2. Elasticity

7. Averaged elasticity of composite materials

7.1 Introduction

In this chapter, we discuss how to evaluate bulk elastic moduli of the composite solids whose components have different elastic properties. In Hooke's law, the stress (σ) is proportional to the strain (ε) with elasticity (E); $\sigma = E\varepsilon$. Now, we consider the composite solid with different elastic moduli, so the bulk elastic moduli are changed depending on the condition where the materials deform. That is because each phase follows Hooke's law, though the whole of the material also follows. From this perspective, it is implicated that conditions of loaded stress and strain play an important role to determine the elastic properties of composite solids.

In the following section, we first introduce two extreme cases for isotropic bodies, next consider more realistic conditions to provide the elastic moduli such as intermediate stress-strain condition and cases for non-isotropic materials, and finally show some geoscientific examples.

7.2 Voigt average

First, let us consider the situation where two solids with different elasticities aligned in parallel to the direction of stress (Fig1.1). Let the elasticity of each phase be E_α, E_β and the mass of each phase is referred to as m_A, m_B and their summation is unity, which can be regarded as the mass fraction of each phase.

$$m_\alpha + m_\beta = 1 \tag{2.7.1}$$

Then, Hooke's law for each phase is described as

$$\sigma_\alpha = E_\alpha \varepsilon_\alpha \tag{2.7.2}$$

$$\sigma_\beta = E_\beta \varepsilon_\beta \tag{2.7.3}$$

where σ is stress and ε is strain. In the situation we consider now, loaded stresses are different on each phase but strains are equal, and the evaluated elastic moduli are called Voigt average.

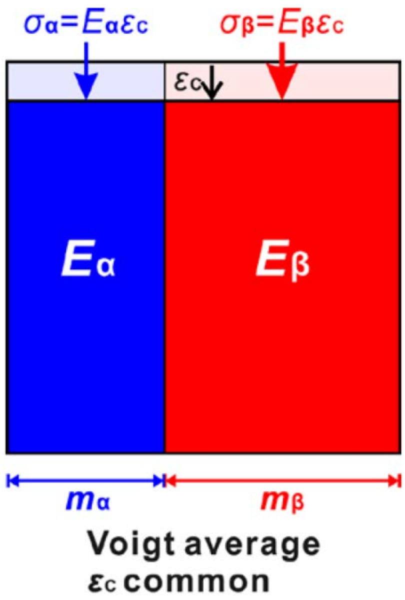

Fig 1.1 Condition assumed in Voigt. Two phases with different elasticities are aligned in parallel to the stress direction. The volume fractions are proportional to the mass fractions as shown in the figure with the areas. The strain is the same between the phases, but the stress is different now.

In addition, Hooke's law for the whole of material is

$$\sigma_V = E_V \varepsilon_C \tag{2.7.4}$$

where σ_V is average stress loaded on the whole of material, E_V is bulk elasticity in Voigt average, and ε_C is a common strain. Again, note that the strain is uniform, and the stress is not equal on each phase now. Therefore,

$$\varepsilon_C = \varepsilon_\alpha = \varepsilon_\beta \tag{2.7.5}$$

$$\sigma_V \neq \sigma_\alpha \neq \sigma_\beta \tag{2.7.6}$$

Let us assume the average stress is proportional to volume fraction. It also can be represented by the mass of each phase, so the average stress can be described by the following relation.

$$\sigma_V = m_\alpha \sigma_\alpha + m_\beta \sigma_\beta \tag{2.7.7}$$

Then, from (2.7.2), (2.7.3), and (2.7.7), the average stress is expressed by the strain.

$$\sigma_V = m_\alpha E_\alpha \varepsilon_C + m_\beta E_\beta \varepsilon_C = [m_\alpha E_\alpha + m_\beta E_\beta]\varepsilon_C \tag{2.7.8}$$

Referring to (2.7.4), bulk elasticity in Voigt average can be given by the following form from the average stress.

$$E_V = \frac{\sigma_V}{\varepsilon_C} = m_\alpha E_\alpha + m_\beta E_\beta \tag{2.7.9}$$

(2.7.9) suggests that the average elastic moduli are equal to the volume fraction weighted average of elastic moduli of each phase in Voigt average. In other words, it is given by the proportional distribution of elastic moduli of each phase to volume fraction in this situation.

