Incorporation of Microstructural Effects in Green's Function and Boundary Element Calculations: Single-Phase Cellular Solids

J. R. Berger

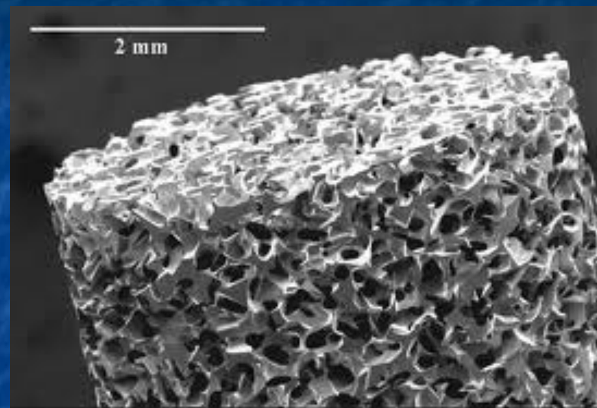
Division of Engineering

Colorado School of Mines

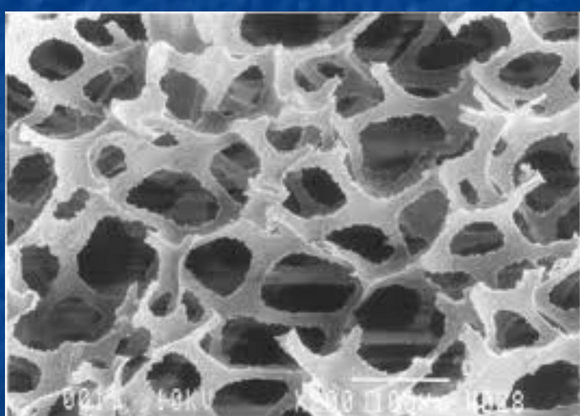
Outline for the talk

1. Examples of porous/cellular solids in engineering
2. Stress analysis: two approaches.
3. Homogenization: microstructural parameters, fabric tensor
4. Modeling of representative volume elements (RVEs)
5. Issues in elastic modeling
6. Issues in strength and fracture

