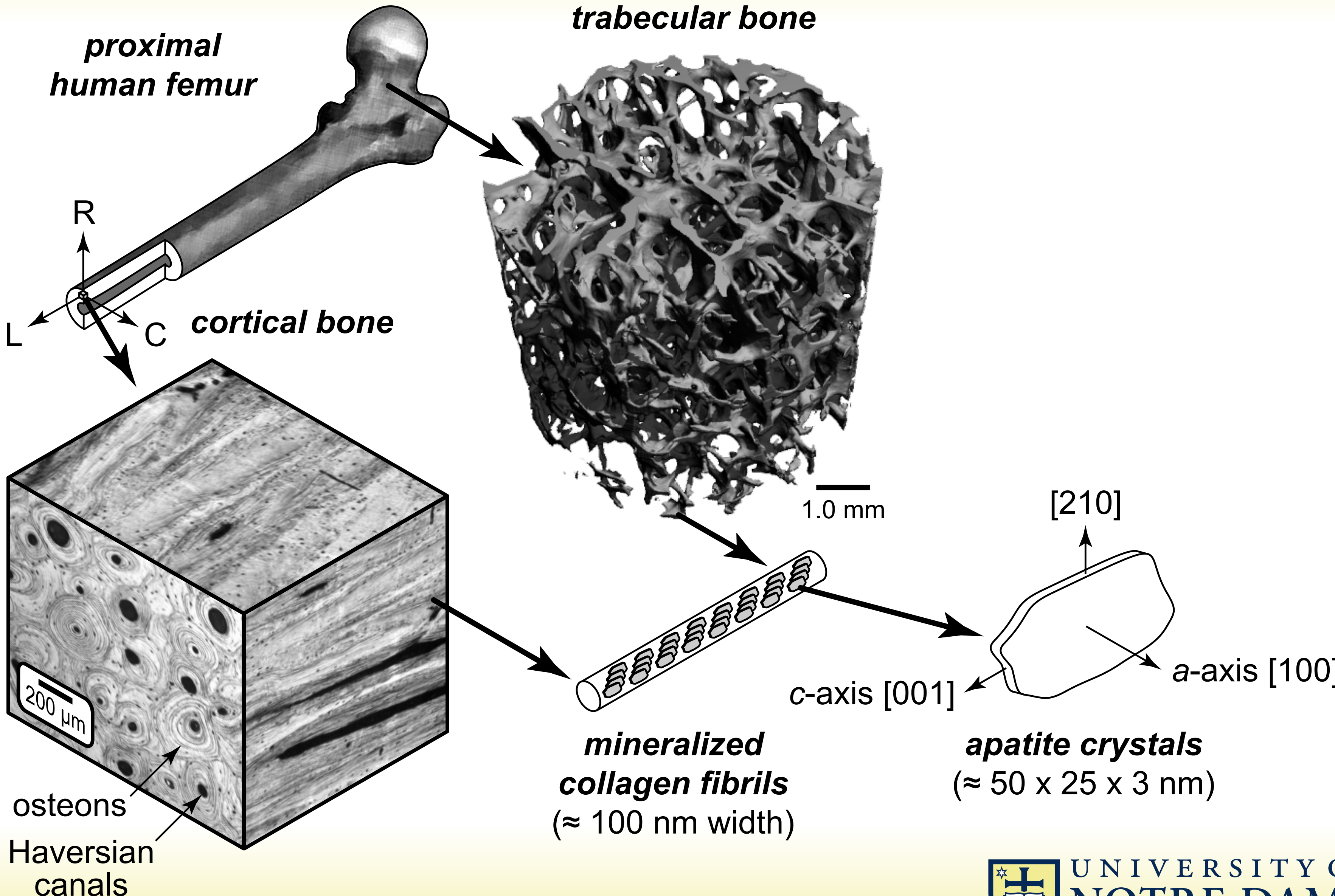
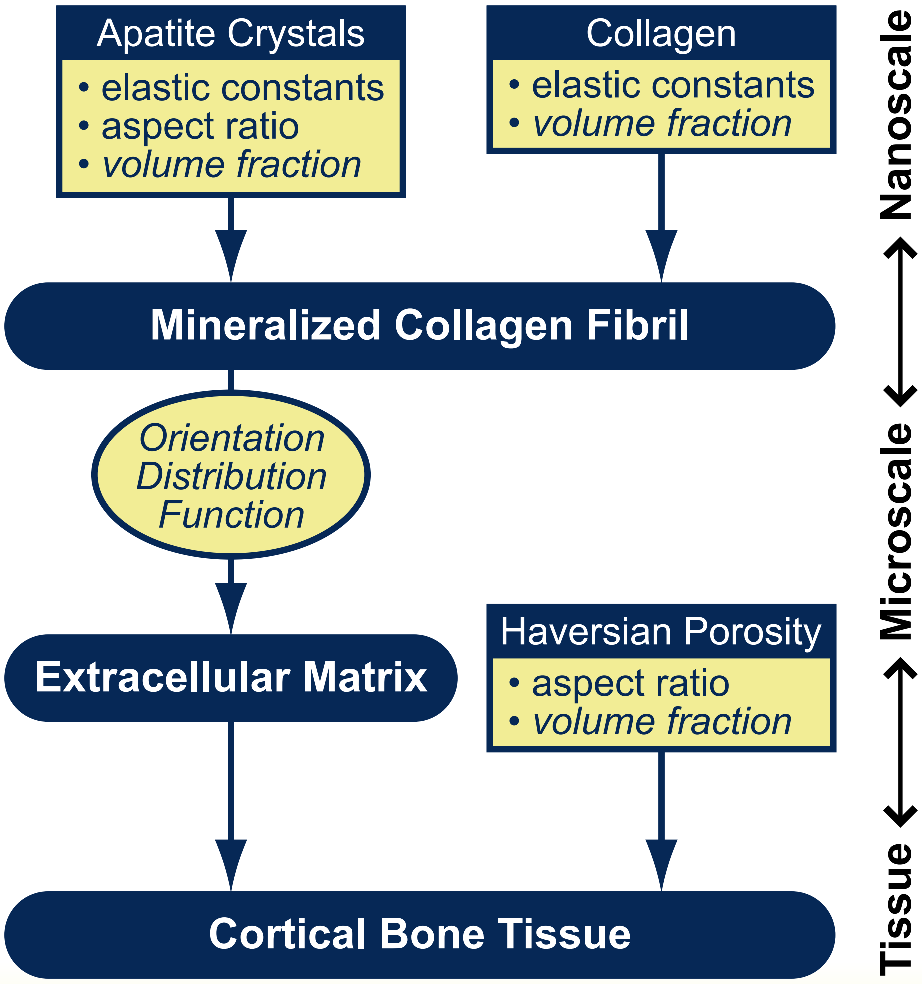
Hierarchical Structure of Bone Tissue