7.3 Reuss average

Next, let us consider the situation where two solids with different elasticities aligned in serial to the direction of stress (Fig1.2). In this situation, loaded stress is the same for each phase resulting in the difference of strains. Evaluation under this condition is called Reuss average.

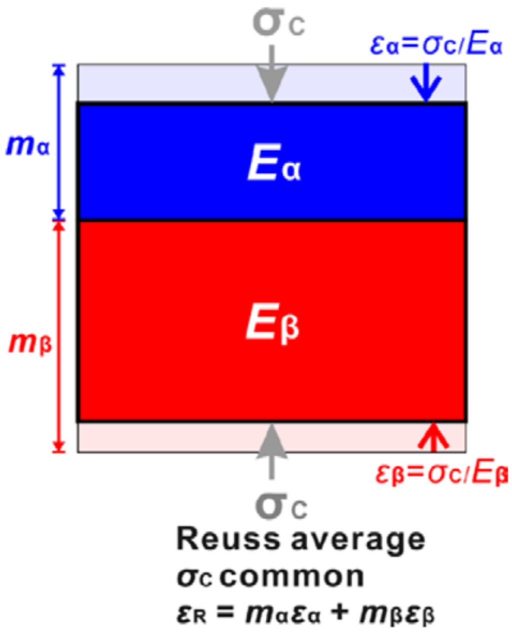

Fig 1.2 Condition assumed in Reuss. Two phases with different elasticities are aligned in serial to stress direction. As same as Voigt, the volume fractions are proportional to the mass fractions. On the other hand, the stress is the same between the phases, but the strain is different now.

The Hooke's law of each phase is also the same as (2.7.2) and (2.7.3), and of the bulk is

$$\sigma_C = E_R \varepsilon_R \tag{2.7.10}$$

where σ_C is the common stress, E_R is the averaged bulk elasticity in Reuss average, and ε_R is the averaged strain. Again, note that the stress is uniform, and the strain is not equal on each phase now. Therefore,

$$\sigma_C = \sigma_\alpha = \sigma_\beta \tag{2.7.11}$$

$$\varepsilon_R \neq \varepsilon_\alpha \neq \varepsilon_\beta \tag{2.7.12}$$

Let us assume the average strain proportionally depends on the volume fraction represented by the mass of each phase.

$$\varepsilon_R = m_\alpha \varepsilon_\alpha + m_\beta \varepsilon_\beta \tag{2.7.13}$$

By transforming and substituting (2.7.2) and (2.7.3) for strain terms in (2.7.13), we can get the averaged strain as follows:

$$\varepsilon_R = m_\alpha \frac{\sigma_C}{E_\alpha} + m_\beta \frac{\sigma_C}{E_\beta} = \left(\frac{m_\alpha}{E_\alpha} + \frac{m_\beta}{E_\beta}\right)\sigma_C \tag{2.7.14}$$

Considering to (2.7.10), bulk elasticity in Reuss average can be given by the following form from the averaged strain.

$$\frac{1}{E_R} = \frac{\varepsilon_R}{\sigma_C} = \frac{m_\alpha}{E_\alpha} + \frac{m_\beta}{E_\beta} \tag{2.7.15}$$

(2.7.15) suggests that the inversed average elastic moduli are equal to the volume fraction weighted average of inversed elastic moduli of each phase in Reuss average. In other words, it is given by the inverse proportional distribution of elastic moduli of each phase to volume fraction in this situation.

