Mineral Physics I
Chapter 2. Elasticity
Section 7. Averaged elasticity of composite materials

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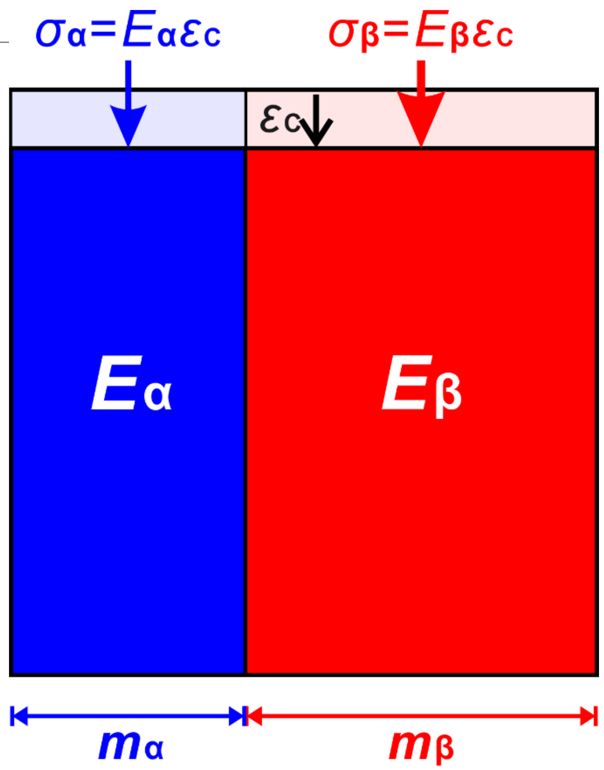
Why do we need a special argument about average of elasticity?

- Hooke's law
  - $\sigma = E\varepsilon$
  - If more than two solids with different elastic constants are mixed, we want to know the bulk elastic constants of the composite solid.

- There are two extreme cases
  - The strain of each grain is equal: the stress on each grain is different with each other.
    - ✓ Voigt average
  - The stress on each grain is equal: the strain of each grain is different with each other
    - ✓ Reuss average

Voigt average

- Elasticity of composite material
  - Mixture of solid α and β
    - ✓ Elastic constants $E_\alpha \neq E_\beta$
    - ✓ Volume fraction: m_α and m_β, $m_\alpha + m_\beta = 1$
- The Hooke's law of each phase
  - $\sigma_\alpha = E_\alpha \varepsilon_\alpha,\ \sigma_\beta = E_\beta \varepsilon_\beta$ (2.7.1)
- Elastic constant of the composite material, E_V
  - the phases area aligned in parallel, and strains are common.
  - uniform strains: $\varepsilon_C = \varepsilon_\alpha = \varepsilon_\beta$, Average stress $\sigma_V \neq \sigma_\alpha \neq \sigma_\beta$
    - $\sigma_V = m_\alpha \sigma_\alpha + m_\beta \sigma_\beta = m_\alpha E_\alpha \varepsilon_C + m_\beta E_\beta \varepsilon_C = [m_\alpha E_\alpha + m_\beta E_\beta]\varepsilon_C$
    - $E_V = \sigma_V / \varepsilon_C = m_\alpha E_\alpha + m_\beta E_\beta$ (2.7.2)
      - Voigt average



Voigt average

ε_C common

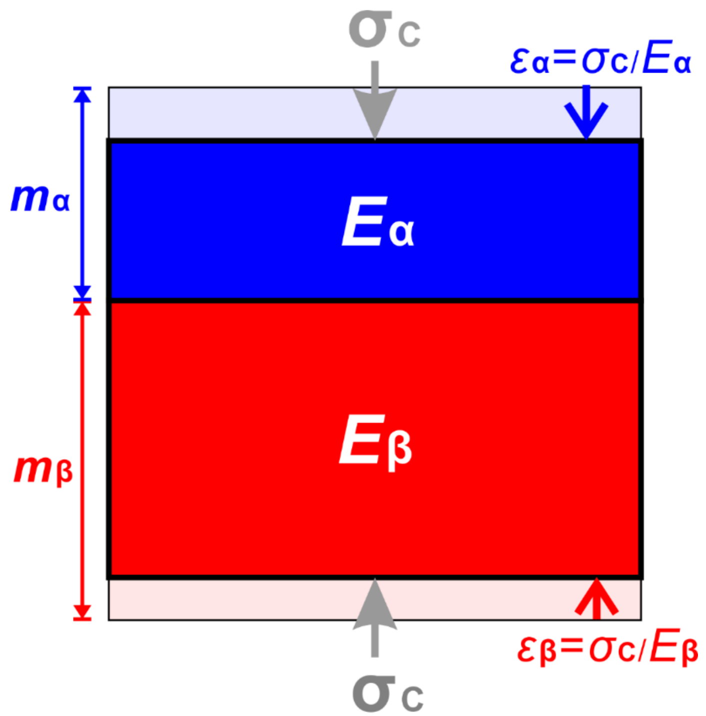
$\sigma_V = m_\alpha \sigma_\alpha + m_\beta \sigma_\beta$

