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RANDOM POLYCRYSTALS OF GRAINS WITH CRACKS: MODEL OF ELASTIC BEHAVIOR FOR FRACTURED SYSTEMS

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OUTLINE

- Part I: Anisotropy due to low density of cracks/fractures
  - Sayers-Kachanov (1991) method
  - Effective medium theories (NI, DS, CPA, SC)
  - Crack influence parameters: η_1 and η_2.
- Part II: Analysis for denser systems of fractures
  - Grechka-Kachanov (2006) numerical simulations
  - Hashin-Shtrikman (HS) bounds
  - Voigt-Reuss (V, R) bounds
  - Voigt-Reuss-Hill (VRH) estimates
  - Crack influence parameters: η_3, η_4, and η_5.
- Conclusions

PART I:
DEFINITION OF CRACK DENSITY ρ

A key parameter is crack density $\rho = na^3$, where a is the radius of a penny-shaped crack and $n = N/V$ is the number (N) of cracks per unit volume (V).

A penny-shaped crack is an oblate spheroidal void *i.e.*, an ellipsoid having principal axis dimensions $a \geq b \geq c$ such that $a = b$ and $c = \alpha a$, where $\alpha < 1$ is the aspect ratio. For flat cracks, α can be very small. Crack density does not depend on α.

Porosity $\phi = 4\pi\rho\alpha/3$, and therefore depends on α.

Anisotropy Due to Fractures (1)

Using Voigt matrix notation, the isotropic compliance matrix (inverse of the stiffness matrix) for an elastic material is often written as $S =$

$$\begin{pmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & & & \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & & & \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & & & \\ & & & \frac{1}{G} & & \\ & & & & \frac{1}{G} & \\ & & & & & \frac{1}{G} \end{pmatrix}$$

where E is Young's modulus, ν is Poisson's ratio, and $G = E/2(1+\nu)$ is the shear modulus.

Anisotropy Due to Fractures (2)

Sayers and Kachanov (1991) show that corrections to the **isotropic** matrix S_{ij}, caused by low crack densities ($\rho << 1$), can be written as

$$\Delta\left(\frac{1}{G}\right) = 4\eta_2\rho/3,$$

$$\Delta\left(-\frac{\nu}{E}\right) = 2\eta_1\rho/3,$$

$$\Delta\left(\frac{1}{E}\right) = 2(\eta_1 + \eta_2)\rho/3,$$

where η_1 and η_2 are parameters to be found from EMT.

Anisotropy Due to Fractures (3)

Thus, in the **isotropic** case, again using Voigt notation, we have

$$\Delta S_{ij} = (2\rho/3)\times$$

$$\begin{pmatrix} (\eta_1+\eta_2) & \eta_1 & \eta_1 & & & \\ \eta_1 & (\eta_1+\eta_2) & \eta_1 & & & \\ \eta_1 & \eta_1 & (\eta_1+\eta_2) & & & \\ & & & 2\eta_2 & & \\ & & & & 2\eta_2 & \\ & & & & & 2\eta_2 \end{pmatrix}.$$

Anisotropy Due to Fractures (4)

For horizontal cracks, we get an anisotropic (being a **TI** or **VTI**) medium whose correction matrix is

$$\Delta S_{ij} = \rho \times$$

$$\begin{pmatrix} 0 & 0 & \eta_1 & & & \\ 0 & 0 & \eta_1 & & & \\ \eta_1 & \eta_1 & 2(\eta_1 + \eta_2) & & & \\ & & & 2\eta_2 & & \\ & & & & 2\eta_2 & \\ & & & & & 0 \end{pmatrix}.$$

Anisotropy Due to Fractures (5)

For vertical cracks whose axis of symmetry is randomly oriented in the xy-plane, we have another anisotropic medium (also **TI** or **VTI**) whose correction matrix is

$$\Delta S_{ij} = \rho \times$$

$$\begin{pmatrix} (\eta_1 + \eta_2) & \eta_1 & \eta_1/2 & & & \\ \eta_1 & (\eta_1 + \eta_2) & \eta_1/2 & & & \\ \eta_1/2 & \eta_1/2 & 0 & & & \\ & & & \eta_2 & & \\ & & & & \eta_2 & \\ & & & & & 2\eta_2 \end{pmatrix}.$$

Anisotropy Due to Fractures (6)

Examples of the values of the η's for **isotropic** "quartz" found using various effective medium theories are:

EMT	η_1	η_2
NI	-0.000216	0.0287
DS	-0.000216	0.0290
CPA	-0.000258	0.0290
SC	$-.0000207$	0.0290

Note that $|\eta_1|/\eta_2 < 0.01$ in all cases here. So only one parameter is important for isotropic quartz.