7.4 Averaged elastic moduli under intermediate conditions

In the previous section, we introduce the extreme cases where strain or stress is completely the same on phases, but the elastic conditions are always somewhere between the two. Some restrictive averaging methods have been suggested for such a condition.

Hill average is the simplest example, which is the arithmetic average of the Voigt and Reuss averages.

$$E_H = \frac{E_V + E_R}{2} \tag{2.7.16}$$

Hashin-Shtrikman bounds are the most frequently used in geophysics to constraint the elastic condition for isotropic materials more strictly than the Voigt and Reuss averages. Let us assume the aggregates of spheres with shells and cores composed of the phases with different stiffnesses to estimate the bounds (Fig.1.3). Note that this assumption is implicated that these bounds are only determined when the materials are highly almost isotropic (Hashin and Shtrikman, 1962). Though they have calculated them by complicated variational method, in short, the upper and lower bounds of bulk modulus $K_{HS}^{\pm}$ and rigidity (shear modulus) $\mu_{HS}^{\pm}$ are described as follows:

$$K_{HS}^{\pm} = K_\alpha + \frac{f_\beta}{\left(K_\beta - K_\alpha\right)^{-1} + f_\alpha \left(K_\alpha + \frac{4}{3}\mu_\alpha\right)^{-1}} \tag{2.7.17}$$

$$\mu_{HS}^{\pm} = \mu_\alpha + \frac{f_\beta}{\left(\mu_\beta - \mu_\alpha\right)^{-1} + \frac{2 f_\alpha (K_\alpha + 2\mu_\alpha)}{5\mu_\alpha \left(K_\alpha + \frac{4}{3}\mu_\alpha\right)}} \tag{2.7.18}$$

where $K_{A,B}$, $\mu_{A,B}$, $f_{A,B}$ is the bulk modulus, rigidity, and volume fraction of each phase, respectively. The upper bound is given when the phase α is stiffer than β, i.e., $K_\beta < K_\alpha$ or $\mu_\beta < \mu_\alpha$. In the opposite condition, the lower bound is obtained.

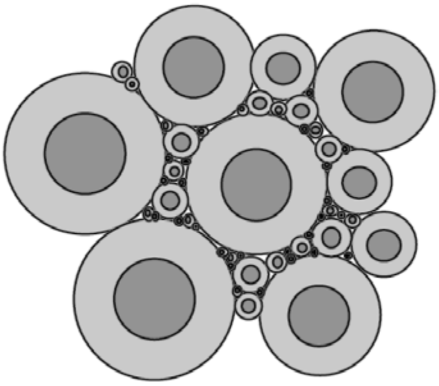

Fig 1.3 Schematic drawing of grains assumed by Hashin and Strikman. They have shells and cores with different stiffnesses. Note that it is suggested that isotropy is highly required in this theory.

7.5 Difference between the bounds of elastic moduli of two mineral mixtures

Let us compare the averaged elastic moduli shown above using two concrete examples where the relative stiffness between the phases is different.

First, we consider the mixed material consisted of phase α (K_S^α = 240 GPa) and β (K_S^β = 160 GPa), which represent bridgmanite for α and periclase for β respectively, in terms of earth science. In this case, note that phase α is stiffer than β but their difference is not significant. Fig.1.4 shows the bulk modulus of the whole body obtained by Voigt average, Reuss average, and Hashin-Shtrikman bounds, and their differences. Voigt average is always higher than Reuss average, and their difference is up to ~8 GPa when the volume fraction of A is ~45 %. On the other hand, a difference of Hashin-Shtrikman upper and lower bounds is so negligible that we cannot distinguish each other on the graph, whose maximum is up to only ~0.4 GPa. In other words, Hashin-Shtrikman bound can limit the available value of elastic moduli in this situation. Therefore, it will be useful to estimate the elastic properties when the material consists of phases with similar stiffnesses.