Adapted from R.K. Roeder, *et al.*, *JOM*, 2008.

Specimen-Specific, Multiscale Micromechanical Model of Cortical Bone



Deuerling, *et al.*, *J. Biomechanics*, 2009.

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Specimen-Specific, Multiscale Micromechanical Model of Cortical Bone

Phase	Parameter	Value(s)	Reference
Apatite Crystals	Elastic Constants (transversely isotropic)	C_{11} = 137 GPa C_{33} = 172 GPa C_{12} = 42.5 GPa C_{13} = 54.9 GPa C_{44} = 39.6 GPa	Katz and Ukraincik, 1971
	ODF	*measured*	
	Volume Fraction	*measured*	
	Mean Aspect Ratio	20	Eppel *et al*., 2001
Collagen	Elastic Constants (isotropic)	C_{11} = 3.9 GPa C_{12} = 1.1 GPa	Sasaki and Odajima, 1996
	Volume Fraction	*measured*	
Haversion Porosity	Aspect Ratio	60	Sevostianov and Kachanov, 2000
	Volume Fraction	*measured*	

Deuerling, *et al*., *J. Biomechanics*, 2009.

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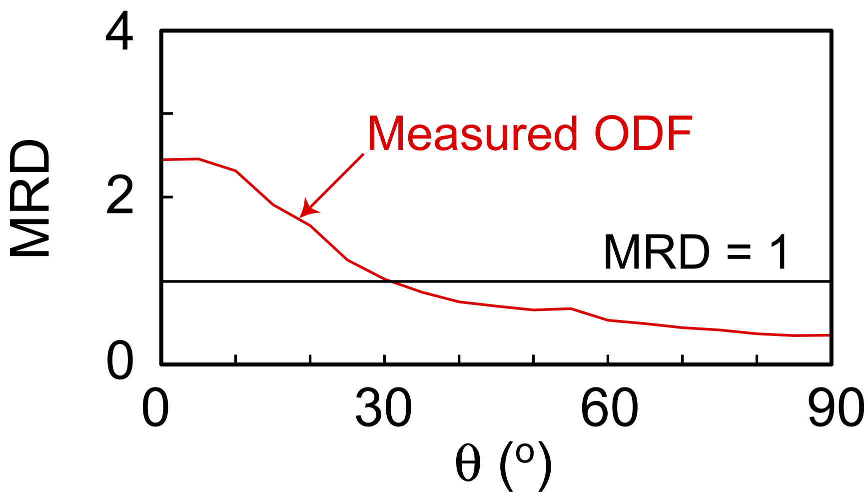