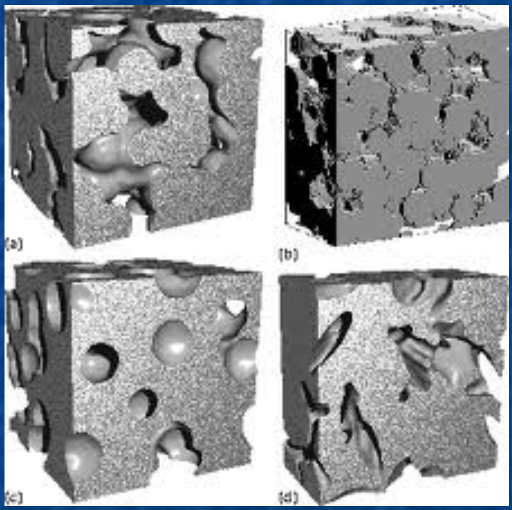
Examples of Porous/Cellular Solids



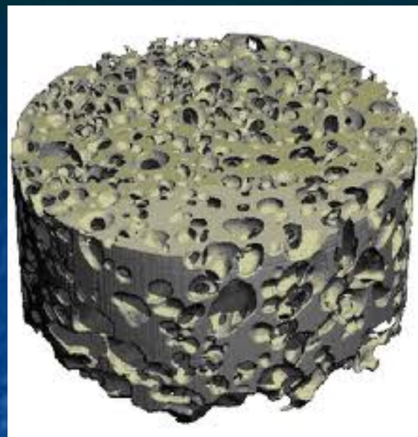
Metallic Foams



Cellular Polymeric Foams

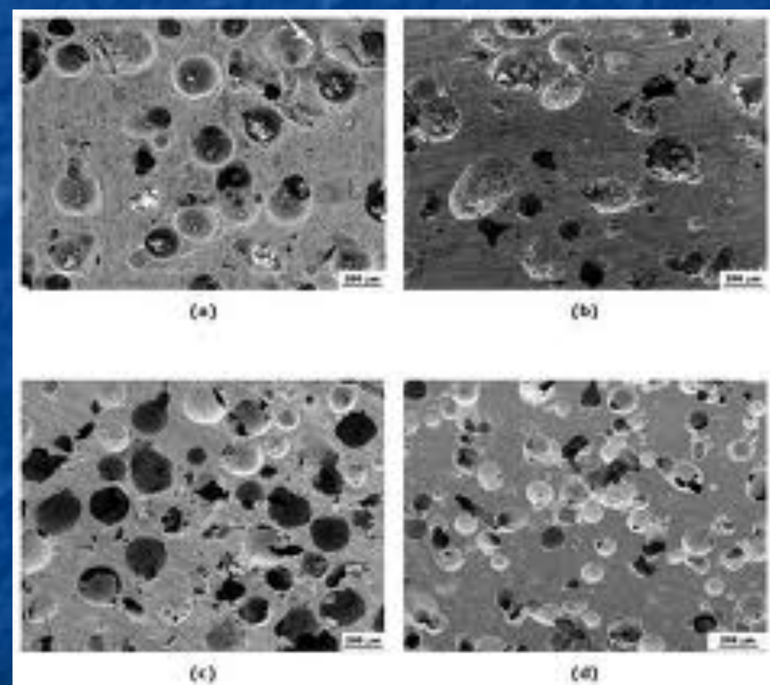


Porous Ceramics



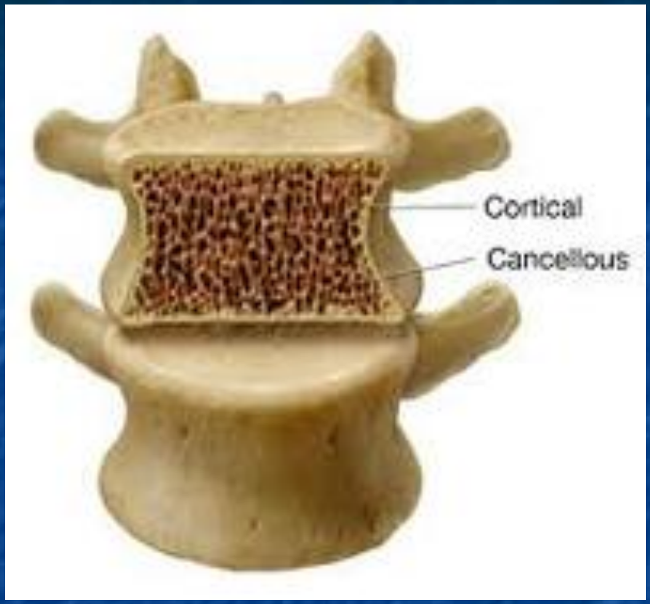
Porous ceramic for biomedical application (dental)

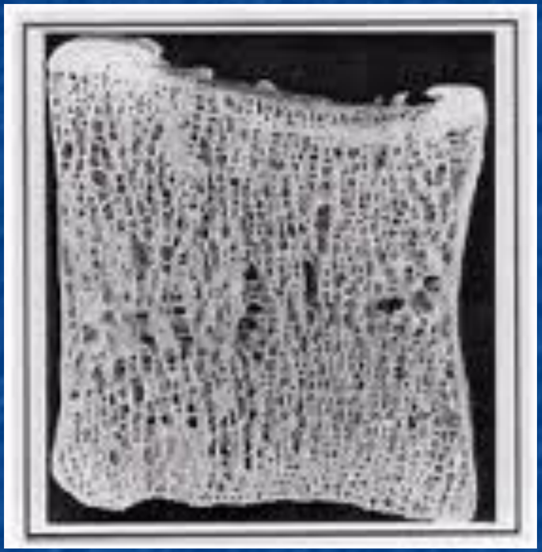
Porosity is controlled by design for desired properties, i.e., tissue growth, metallic diffusion

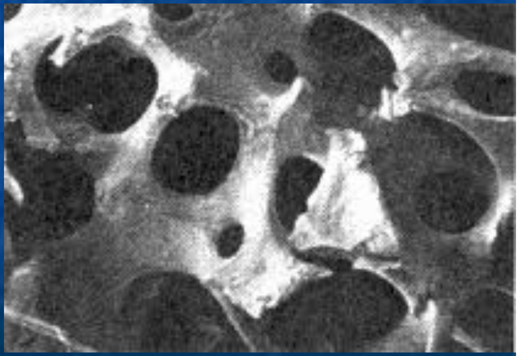


Zirconia

Cancellous Bone
(of bone: having a porous structure)