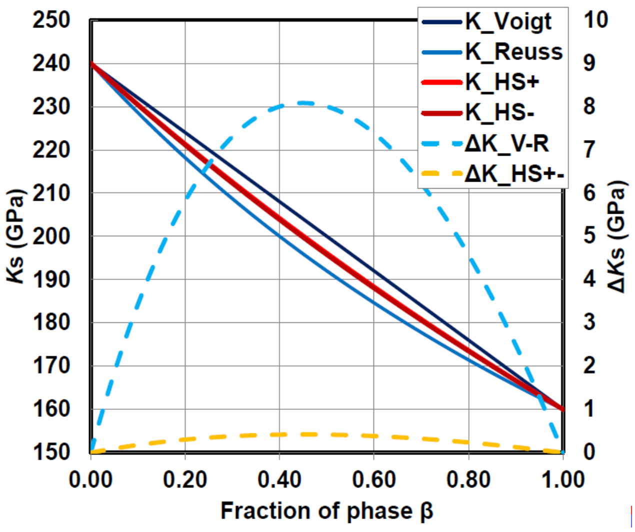

Fig 1.4. The bulk moduli (left axis) and their difference between the bounds (right axis) when the stiffnesses are similar with each phase. The horizontal axis shows the fraction of phase β, so the left end is pure α and the right is pure β. The difference in Hashin-Strikman bound is quite small here.

Next, let us assume that the material consists of phase α and β but α is much stiffer than β (K_s^α = 130 GPa, K_s^β = 10 MPa). This is the case where α is the analogue of olivine and β is of pores filled with fluid phase. Fig1.5 shows averaged elastic moduli of it. As shown, bulk modulus in Voigt average is almost the same as pure phase α while one in Reuss is identical to pure pore phase β. As same as the two, Hashin-Strikman upper bound is almost the same as pure α, and the lower bound is almost identical to pure β. Even if the porosity is only 1%, the bulk modulus goes less than 10% to the value of pure α. In this situation, therefore, Hashin-Strikman bounds also cannot be representative of available elastic moduli. It suggests that every average shown here does not have any essential meaning to evaluate the elastic properties of composite material in this situation. These tendencies also can be expected by their formulas. Because of $K_s^\alpha \gg K_s^\beta$ now, bulk modulus in Voigt average seems to be dominated by the value of K_s^α referring to (2.7.9). As for Hashin-Strikman upper bound, it is also estimated that it will be almost the same as K_s^α, especially when the fraction of phase β is small, with (2.7.17).

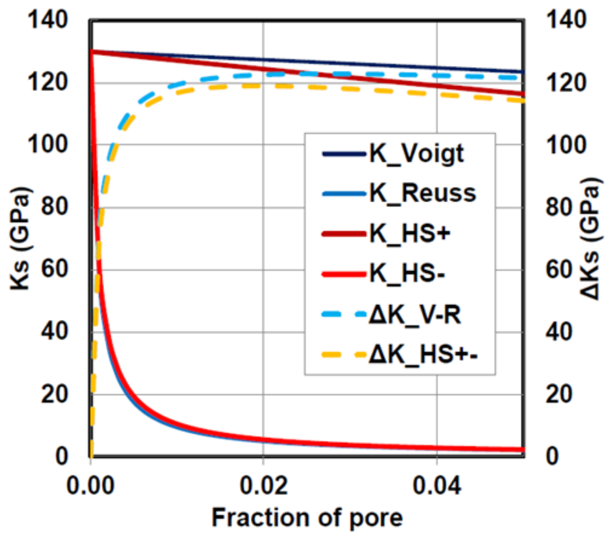

Fig 1.5 The bulk moduli (left axis) and the differences (right axis) when the stiffnesses are very different. The horizontal axis shows the fraction of phase β. The left end is pure α, but the right is only 5% of pure β. The difference in Hashin-Strikman bound is also large as in Voigt and Reuss.

In conclusion, it is very difficult to estimate the bulk modulus of composite materials when they consist of phases with quite different stiffnesses such as materials with fluid pores.