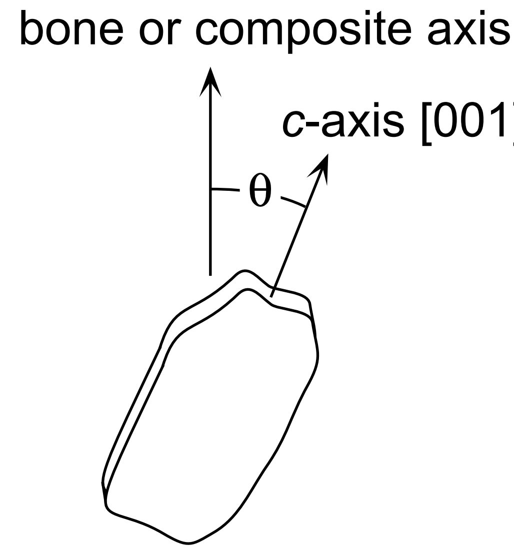

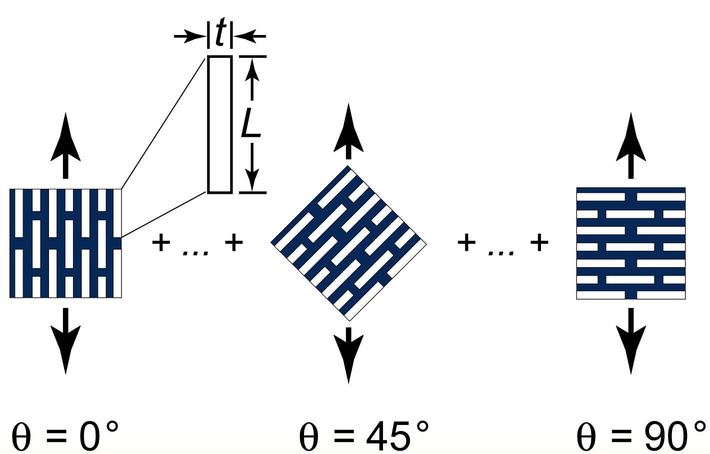

$$\bar{E}_{ij}(\theta) = \frac{\int_{\theta} g(\theta)\cdot E_{ij}(\theta)\cdot d\theta}{\int_{\theta} g(\theta)\cdot d\theta}$$

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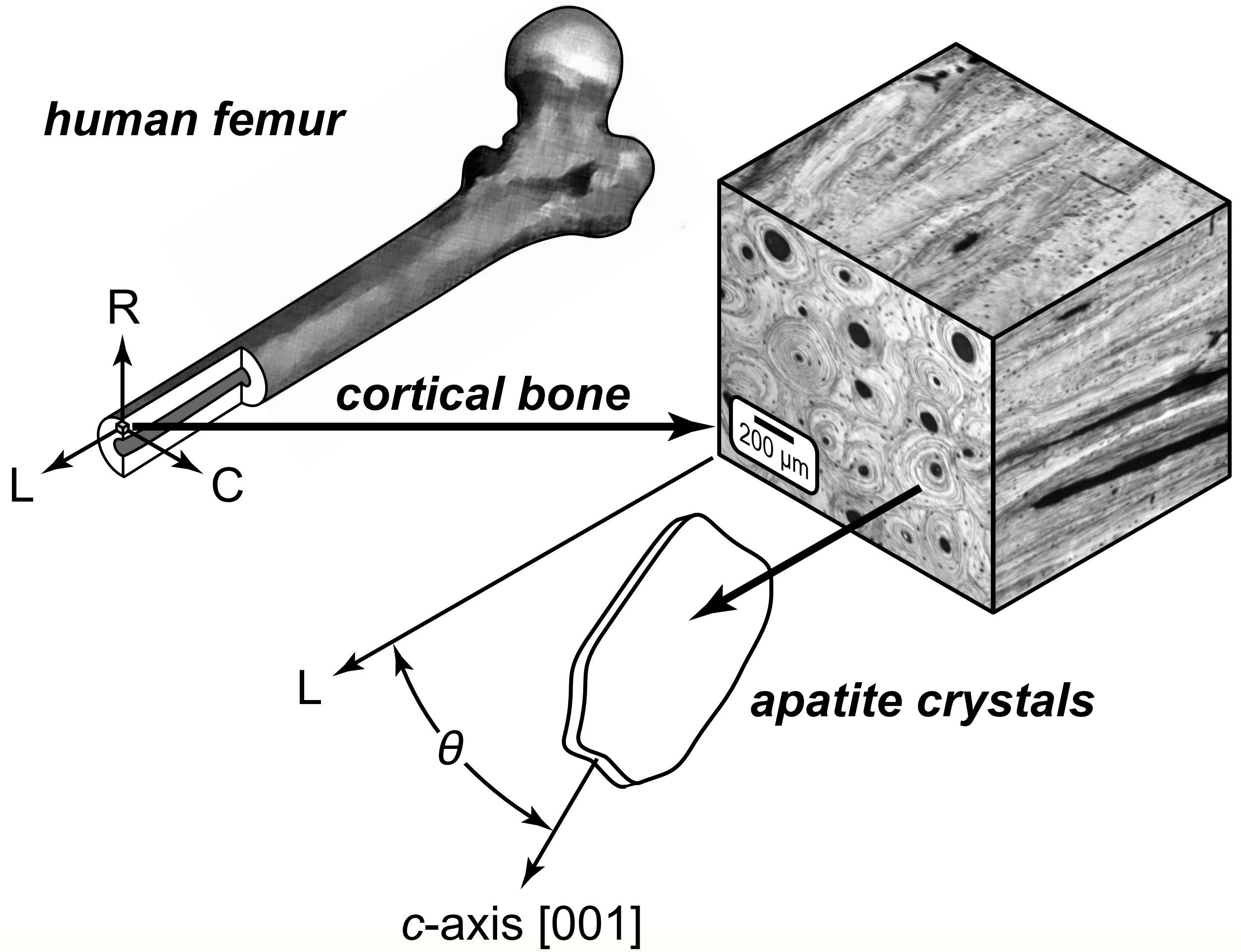