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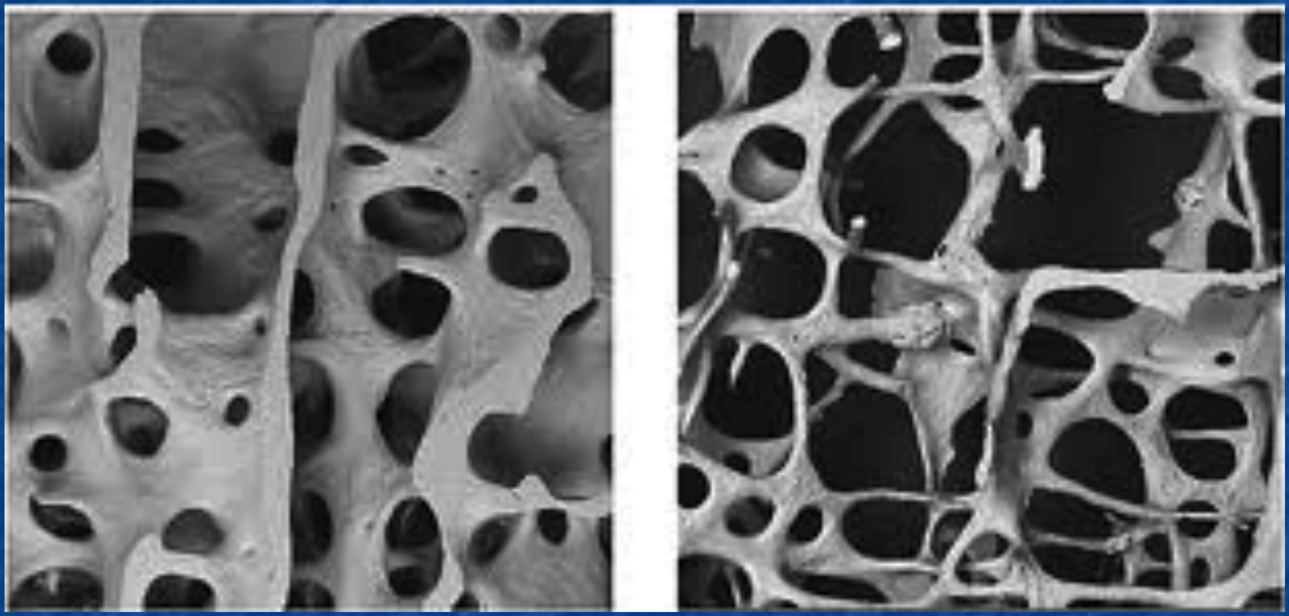
Degradation of bone due to osteoporosis:



Note: the trabecular “structure” stays the same but the solid density clearly changes.

Some Terminology

Solid volume fraction: $V_s = \dfrac{V_m}{V_m + V_p}$

V_m : volume of the solid matrix

V_p : volume of the pores

Porosity, $\phi = 1 - V_s$

For $V_s > 0.3$, transition from a cellular solid to a solid containing isolated pores. The *structural density* ρ_s is also frequently used.

Stress Analysis of Porous Solids

• Key point of understanding: porosity (or solid density) is a necessary but *insufficient* parameter for describing the elastic properties.

• In foams and sintered materials, the elastic properties are independent of the absolute dimensions of the microstructure.

• We also need a measure of the shape, orientation, and distribution of the pores. This is often (but not always) a *tensor* property. Cell shape matters much more than cell size.

• Most (but not all) cellular solids are *structurally anisotropic*: the anisotropy occurs due to the shape and distribution of the cells. The “matrix” material is itself isotropic.

How can Boundary Element/Green's Function analysis be helpful???

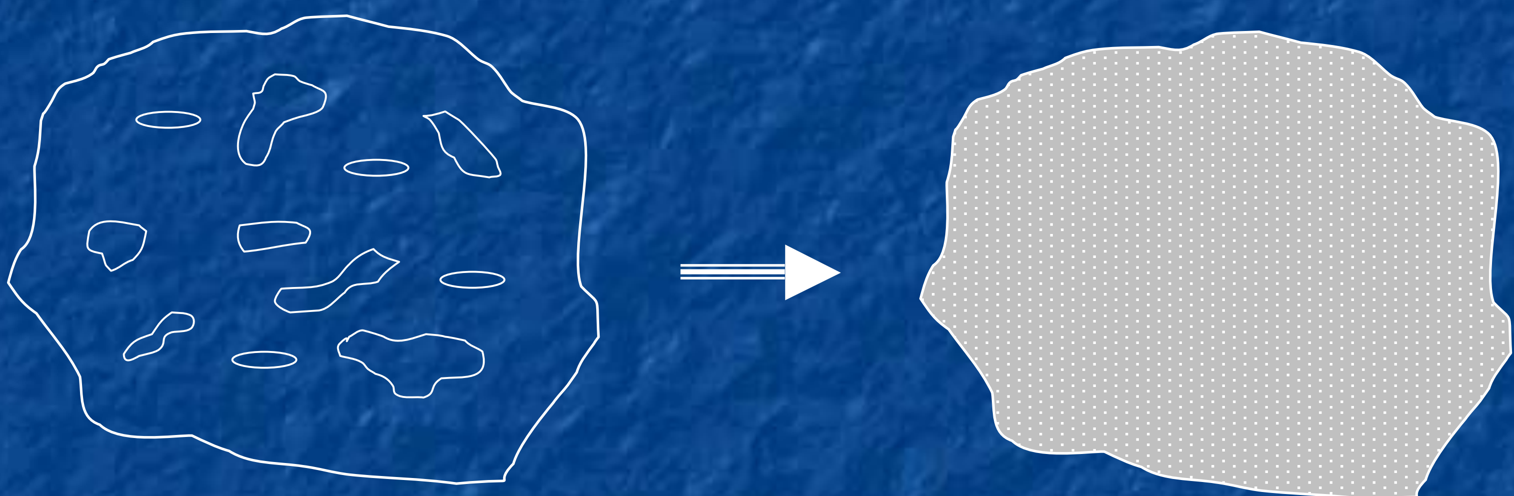
1. Stress analysis of a homogenized, anisotropic material.