NIA EXAMPLES (1)

Since it makes little difference at low crack densities which theoretical method is used, we might as well consider the simplest one which is surely the non-interaction approximation (NIA).

It is well-known (e.g., see Zimmerman's book) for the **isotropic** case that:

$$\frac{1}{K_{NI}} - \frac{1}{K} = \frac{\rho}{K}\frac{16(1-\nu^2)}{9(1-2\nu)}$$

$$\frac{1}{G_{NI}} - \frac{1}{G} = \frac{\rho}{G}\frac{32(1-\nu)(5-\nu)}{45(2-\nu)},$$

where $K =$ bulk modulus, $G =$ shear modulus, and $\nu =$ Poisson's ratio of the **isotropic** background medium.

NIA EXAMPLES (2)

But we can also backsolve these equations to obtain

$$\eta_2 = \frac{3}{4\rho}\left(\frac{1}{G^*} - \frac{1}{G}\right)$$

and

$$\eta_1 = \frac{1}{6\rho}\left(\frac{1}{K^*} - \frac{1}{K}\right) - \frac{1}{4\rho}\left(\frac{1}{G^*} - \frac{1}{G}\right),$$

for these two Sayers-Kachanov (1991) crack influence parameters.

NIA EXAMPLES (3)

Thus, we find directly that

$$\eta_2 = \tfrac{1}{G}\tfrac{8(1-\nu)(5-\nu)}{15(2-\nu)} \geq 0$$

and

$$\eta_1 = -\tfrac{1}{G}\tfrac{4\nu(1-\nu)}{15(2-\nu)} \leq 0 \qquad ,$$

where we also used the easily shown fact that $1/2G = (1+\nu)/3K(1-2\nu)$.

Especially note that, in the NIA, η_1 is negative and directly proportional to Poisson's ratio ν.

Random Polycrystals of Laminates

One approach I have taken in related work has used the same "random polycrystals" approach to treat grains as if they are anisotropic due to layering of different isotropic materials.

Thus, the grains have hexagonal symmetry (same as **TI** or **VTI**).

I will not discuss this any more here today since I am focusing instead on fractured media, composed of grains having the same symmetry, *i.e.*, hexagonal.

HS BOUNDS ON K FOR POLYCRYSTALS (1)

General HS (Hashin-Shtrikman-type) bounds for elastic constants of isotropic random polycrystals are known, given first by Peselnick and Meister (1965), and later improved by Watt and Peselnick (1980).
Some caveats about HS bounds will be mentioned later.

These bounds for the bulk modulus can be expressed in terms of these uniaxial shear energies per unit volume as

$$K_{PM}^{\pm} = K_V \frac{G_{eff}^r + \zeta_\pm}{G_{eff}^v + \zeta_\pm}$$

HS BOUNDS ON K FOR POLYCRYSTALS (2)

where

$$\zeta_\pm = \frac{G_\pm}{6}\left(\frac{9K_\pm + 8G_\pm}{K_\pm + 2G_\pm}\right).$$

Parameters $G_\pm$, $K_\pm$ were defined by Watt and Peselnick.

Uniaxial Shear Energy per Unit Volume and the Product Formula

For an applied uniaxial shear *strain* applied along the symmetry axis, *i.e.*, $(e_{11}, e_{22}, e_{33}) = (1, 1, -2)/\sqrt{6}$.

$$G^{v}_{eff} \equiv (c_{11} + c_{33} - 2c_{13} - c_{66})/3$$

For an applied uniaxial shear *stress* applied along the symmetry axis, *i.e.*, $(\sigma_{11}, \sigma_{22}, \sigma_{33}) = (1, 1, -2)/\sqrt{6}$.

$$G^{r}_{eff} \equiv K_{Reuss} G^{v}_{eff} / K_{Voigt}.$$

The latter expression is the **product formula**, relating the shear energies per unit volume to Voigt and Reuss bounds on K.

HS BOUNDS ON G FOR POLYCRYSTALS (1)

The bounds on shear modulus can be expressed similarly as

$$\frac{5}{G_{PM}^{\pm}+\zeta_{\pm}} = \frac{1-X_{\pm}}{G_{eff}^{v}+\zeta_{\pm}+Y_{\pm}} + \frac{2}{c_{44}+\zeta_{\pm}} + \frac{2}{c_{66}+\zeta_{\pm}}$$

where $X_{\pm}$ and $Y_{\pm}$ are additional parameters depending on $G_{\pm}$ and $K_{\pm}$.

Note that in both cases when $\zeta_{-} \to 0$ the bounds go to the Reuss average (lower bound), and when $\zeta_{+} \to \infty$ the bounds go to the Voigt average (upper bound).