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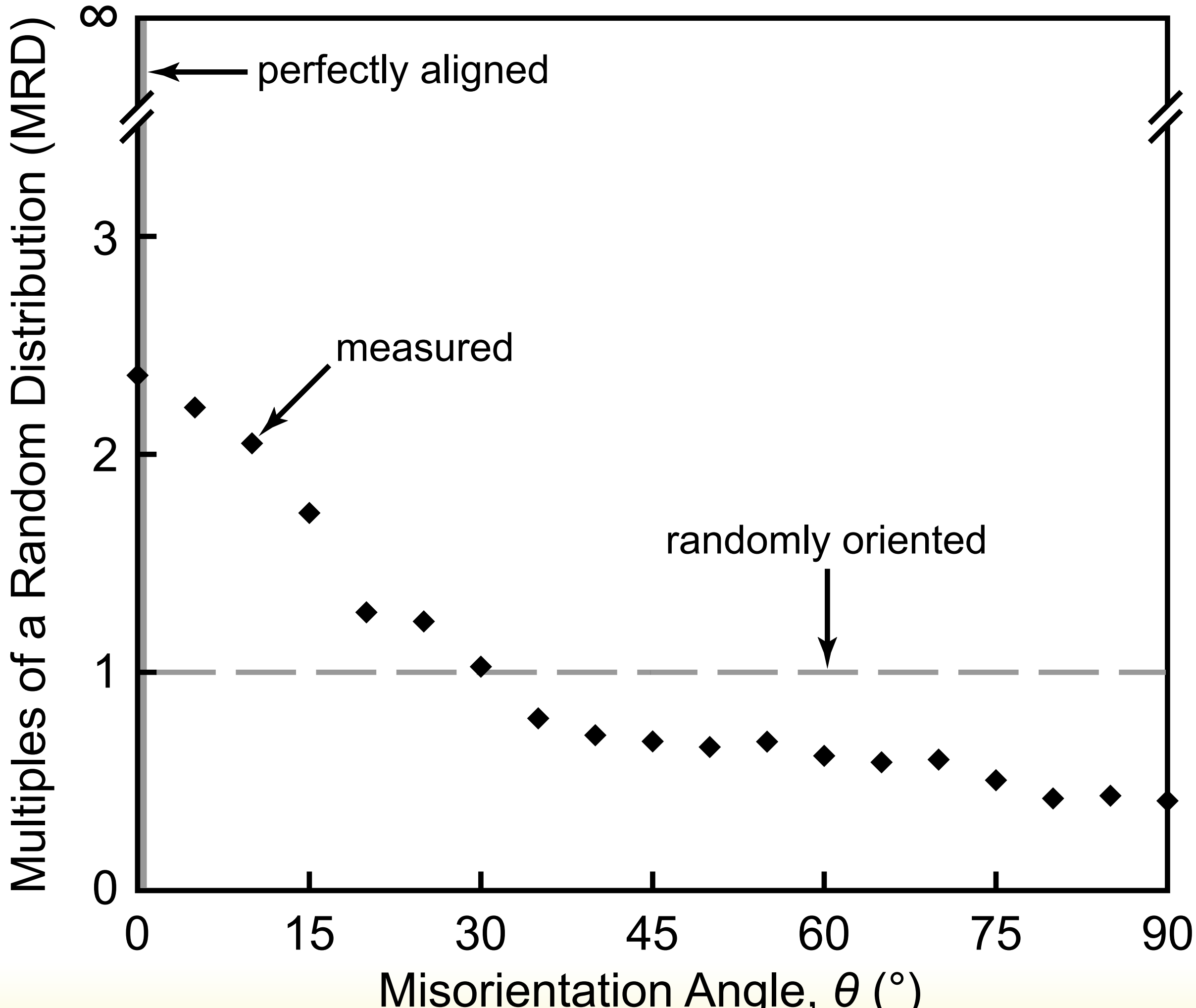