2. Mechanical property analysis on Representative Volume Elements (RVEs).

3. Efficient three-dimensional strength analysis on RVEs.

Homogenization Approach

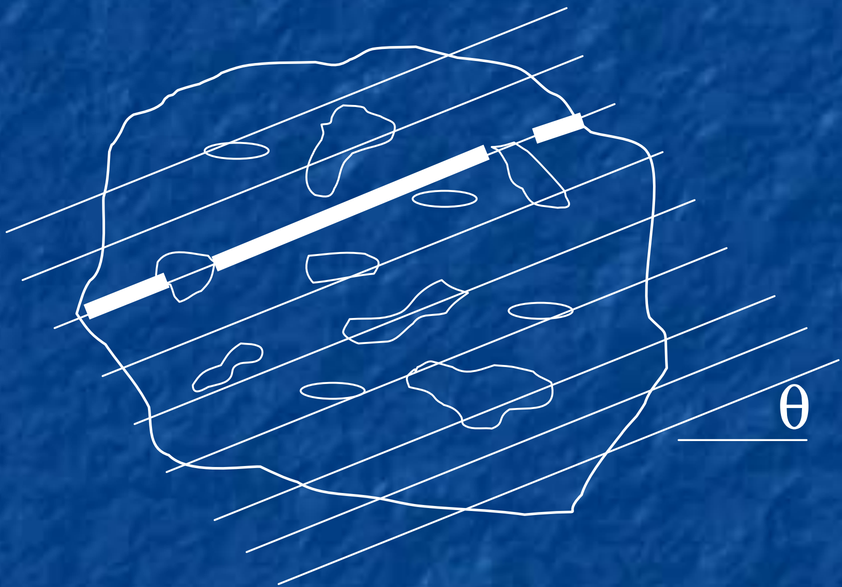
For any homogenization approach, we assume that the length scale of interest for stress analysis is longer than any microstructurally important length scale (pore diameter, grain size, inclusion spacing, etc.).

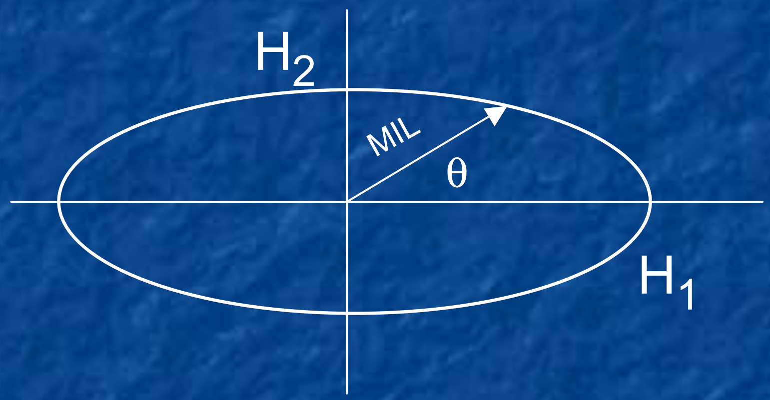


$\sigma_{ij} = C_{ijkl}\,(\boldsymbol{x})\,\varepsilon_{kl} \quad \Longrightarrow \quad \sigma_{ij} = C^*_{ijkl}\,\varepsilon_{kl}$

Homogenization: Fabric Tensor Approach

Whitehouse (1974) and Harrigan and Mann (1984) noted that the *Mean Intercept Length* (MIL) in a voided/cellular solid plots as an ellipsoid





(2-dimensional example)

Note: a similar approach has been used for contact normal distributions in granular media (Oda, or Satake, for example) and for crack density/orientation in rock (Harrigan and Mann)

Ellipsoid:

$$Ax_1^2 + Bx_2^2 + Cx_3^2 + 2Dx_1x_2 + 2Ex_1x_3 + 2Fx_2x_3 = 0$$

Or

$$H = \begin{bmatrix} A & D & E \\ D & B & F \\ E & F & C \end{bmatrix} \xrightarrow{Diag} \begin{bmatrix} H_1 & 0 & 0 \\ 0 & H_2 & 0 \\ 0 & 0 & H_3 \end{bmatrix}$$

H is the ***Fabric Tensor***, a measure of structural anisotropy

The orientation distribution function (ODF) describing the structural anisotropy is then (Zysset, 1998)

$$L(\mathbf{n}) = \frac{1}{\sqrt{\mathbf{n}^T \mathbf{H} \mathbf{n}}}$$

Where ***n*** is a unit direction in space.