7.6 Bulk modulus of non-isotropic composite materials

Up to this point, though we have assumed isotropic materials, we now consider the bulk modulus of non-isotropic composite bodies. Reuss and Voigt averages are calculated in this situation as same as isotropic. Again, note that bulk modulus K is defined as the volume-normalized derivative of pressure (P) with respect to volume (V).

$$K \equiv -V\frac{\Delta P}{\Delta V} = -\frac{\Delta P}{\frac{\Delta V}{V}} \tag{2.7.19}$$

Therefore, if we know the relative volume change $\Delta V/V$ and confining pressure ΔP under elastic deformation, we can obtain bulk modulus. In the following, we focus on these values and estimate them in Reuss and Voigt averaging conditions to evaluate bulk moduli of non-isotropic bodies.

In Reuss average where stresses are identical, suppose that crystals are under hydrostatic pressure. In this condition, normal stresses are equal to confining pressure and shear stresses are zero. Therefore, stress components are described as

$$\sigma_1 = \sigma_2 = \sigma_3 = -\Delta P \tag{2.7.20}$$

$$\sigma_4 = \sigma_5 = \sigma_6 = 0 \tag{2.7.21}$$

respectively, where σ_i is stress components and P is confining pressure. In generalized Hooke's law in the inversed expression, strain can be written as follows:

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} S_{11} & \cdots & S_{16} \\ \vdots & \ddots & \vdots \\ S_{61} & \cdots & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = [S_{ij}] \begin{bmatrix} -\Delta P \\ -\Delta P \\ -\Delta P \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{2.7.22}$$

where ε_i is strain and S_{ij} is elastic compliance constant. Using from (2.7.20) to (2.7.22), we can obtain each strain component as

$$\begin{gathered} \varepsilon_1 = S_{11}\sigma_1 + S_{12}\sigma_2 + S_{13}\sigma_3 = -\Delta P(S_{11} + S_{12} + S_{13}) \\ \vdots \\ \varepsilon_6 = S_{61}\sigma_1 + S_{62}\sigma_2 + S_{63}\sigma_3 = -\Delta P(S_{61} + S_{62} + S_{63}) \end{gathered} \tag{2.7.23}$$

Where, relative volume change $\Delta V/V$ is the summation of compressional strains, so

$$\frac{\Delta V}{V} = \sum_{i=1}^{3} \varepsilon_i \tag{2.7.24}$$

and now, from $i = 1\sim3$ of (2.7.23), we can get

$$\frac{\Delta V}{V} = \sum_{i,j=1}^{3} S_{ij}\sigma_j = -\Delta P \sum_{i,j=1}^{3} S_{ij} \tag{2.7.25}$$

That is why the bulk modulus in Reuss average is described as follows:

$$\frac{1}{K_R} = -\frac{\frac{\Delta V}{V}}{\Delta P} = \sum_{i,j=1}^{3} S_{ij} \tag{2.7.26}$$

$$K_R = \frac{1}{S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{23} + S_{13})} \tag{2.7.27}$$

We can find that the bulk modulus in Reuss average is expressed by the inverse of summation of the elastic compliance constants. This tendency is consistent with the fact that Reuss average for isotropic material depended on the inversed elasticity, which is the proportional constant in inversed Hooke's law, because the compliance constants are also proportional constant in the generalized law.