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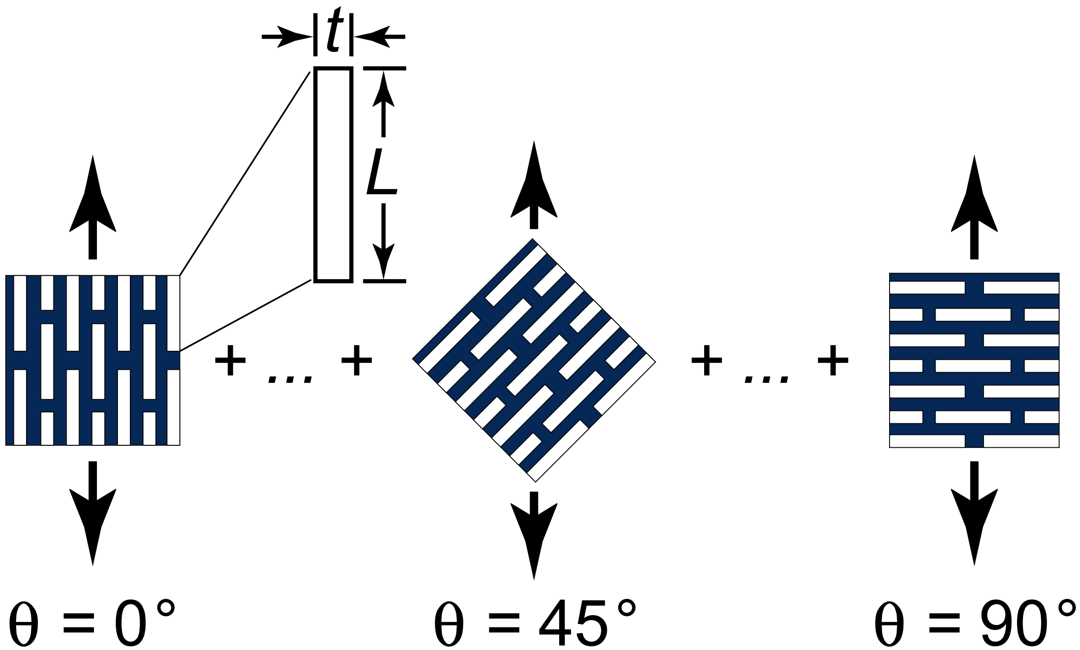

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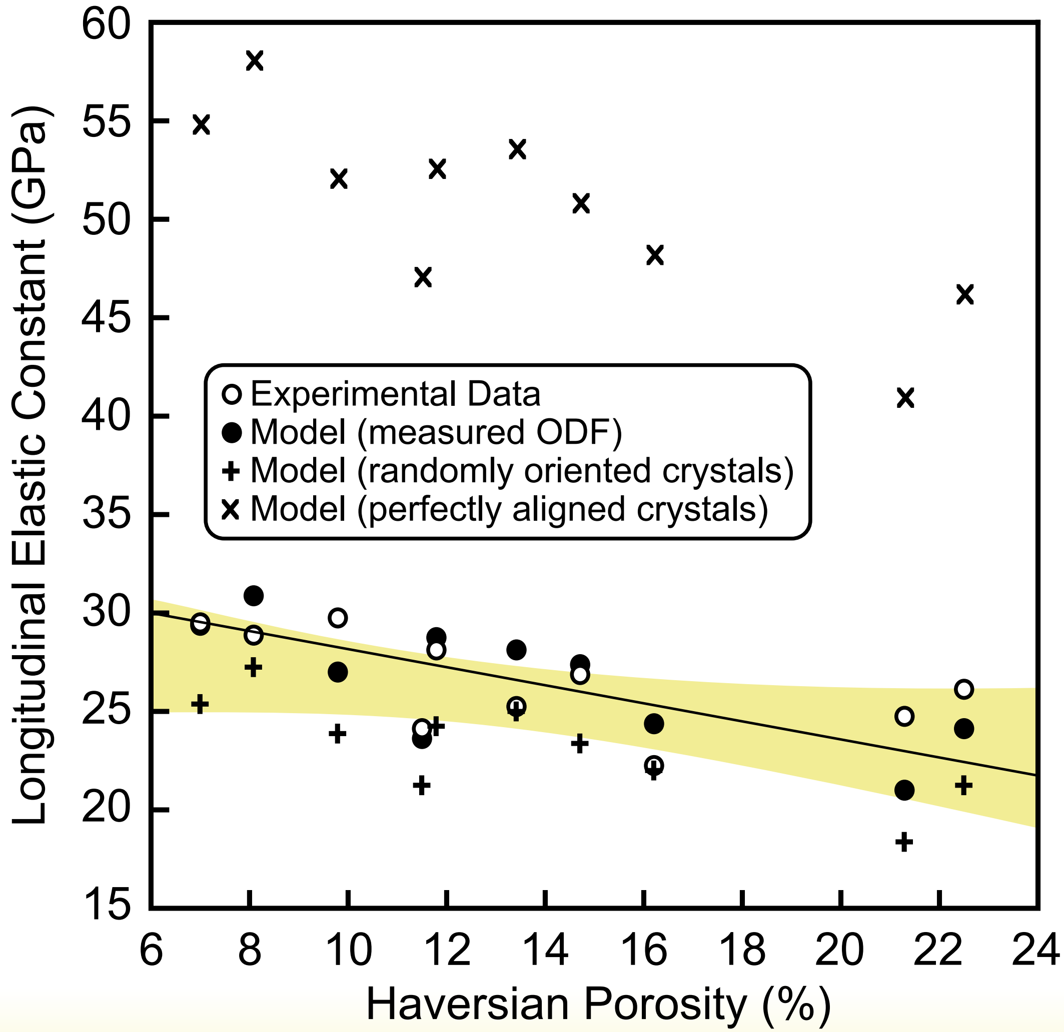