This ODF can be expanded in the tensor form of a spherically-harmonic Fourier series (Kanatani, 1984) as

$$L(\mathbf{n}) = f \cdot g + \mathbf{G} : \mathbf{F}(\mathbf{n}) + \mathbf{G}' :: \mathbf{F}'(\mathbf{n}) + \cdots$$

Where *f (=1)*, **F**, **F’** are (known) even-ranked tensorial basis coefficients and *g*, **G**, and **G’** are even-ranked generalized fabric tensors.

If we restrict ourselves to *isotropic*, *transversely isotropic*, and *orthotropic* structural anisotropies, the series can be truncated as

$$L(\mathbf{n}) = f \cdot g + \mathbf{G} : \mathbf{F}(\mathbf{n})$$

Other material symmetries require retaining higher-order terms in the expansion. Also, **G** and **H** are related, **H** = g**I**+**G**.

The fabric tensor can be related to the elastic constants.

Cowin (mid to late 1980's): stress is an isotropic function of strain and fabric. Leads to expressions for the orthotropic stiffnesses of the form

$$E_i = m_1 + m_2 II_H + m_3 H_i + m_4 H_i^2, \quad i = 1,2,3$$

$$G_{ij} = m_5 + m_6 II_H + m_7 \left(H_i + H_j \right) + m_8 \left(H_i^2 + H_j^2 \right), \quad i, j = 1,2,3, \ i \neq j$$

Issues with the Cowin formulation:

- Numerous parameters to determine
- Invertibility of compliance to stiffness tensors not guaranteed
- Positive definiteness of strain energy not guaranteed.

Zysett approach (late 1990's):

• Similar approach, but enforced positive-definiteness of the stiffness tensor.

• Homogenization assumption: the anisotropy of the constitutive law is independent of the physical units of the microstructural property,

$$S(\lambda g, \lambda G) = \lambda^k S(g, G) \quad \forall \lambda > 0$$

• Through a free-energy potential formulation, the fabric-stiffness relations are

$$E_i = E_0 \rho_s^k H_i^{2m}$$

$$\nu_{ij} = \nu_0 \left(\frac{H_j}{H_i} \right)^{2m}$$

$$G_{ij} = G_0 \rho_s^k H_i^m H_j^m$$

With either approach, the unknown constants must be determined either from physical or numerical experiments.

For example, from the Zysett 2003 review article, for trabecular bone specimens,

$$E_i = 17607\,\rho_s^{3.2} H_i^{3.2} \quad \text{MPa}$$

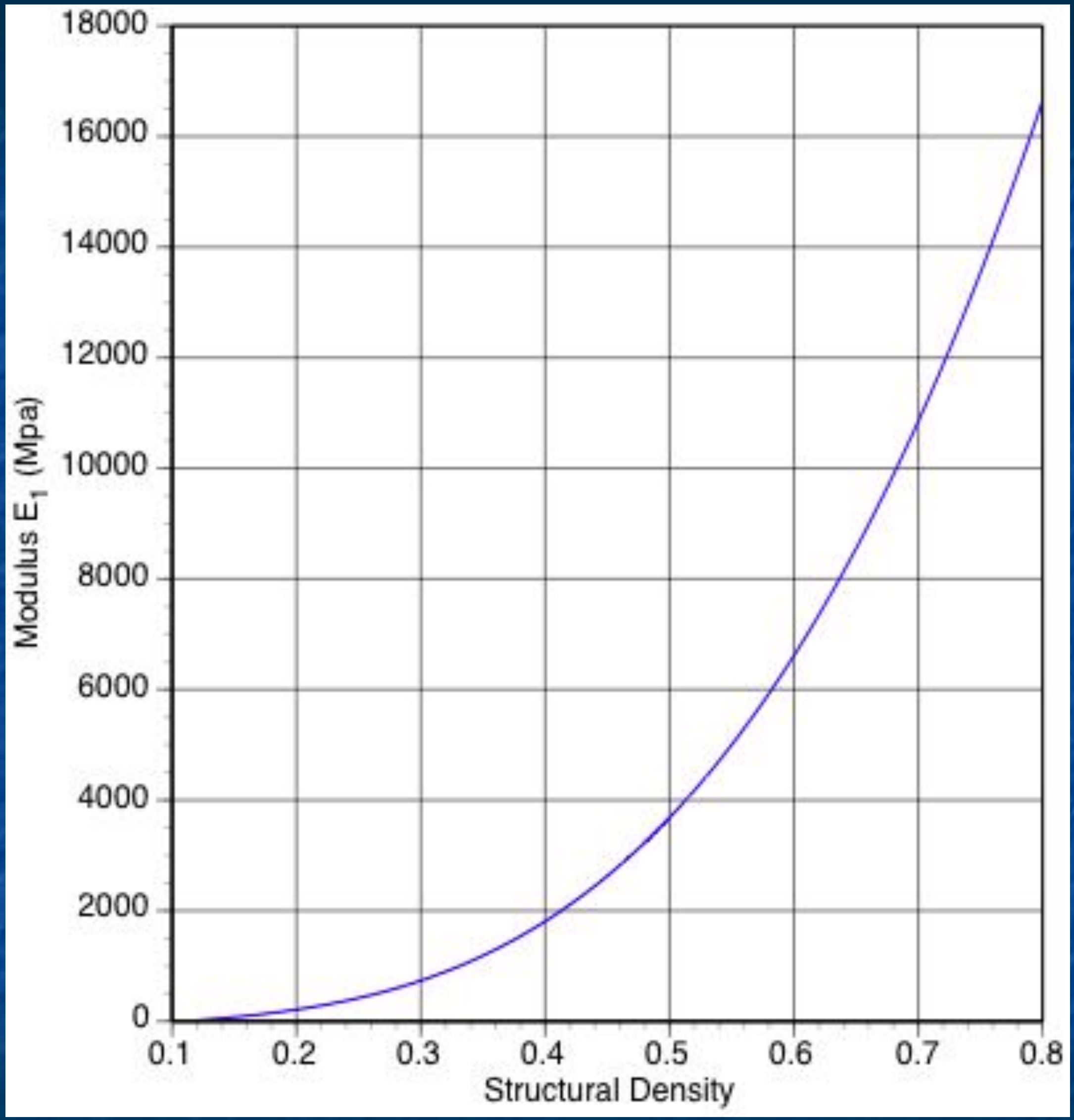
$$\frac{E_i}{\nu_{ij}} = 45800\,\rho_s^{3.2} H_i^{2.4} H_j^{2.4} \quad \text{MPa}$$