Reuss average

- The phases area aligned in serial, and the stresses are common.
  - ✓ $\sigma_C = \sigma_\alpha = \sigma_\beta$, $\varepsilon_R \neq \varepsilon_\alpha \neq \varepsilon_\beta$
  - ✓ $\varepsilon_R = m_\alpha \varepsilon_\alpha + m_\beta \varepsilon_\beta = m_\alpha E_\alpha^{-1} \sigma_C + m_\beta E_\beta^{-1} \sigma_C$

    $\varepsilon_R = \left[m_\alpha E_\alpha^{-1} + m_\beta E_\beta^{-1} \right] \sigma_C$
  - ✓ $E_R^{-1} = \varepsilon_R / \sigma_C = m_\alpha E_\alpha^{-1} + m_\beta E_\beta^{-1}$ (2.7.3)
    - Reuss average

- Hill average
  - Simply arithmetic average of the Voigt and Reuss averages
    - $E_{\text{Hill}} = \left(E_{\text{Voigt}} + E_{\text{Reuss}} \right)/2$ (2.7.4)

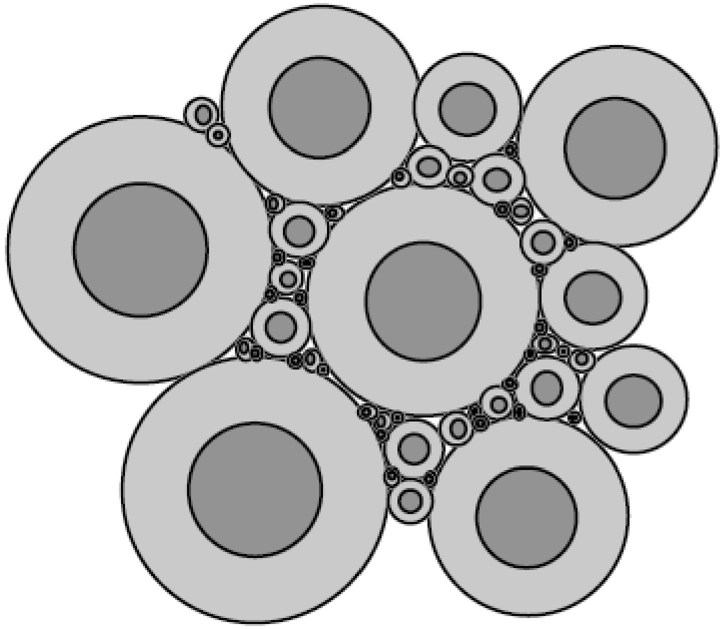


Reuss average
σC common
$\varepsilon_R = m_\alpha \varepsilon_\alpha + m_\beta \varepsilon_\beta$