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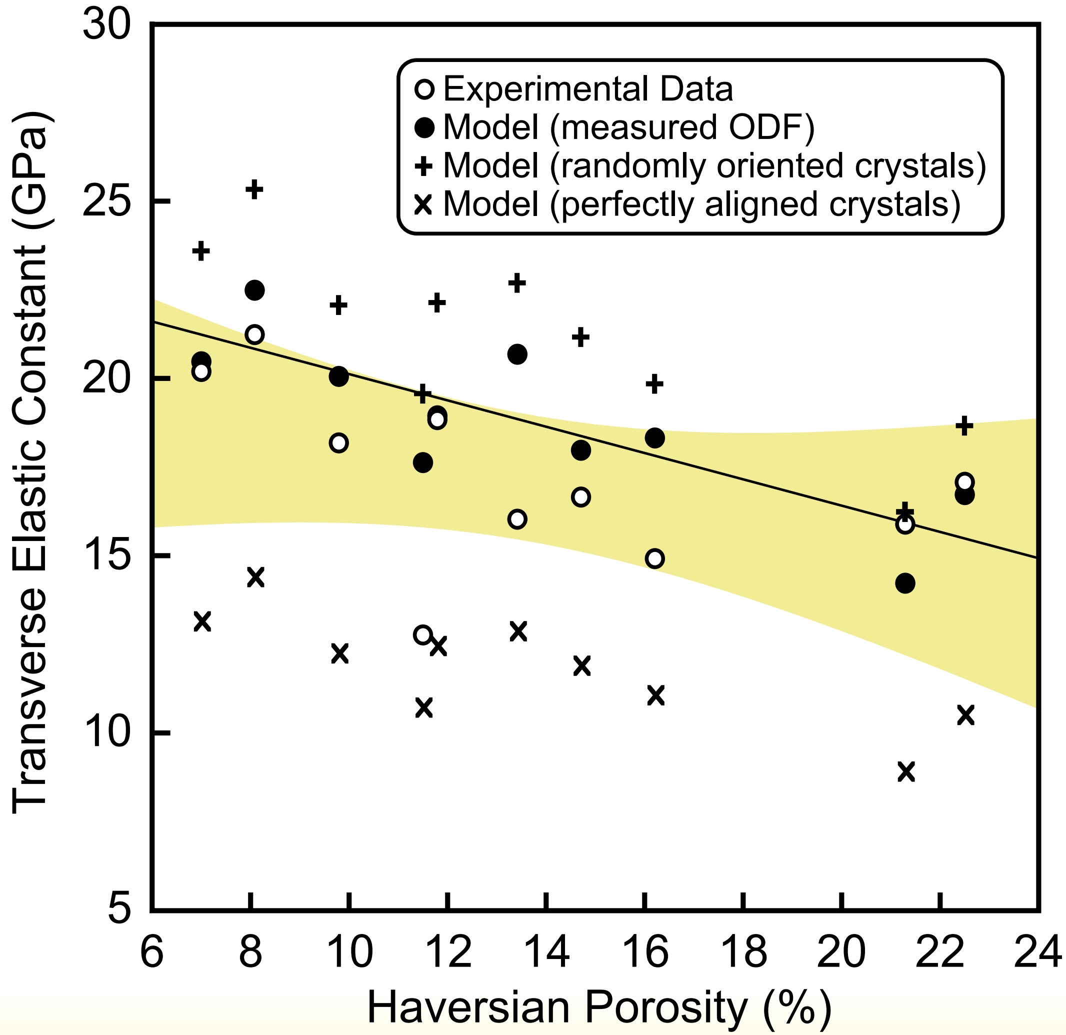