$$G_{ij} = 7799\,\rho_s^{3.3} H_i^{1.6} H_j^{1.6} \quad \text{MPa}$$

Note:

• The principal axes of the fabric tensor and the principal material axes are coincident (Cowin, 1985; Odgaard, 1997)

• Poisson ratios are independent of structural density (Gibson and Ashby, 1999)



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Boundary Element Analysis with Anisotropic Green's Functions

In plane-strain, the displacement Green's function is of the form

$$U_{ij}(P,Q) = \sum_n \gamma_{ij}(p_n) \log(z_n - z'_n)$$

where

$$z_n = x_1 + p_n x_2, \quad z'_n = x'_1 + p_n x'_2$$

$$P = (x'_1, x'_2), \quad Q = (x_1, x_2)$$

The Stroh-roots p_n for an orthotropic solid are determined in plane-strain from

$$p^4 + p^2\left(\frac{C_{11}}{C_{66}} + \frac{C_{66}}{C_{22}} - \frac{(C_{12}+C_{66})^2}{C_{22}C_{66}}\right) + \frac{C_{11}}{C_{22}} = 0$$

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In terms of fabric, the roots are given by

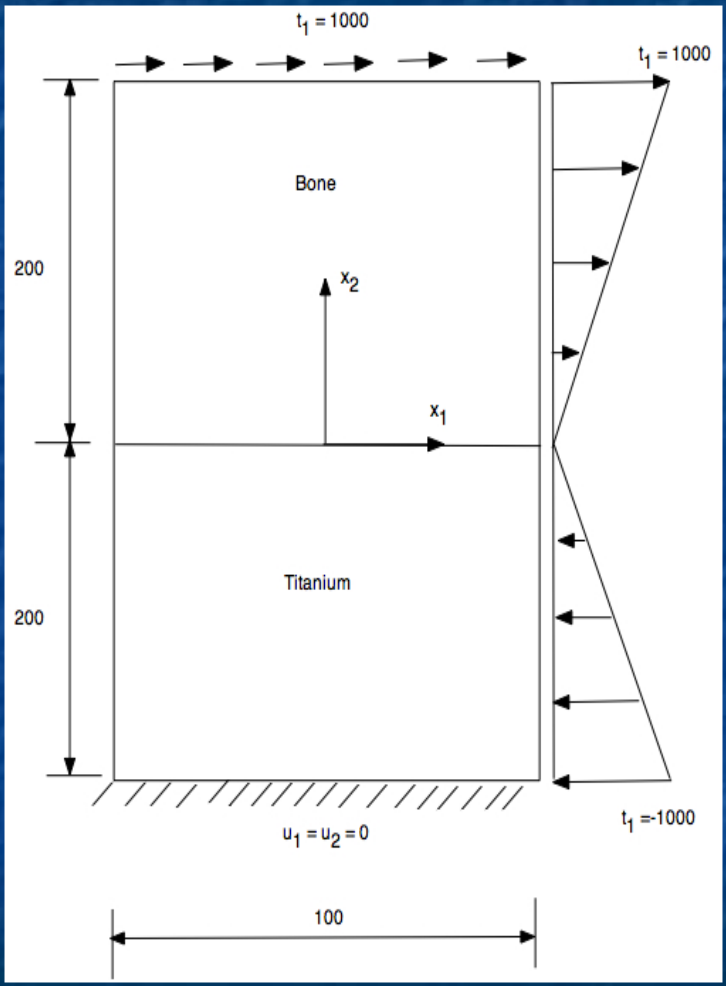
$$p^4 + p^2\left(\frac{\Lambda_0 E_0}{G_0}\left(\frac{H_1}{H_2}\right)^{m} - \frac{2\Gamma_0}{\Lambda_0}\left(\frac{H_1}{H_2}\right)^{3m} - \frac{\Gamma_0^2 E_0}{\Lambda_0 G_0}\left(\frac{H_1}{H_2}\right)^{5m}\right) + \left(\frac{H_1}{H_2}\right)^{m} = 0$$