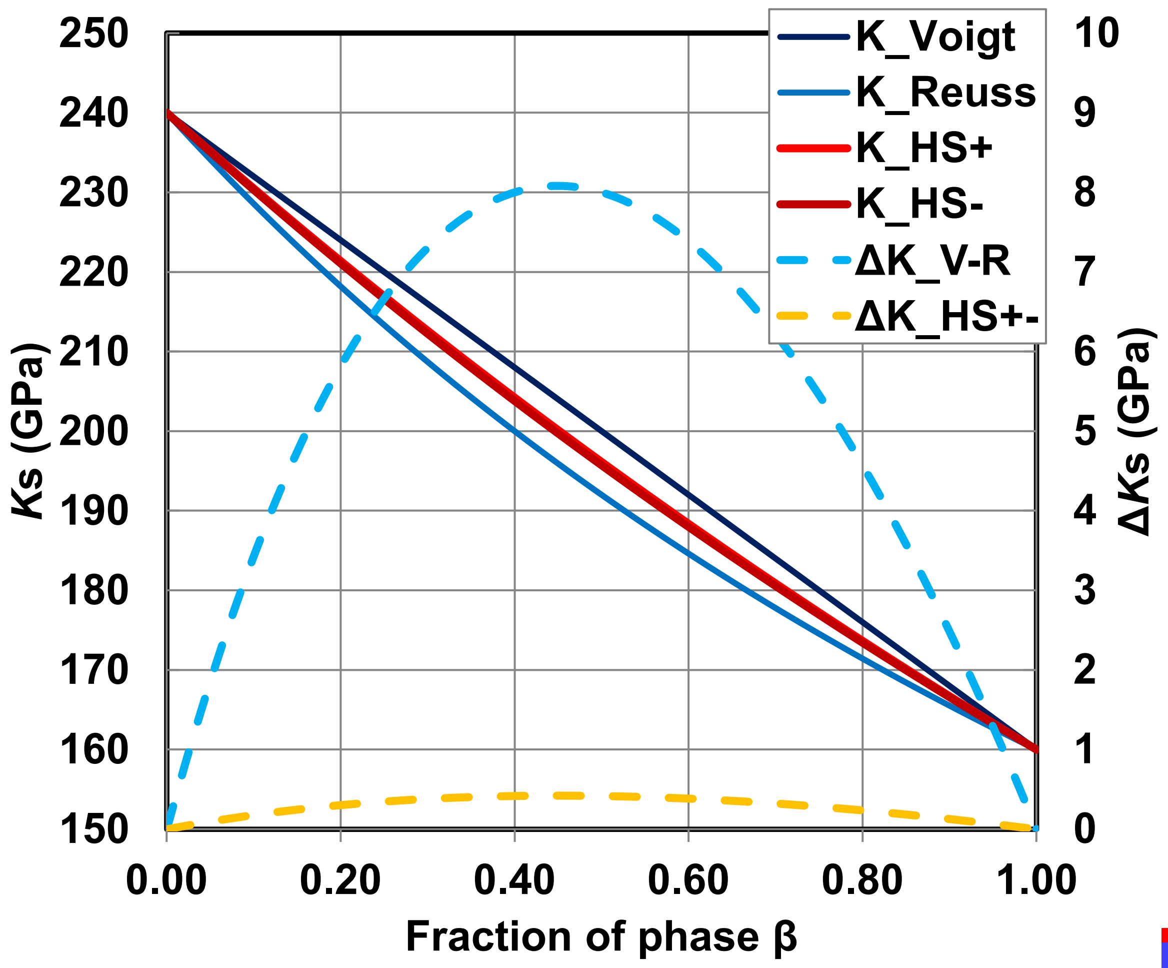
Hashin-Shtrikman bounds

- Aggregates of spheres of one material, and shells of the other material.
  - The narrowest possible bounds on moduli that we can estimate for an isotropic material

- Hashin-Shtrikman bounds of phase α and β
  - $K^{HS\pm} = K_\alpha + \frac{f_\beta}{(K_\beta - K_\alpha)^{-1} + f_\alpha\left(K_\alpha + \frac{4}{3}\mu_\alpha\right)^{-1}}$ (2.7.4)
  - $\mu^{HS\pm} = \mu_\alpha + \frac{f_\beta}{(\mu_\beta - \mu_\alpha)^{-1} + \frac{2 f_\alpha (K_\alpha + 2\mu_\alpha)}{5\mu_\alpha\left(K_\alpha + \frac{4}{3}\mu_\alpha\right)}}$ (2.7.5)
    - ✓ f_α, f_β: volume fractions of phases α and β
    - ✓ The upper bound is given if phase α is stiffer than β, and vice versa.