HS BOUNDS ON G FOR POLYCRYSTALS (2)

For example,

$$K^{-}_{PM} \rightarrow K_V G^r_{eff}/G^v_{eff} \equiv K_R$$

from the product formulas.

SELF-CONSISTENT MODULI K^*_{SC} & G^*_{SC} (1)

Self-consistent estimates are obtained (approximately)

by taking $K_\pm \to K^*_{SC}$ and $G_\pm \to G^*_{SC}$.

The resulting formulas are:

$$K^*_{SC} = K_V \frac{G^r_{eff} + \zeta^*_{SC}}{G^v_{eff} + \zeta^*_{SC}}$$

where

$$\zeta^*_{SC} = \frac{G^*_{SC}}{6}\left(\frac{9K^*_{SC} + 8G^*_{SC}}{K^*_{SC} + 2G^*_{SC}}\right),$$

and

$$\frac{5}{G^*_{SC} + \zeta^*_{SC}} = \frac{1 - X^*_{SC}}{G^v_{eff} + \zeta^*_{SC}} + \frac{2}{c_{44} + \zeta^*_{SC}} + \frac{2}{c_{66} + \zeta^*_{SC}}.$$

SELF-CONSISTENT MODULI K^*_{SC} & G^*_{SC} (2)

These formulas can then be used together with the bounds to compute both bounds and estimates for the effective quasi-static elastic constants of fractured media.

Voigt and Reuss bounds are always rigorous and available. However, the validity of the HS bounds for anisotropic media is limited to certain microgeometries such as cell materials. We will see what this means in the next section of the talk.

PART II:

Analysis for denser systems of fractures

ANISOTROPY FOR HIGHER CRACK DENSITY

For horizontal cracks, we get an anisotropic medium whose second order compliance correction matrix is

$$\Delta^{(2)}S_{ij} = \rho^2 \times$$

$$\begin{pmatrix} 0 & 0 & \eta_4 & & & \\ 0 & 0 & \eta_4 & & & \\ \eta_4 & \eta_4 & 2(\eta_3+\eta_4+\eta_5) & & & \\ & & & 2\eta_5 & & \\ & & & & 2\eta_5 & \\ & & & & & 0 \end{pmatrix}.$$

where η_3, η_4, and η_5 are three more Sayers-Kachanov crack influence parameters.

NUMERICAL EXAMPLES

CRACK-INFLUENCE PARAMETERS

Examples of the values of the η's found this way from the simulation results supplied by V. Grechka are:

Parameter	$\nu_0 = 0.00$	$\nu_0 = 0.4375$
η_1	0.0000	−0.0192
η_2	0.1941	0.3994
η_3	−0.3666	−1.3750
η_4	0.0000	0.0000
η_5	−0.0917	0.5500

CONCLUSIONS

- The Sayers and Kachanov (1991) approach has some powerful advantages for forward and inverse modeling in fractured systems, especially when used together with measured seismic (Thomsen) parameters.
- For a given material (*e.g.*, quartz) and a given crack shape (*e.g.*, penny-shaped), η_1 and η_2 can be computed once and for all.
- Measured seismic (Thomsen) parameters can then be inverted for crack density.
- Incorporating fluid dependence rigorously into this problem is also easy to do using the Sayers-Kachanov parameters, but that is another (poroelastic) talk.

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Random Polycrystals of Laminates (1)

- Assume building blocks (crystalline grains) composed of layers

  - Use Backus averaging scheme to compute effective properties of these grains

  - Use Hashin-Shtrikman bounds based on layer properties to estimate behavior using only volume fraction and layer property information

Random Polycrystals of Laminates (2)

- Assume also that the grains are equi-axed: when all grains are considered, the axis of anisotropic grain symmetry due to the layering has no preferred direction

  - Use bounds based on these "anisotropic crystals" to estimate overall behavior of the resulting random polycrystal

  - Use self-consistent method to provide one type of direct estimate of the overall behavior

Random Polycrystals of Laminates (3)

- For poroelasticity, we have two kinds of exact results:
  - ∘ If layers are poroelastic Gassmann materials (i.e., microhomogeneous), then with just two types of layers exact results are available for Biot-Willis parameter and Skempton's coefficient.

  - ∘ If, in addition, the permeability of these two types of layers are very different, the double-porosity modeling can also be pursued and this also gives exact results for two components.

Random Polycrystals of Laminates (4)

◦ The exact results do not predict the drained constants for poroelastic media, but the random polycrystals of laminates model gives very close bounds. The rigor of these HS bounds may be questionable, but the related self-consistent estimates nevertheless remain useful.