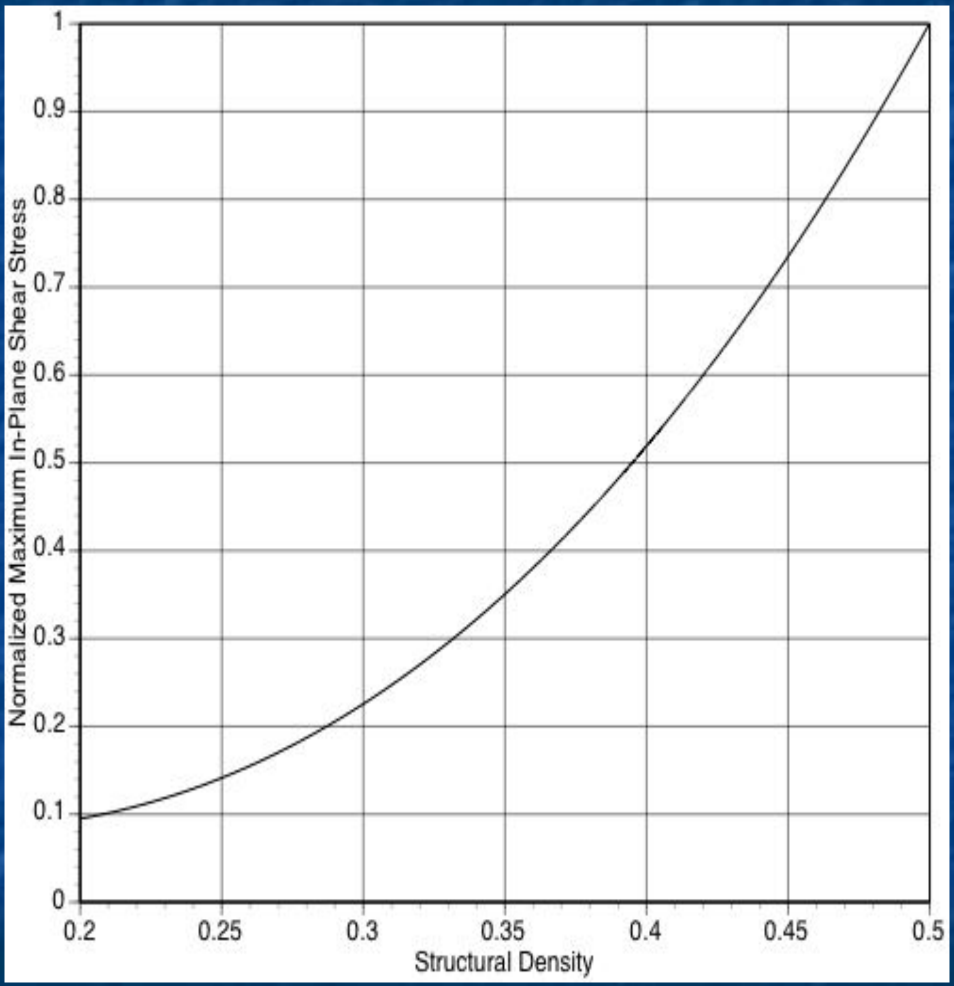
where

$$\Lambda_0 = \frac{1-\nu_0}{(1+\nu_0)(1-2\nu_0)}, \quad \Gamma_0 = \frac{\nu_0}{(1+\nu_0)(1-2\nu_0)}$$

Note that the Stroh roots are *independent* of the solid density -- they are a measure of the structural anisotropy.

Example calculation: principal stress variation with bone density in a bone/titanium specimen (anisotropic, bimaterial Green's function)





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Another approach: the *Micromechanical Approach* (see, for example, the review article by Kachanov, 2005). Relies on forming an elastic potential for stress as

$$f = f_0 + \Delta f$$

Where f_0 is the potential with no inhomogeneities and Δf is the potential due to the inhomogeneities. Furthermore, Δf is formed as

$$\Delta f = \sum_{j=1}^{J} \Delta f^{j}$$

Where Δf^{j} is due to an individual inhomogeneity.