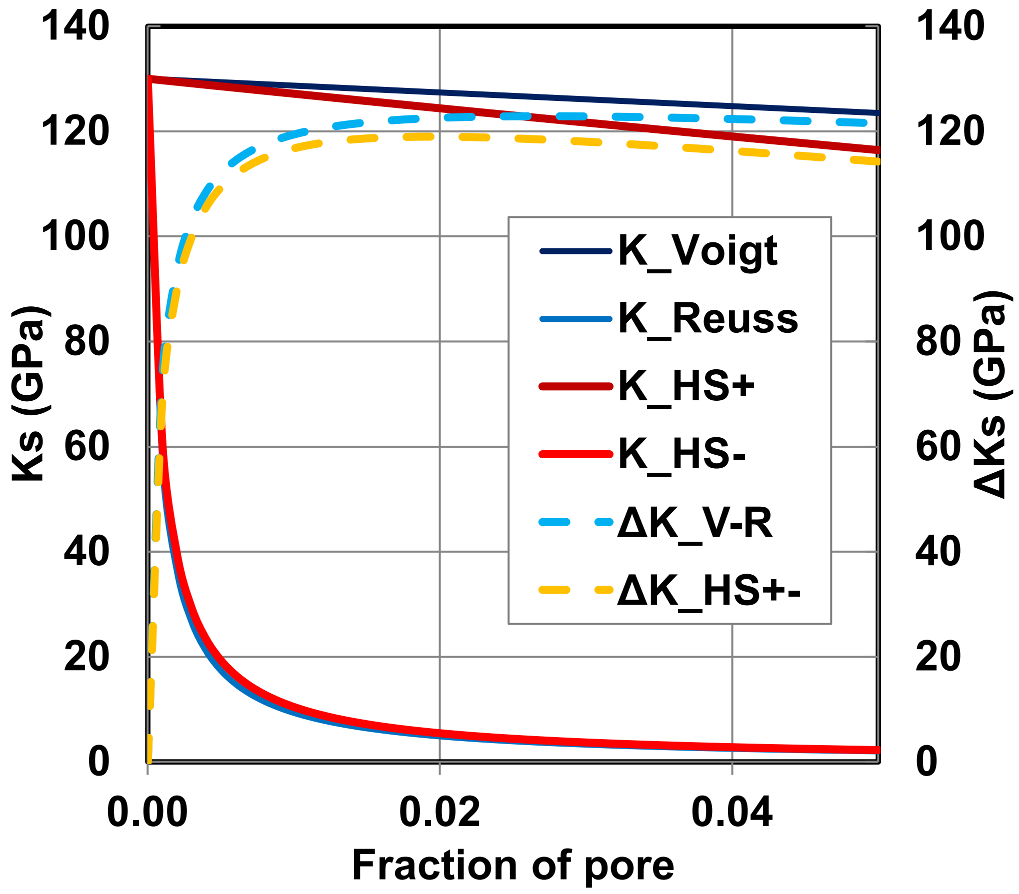


Difference between the upper and lower bounds of two mineral mixtures



- Ks_{α} = 240 GPa, Ks_{β} = 160 GPa
  - Difference between the Voigt and Reuss average: up to 8 GPa
    - ✓ Not negligible
  - Difference between the Hashin-Shtrikman upper and lower bounds: up to 0.4 GPa
    - ✓ Negligible

Evaluation of elasticity of mineral aggregate with pore



- ❑ Ks_α = 130 GPa, Ks_β = 10 MPa
  - ➢ The values of the Reuss average and HS lower bound are against our expectation
    - ✓ Very low
      - ▪ Even 1% of pores make the bulk modulus by less than 1/10.
    - ✓ Almost useless

Bulk modulus of composite materials composed of non-isotropic phases
Reuss average -1

- Reuss average: stresses are identical
  - Crystals under hydrostatic pressure conditions
    - $\sigma_1 = \sigma_2 = \sigma_3 = -\Delta P$ (2.7.6)
    - $\sigma_4 = \sigma_5 = \sigma_6 = 0$ (2.7.7)
- Generalized Hooke's law in the inversed expression
  - $$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} & S_{56} \\ S_{61} & S_{62} & S_{63} & S_{64} & S_{65} & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = [S_{ij}] \begin{bmatrix} -\Delta P \\ -\Delta P \\ -\Delta P \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (2.7.8)$$

Bulk modulus of composite materials composed of non-isotropic phases
Reuss average -2

- The strains under hydrostatic conditions are:
  - $\varepsilon_1 = S_{11}\sigma_1 + S_{12}\sigma_2 + S_{13}\sigma_3 = -\Delta P(S_{11} + S_{12} + S_{13})$
  - $\varepsilon_2 = S_{21}\sigma_1 + S_{22}\sigma_2 + S_{23}\sigma_3 = -\Delta P(S_{21} + S_{22} + S_{23})$
  - $\ldots$
  - $\varepsilon_6 = S_{61}\sigma_1 + S_{62}\sigma_2 + S_{63}\sigma_3 = -\Delta P(S_{61} + S_{62} + S_{63})$
- The volume change $\frac{\Delta V}{V}$ is:
  - $\frac{\Delta V}{V} = \sum_{k=1}^{3} \varepsilon_k = \sum_{i=1}^{3} \sum_{j=1}^{3} S_{ij}\sigma_i = -\Delta P \sum_{i=1}^{3} \sum_{j=1}^{3} S_{ij}$
- The inverse of the bulk modulus is:
  - $\frac{1}{K} = -\frac{\frac{\Delta V}{V}}{\Delta P} = \sum_{i=1}^{3} \sum_{j=1}^{3} S_{ij} = S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{23} + S_{13})$ (2.7.9)
  - $K_{\text{Reuss}} = \frac{1}{S_{11}+S_{22}+S_{33}+2(S_{12}+S_{23}+S_{13})}$ (2.7.10)