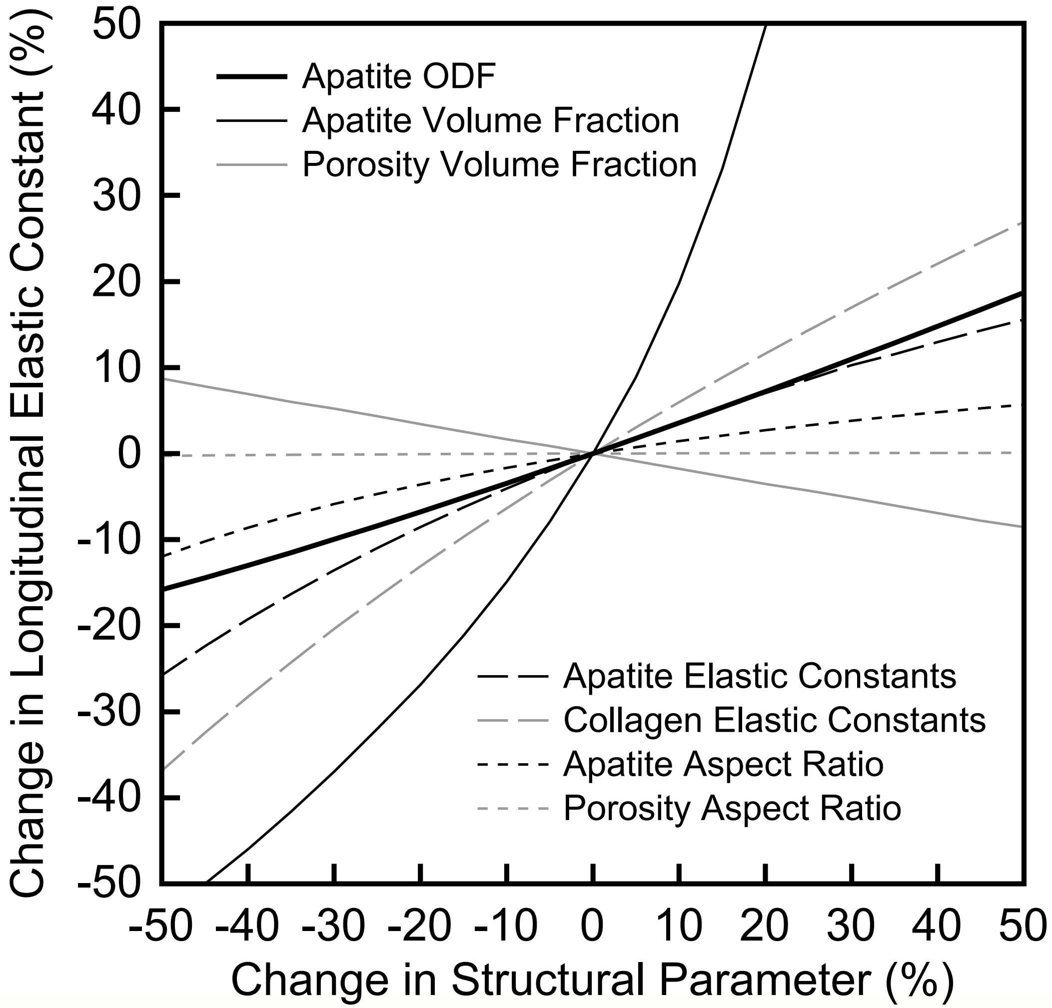
Deuerling, *et al.*, *J. Biomechanics*, 2009.

Specimen-Specific, Multiscale Micromechanical Model of Cortical Bone

	Anisotropy Ratio
Experimental Data	1.56 (0.14)
Model (measured ODF)	1.41 (0.07)
Model (randomly oriented crystals)	1.09 (0.02)
Model (perfectly aligned crystals)	4.27 (0.15)

Deuerling, *et al*., *J. Biomechanics*, 2009.

Specimen-Specific, Multiscale Micromechanical Model of Cortical Bone



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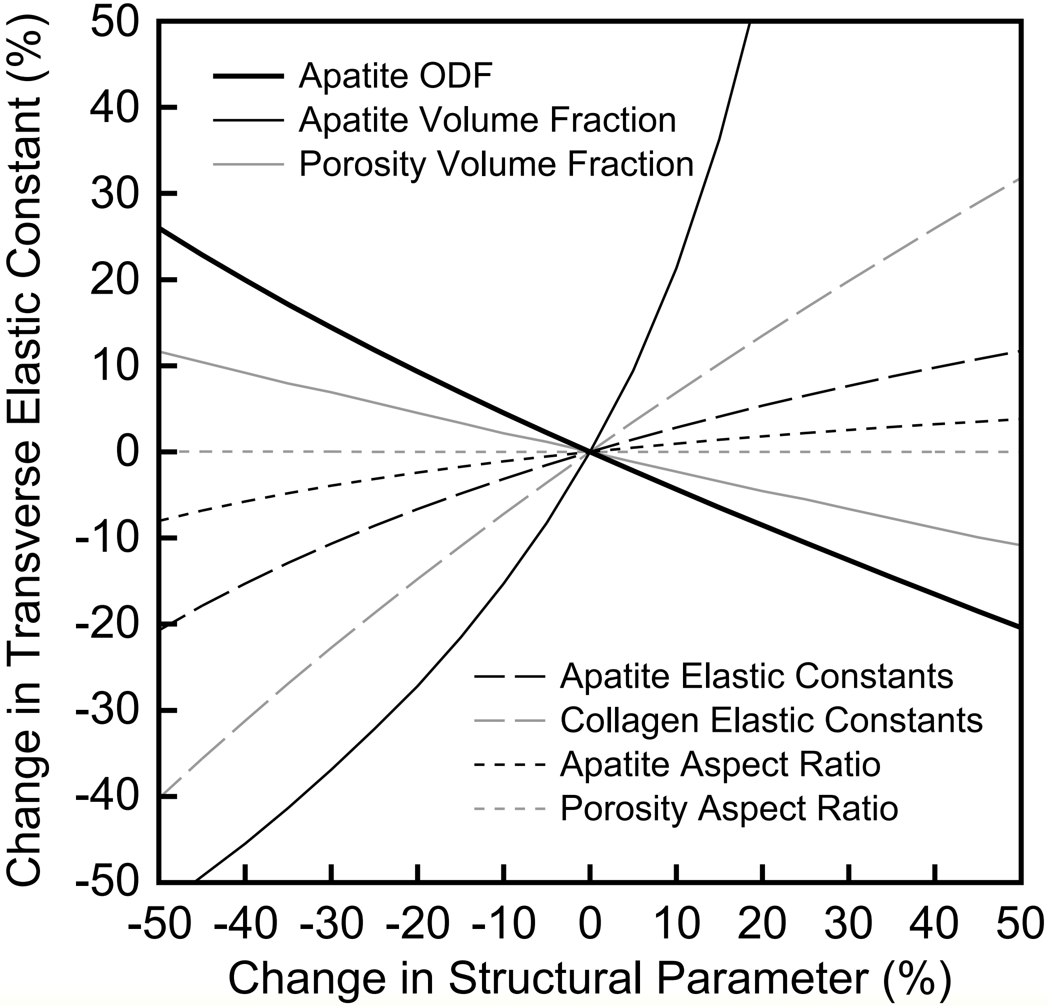