A long history in this area (thanks to Will Parnell, Dept. of Mathematics, Univ. Manchester):

• 1960's: many results for bounds on elastic constants based on arrays of spherical particles. Hill, Hashin, Rosen, Tsai and Halpin.

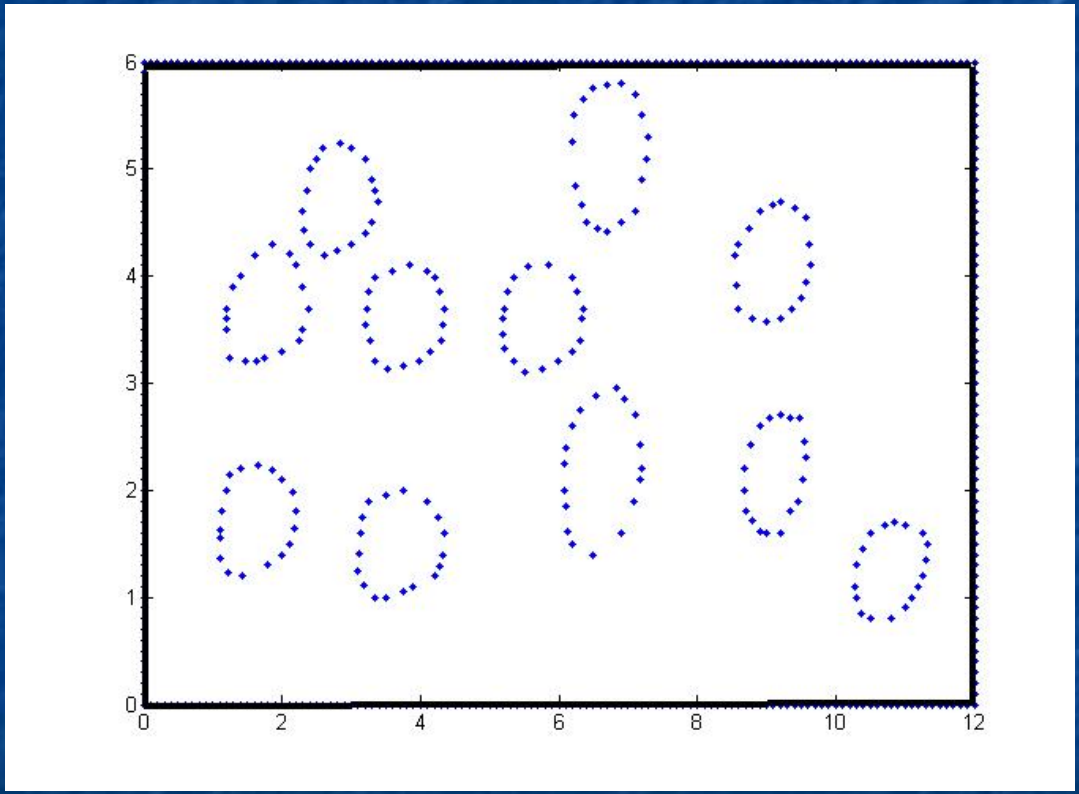
• 1970's: Classical asymptotic homogenization developed. Sanchez-Palencia, Bensoussan, Bakhvalov.

• 1980's: Development of improved bounds using microstructural information.

These techniques are best suited for $V_v > 0.5$

Example BEM calculation: effective orthotropic properties.

Two dimensional computational model of a porous ceramic (ρ_s = 0.52):



Symmetric Galerkin code from L. Gray and A-V Phan used for this analysis.

The model is subjected to simple mechanical tests (tension, shear) to determine the elastic constants.

Bulk material (isotropic): E = 230 MPa, ν = 0.240, G = 92.7 MPa

For the voided material, E_1 = 35.3 MPa, E_2 = 57.8 MPa, ν_{12} = 0.360, ν_{21} = 0.226, and G_{12} = 33.9 MPa.

These results were obtained under displacement boundary conditions, these provide lower bounds on the elastic constants (Hashin, 1965). Traction BC's provide upper bounds.

Next step: determine the fabric tensor, then investigate usefulness of predictions with anisotropic BEM code.

Issues in Elastic Modeling

Relation between fabric tensor and microstructural parameter approach.

Improved bound estimates, static vs dynamic “tests” for elastic constants.

3D RVE modeling for orthotropic properties - speed.

Rapid determination of the fabric tensor from image analysis.

Issues in Strength and Fracture

Main objective is strength prediction with structural density (fracture risk assessment).

Fabric dependence on strength unclear. Cowin (1986) attempted a relation between fabric and Tsai-Wu failure theory.

Damage accumulation/evolution.

Usefulness of homogenized fracture toughness.

Use of combined BEM/DEM models.

Acknowledgments

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