In Voigt average where loaded strains are identical, we can consider crystals are equally compressed from three directions. Therefore, strain components are described as

$$\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = -\frac{1}{3}\frac{\Delta V}{V} \tag{2.7.28}$$

$$\varepsilon_4 = \varepsilon_5 = \varepsilon_6 = 0 \tag{2.7.29}$$

because relative volume change with compression when the strain is identical is written as follows:

$$-\frac{\Delta V}{V} = \sum_{i=1}^{3} \varepsilon_i = 3\varepsilon_1 = 3\varepsilon_2 = 3\varepsilon_3 \tag{2.7.30}$$

Now, generalized Hooke's law is

$$\begin{bmatrix}\sigma_1\\\sigma_2\\\sigma_3\\\sigma_4\\\sigma_5\\\sigma_6\end{bmatrix}=\begin{bmatrix}C_{11}&\cdots&C_{16}\\\vdots&\ddots&\vdots\\C_{61}&\cdots&C_{66}\end{bmatrix}\begin{bmatrix}-\Delta V/3V\\-\Delta V/3V\\-\Delta V/3V\\0\\0\\0\end{bmatrix}\qquad(2.7.31)$$

where C_{ij} is elastic constant. Then, confining pressure is the average of normal stresses, so

$$-\Delta P=\frac{\sigma_1+\sigma_2+\sigma_3}{3}=-\frac{1}{9}\frac{\Delta V}{V}[C_{11}+C_{22}+C_{33}+2(C_{12}+C_{23}+C_{13})]\qquad(2.7.32)$$

Therefore, the bulk modulus in Voigt average is described as follows:

$$K_V=-\frac{\Delta P}{\frac{\Delta V}{V}}=\frac{C_{11}+C_{22}+C_{33}+2(C_{12}+C_{23}+C_{13})}{9}\qquad(2.7.33)$$

This shows that the bulk modulus in Voigt average proportionally depends on the summation of elastic constants. With the same logic for Reuss average, this is also consistent with the fact that Voigt average for isotropic material proportionally depended on the summation of elasticity.

7.7 Rigidity of non-isotropic composite materials

The rigidity of non-isotropic polycrystal can be estimated with elastic modulus components and its definition. Here, it is Reuss average when stresses between adjacent crystals are the same and Voigt average when strains are. Though both have been demonstrated by original authors, the rigidity of orthorhombic crystal is simply described by the following according to Angle et al. (2009).

$$G_R=\frac{15}{4(S_{11}+S_{22}+S_{33})-4(S_{12}+S_{23}+S_{13})+3(S_{44}+S_{55}+S_{66})}\qquad(2.7.34)$$

$$G_V=\frac{(C_{11}+C_{22}+C_{33})-(C_{12}+C_{13}+C_{23})+3(C_{44}+C_{55}+C_{66})}{15}\qquad(2.7.35)$$

where G_R, G_V is rigidity in Reuss and Voigt averages, S_{ij} is elastic compliance constant, and C_{ij} is elastic constant. As same as averaged bulk modulus, Reuss average inversely depends on the summation of elastic compliance constants and Voigt average proportionally depends on the summation of elastic constants.

7.8 Geoscientific examples of averaged elastic moduli

Finally, we show and compare some geoscientific examples of Voigt and Reuss averages of bulk modulus and rigidities (Table1.1). In Table1.1, crystals from gold (Au) to halite (NaCl) are cubic, stishovite is tetragonal, and the others are orthorhombic. The differences of the bulk modulus in Voigt and Reuss averages are all zero in cubic crystals and, even in orthorhombic crystals, they are very small only up to 2 %. This shows that the differences in bulk modulus do not have distinct systematic dependences on crystal systems. In terms of rigidity, they are not identical even in the same crystal systems and they are larger than in bulk modulus. For example, gold has the largest value ~13 % in the table but the difference for pyrope is zero, even though both are cubic. Similarly, fayalite shows a difference of about 5% while the difference in bridgmanite is almost zero in orthorhombic systems. As same as bulk moduli, differences in rigidity do not have a distinct tendency to crystal symmetry. In conclusion, the difference of elastic moduli in Voigt and Reuss averages does not depend on the crystal systems.

Table 1.1 Earth scientific examples of elastic constants (Cij), bulk moduli (K), rigidities (G), and their differences. The crystal systems from Au to Halite are cubic, stishovite is tetragonal, and the others are orthorhombic. By their differences, the blank spaces in Cij sections are caused.

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