Bulk modulus of composite materials composed of non-isotropic phases
Voigt average

- Compress a body equally from three directions

  - Hooke's law:

$$\begin{bmatrix}\sigma_1\\\sigma_2\\\sigma_3\\\sigma_4\\\sigma_5\\\sigma_6\end{bmatrix}=\begin{bmatrix}C_{11}&C_{12}&C_{13}&C_{14}&C_{15}&C_{16}\\C_{21}&C_{22}&C_{23}&C_{24}&C_{25}&C_{26}\\C_{31}&C_{32}&C_{33}&C_{34}&C_{35}&C_{36}\\C_{41}&C_{42}&C_{43}&C_{44}&C_{45}&C_{46}\\C_{51}&C_{52}&C_{53}&C_{54}&C_{55}&C_{56}\\C_{61}&C_{62}&C_{63}&C_{64}&C_{65}&C_{66}\end{bmatrix}\begin{bmatrix}-\Delta V/3V\\-\Delta V/3V\\-\Delta V/3V\\0\\0\\0\end{bmatrix}$$

- $-\Delta P=\frac{\sigma_1+\sigma_2+\sigma_3}{3}=-\frac{\Delta \mathrm{V}}{9\mathrm{V}}[C_{11}+C_{22}+C_{33}+2(C_{12}+C_{13}+C_{23})]$

- $K_{\mathrm{Voigt}}=-\frac{\Delta P}{\frac{\Delta V}{V}}=\frac{C_{11}+C_{22}+C_{33}+2(C_{12}+C_{13}+C_{23})}{9}$ (2.7.11)

Reuss and Voigt averages of rigidity of composite materials composed of non-isotropic phases

- For orthorhombic crystals
  - Reuss average: Stresses are the same between adjacent crystals
    - ✓ $G_{\mathrm{Reuss}} = \frac{15}{[4(S_{11}+S_{22}+S_{33})-4(S_{12}+S_{13}+S_{23})+3(S_{44}+S_{55}+S_{66})]}$ (2.7.12)
  - Voigt averages: strains are the same between adjacent crystals
    - ✓ $G_{\mathrm{Voigt}} = \frac{[(C_{11}+C_{22}+C_{33})-(C_{12}+C_{13}+C_{23})+3(C_{44}+C_{55}+C_{66})]}{15}$ (2.7.13)
  - I do not know the basis, but after Angel et al. [Eur. J. Mineral. 21, 2009]

Examples of Voigt and Reuss averages of bulk moduli and rigidities

Material	c11	c22	c33	C44	C55	C66	C12	C13	C23	K Voigt	K Reuss	K Hill	K Diff %	G Voigt	G Reuss	G Hill	G Diff %
Au	191			42			162			172	172	172	**0.00**	31	24	28	13.11
α-Fe	230			117			135			167	167	167	**0.00**	89	74	82	9.45
Diamond	1079			578			124			442	442	442	**0.00**	538	533	535	0.44
Periclase	294			155			93			160	160	160	**0.00**	133	127	130	2.23
Spinel	282			154			154			154	154	154	**0.00**	118	99	108	8.98
Ringwoodite	327			126			112			184	184	184	**0.00**	119	118	118	0.32
Pyrope	296			92			111			173	173	173	**0.00**	92	92	92	0.00
Halite NaCl	49			13			13			25	25	25	**0.00**	15	15	15	1.46
Stishovite	753		776	252		302	211	203		391	391	391	0.01	262	262	262	0.12
Bridgmanite	515	525	435	179	202	175	117	117	139	247	245	246	0.28	185	184	185	0.37
Enstatite	225	178	214	78	76	82	72	54	53	108	107	108	0.47	75	74	75	0.59
Ferrosilite	198	136	175	59	58	49	84	72	55	103	99	101	2.07	55	53	54	1.64
Forsterite	328	200	235	67	81	81	69	69	73	132	127	129	1.70	80	76	78	2.20
Fayalite	266	168	232	32	46	57	94	92	92	136	131	133	1.85	48	43	45	5.76
Wadslyite	360	383	273	112	118	98	75	110	105	177	176	176	0.50	117	114	115	1.23

- Cubic crystals: identical K_{Voigt} and K_{Reuss}
- G_{Voigt} and G_{Reuss} are different
- Difference between G_{Voigt} and G_{Reuss} is not smaller in cubic crystals than orthorhombic ones.

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