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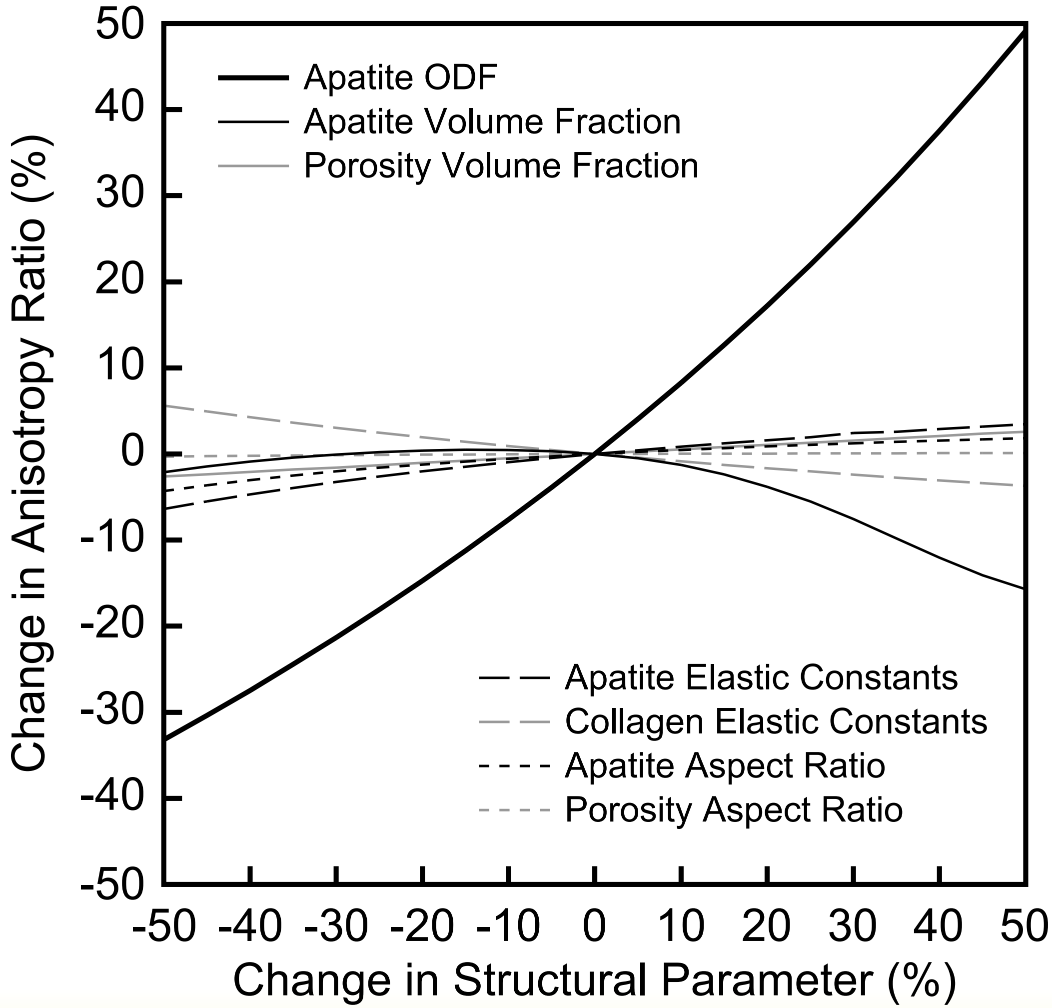
Specimen-Specific, Multiscale Micromechanical Model of Cortical Bone



Deuerling, *et al.*, *J. Biomechanics*, 2009.