

2. Elasticity

7. Averaged elasticity of composite materials

7.1 Why do we need a special argument for the average of elasticity?

Understanding the relation between the [stress](#) (σ) applied on a composite material and the consequent [strain](#) (ε) that is generated, *i.e.* the [elastic constants](#) (E), is critical to discuss the properties of real materials such as rocks and artificial materials (*e.g.* concrete). Rocks are [composite materials](#), since they are made of a variety of different minerals. With time rocks will experience different [pressure](#) fields, resulting on different stresses applied on them. When a stress is applied on a body, this will deform accordingly to the intensity and direction of the stress, and the deformation the body undergoes is represented by the strains. Knowing the relation linking the stresses with the strains for a composite material is vital to understand the property of natural terrestrial material, but also of anthropic materials used in material science and engineering. The parameters used to link the stresses applied to a material and the consequent strains are known as elastic moduli, or elastic constants.

For [elastic materials](#) the relation between the stress and strain is expressed using [Hooke's law](#), which defines the stress as a function of the strain in the following way:

$$\sigma = E\varepsilon \quad (2.7.1)$$

in a monophasic material, σ is the stress applied on the solid, E is a generic elastic constant of the material, and ε is the strain the sample undergoes. In a polyphasic material made of a mixture of two or more different phases however, the stress, strain and elastic constants will be different for every phase. Obviously, the elastic properties of the composite material will depend on the elastic properties of the composing phases, therefore the elastic constants of the composite material will be the result of some average of the elastic constants of the single phases. These averaged elastic constants will always have values between two end-members, namely the [Voigt average](#) and the [Reuss average](#).

7.2 Voigt average

The basic assumption in the calculation of the Voigt average is that there is no slip between the [grains](#). Let's assume a mixture of two materials called α and β , these solids are aligned in parallel with a configuration such as the one shown in Fig. 1. This configuration implies that all the phases will undergo the same strain, but the applied stresses will be different. This parallel alignment is a good analogue of a composite material in which the grains of the different composing phases are locked to each other, preventing any slip along the [grain boundaries](#).

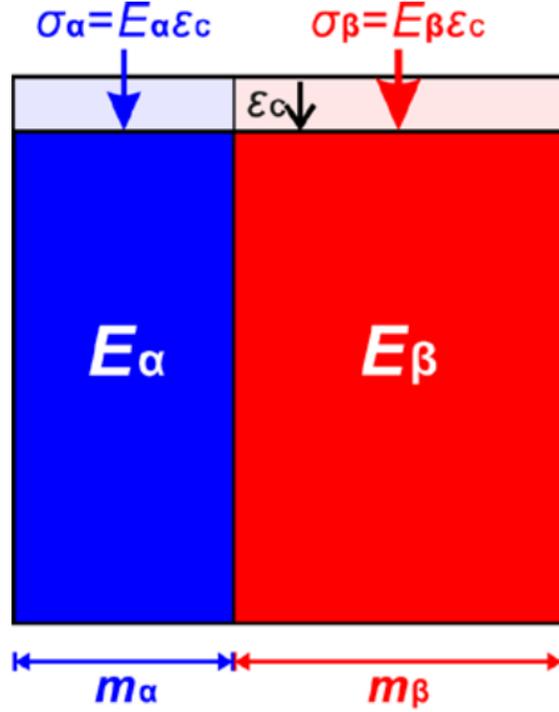


Fig. 1. Schematic representation of the mixture of solid α and solid β in parallel. m_α is the volume fraction of solid α and m_β is the volume fraction of solid β . σ_α is the stress applied on solid α , and σ_β is the one on solid β . ϵ_c is the strain underwent by both the solids.

Using Hooke's law, the definition of the averaged stress on the composite material, and some algebra it is possible to obtain the Voigt average of the elastic constant of a composite material. For a single solid the stress produced by the applied strain is calculated using Hooke's law (Eq. 2.7.1), so, the stresses experienced by solid α and solid β are:

$$\sigma_\alpha = E_\alpha \epsilon_c \quad (2.7.2)$$

$$\sigma_\beta = E_\beta \epsilon_c \quad (2.7.3)$$

where σ_α is the stress on solid α and σ_β is the stress of solid β , E_α is the elastic constant of phase α and E_β is the elastic constant of phase β , and ϵ_c is the strain experienced by solid α and β . Due to the basic assumption of the Voigt average $\sigma_\alpha \neq \sigma_\beta$, $E_\alpha \neq E_\beta$, and $\epsilon_\alpha = \epsilon_\beta = \epsilon_c$. The average stress experienced by the composite material is nothing but the weighted average of the stresses experienced by the single phases composing the solid:

$$\sigma_V = \sigma_\alpha m_\alpha + \sigma_\beta m_\beta \quad (2.7.4)$$

where σ_V is the average stress on the composite material, which is different from both σ_α and σ_β ($\sigma_V \neq \sigma_\alpha \neq \sigma_\beta$), m_α is the volume fraction of phase α and m_β is the volume fraction of phase β , with $m_\alpha + m_\beta = 1$. By substituting Eq. 2.7.2 and 2.7.3 into Eq. 2.7.4 the average stress can also be written as a function of the strain and the elastic constants of the composing materials:

$$\sigma_V = m_\alpha E_\alpha \epsilon_c + m_\beta E_\beta \epsilon_c = [m_\alpha E_\alpha + m_\beta E_\beta] \epsilon_c \quad (2.7.5)$$

Then, by using the Hooke's law to express the elastic constant as a function of the stress and the strains and substituting Eq. 2.7.5 into it, the result is:

$$E_V = \frac{\sigma_V}{\varepsilon_C} = \frac{[m_\alpha E_\alpha + m_\beta E_\beta] \varepsilon_C}{\varepsilon_C} = m_\alpha E_\alpha + m_\beta E_\beta \quad (2.7.6)$$

where E_V is the average elastic constant of the composite material.

What is obtained from Eq. 2.7.6 is the Voigt average (or Voigt bound), in which the average elastic constant of a composite material is the average of the elastic constants of the composing phases, weighted to their volume fraction. The Voigt average represents the upper bound for the elastic constants of a composite material.

7.3 Reuss average

For the calculation of the Reuss average the basic assumption is opposite to the one made for the Voigt average, in this case the grains are free to slip on each other. Let's assume a mixture of two phases called α and β that are aligned in serial with a configuration like the one shown in Fig. 2. This configuration implies that all the phases will experience the same stress but will undergo different strains. This serial alignment is a good analogue of a composite material in which the grains are free to slip on each other along the grain boundaries.

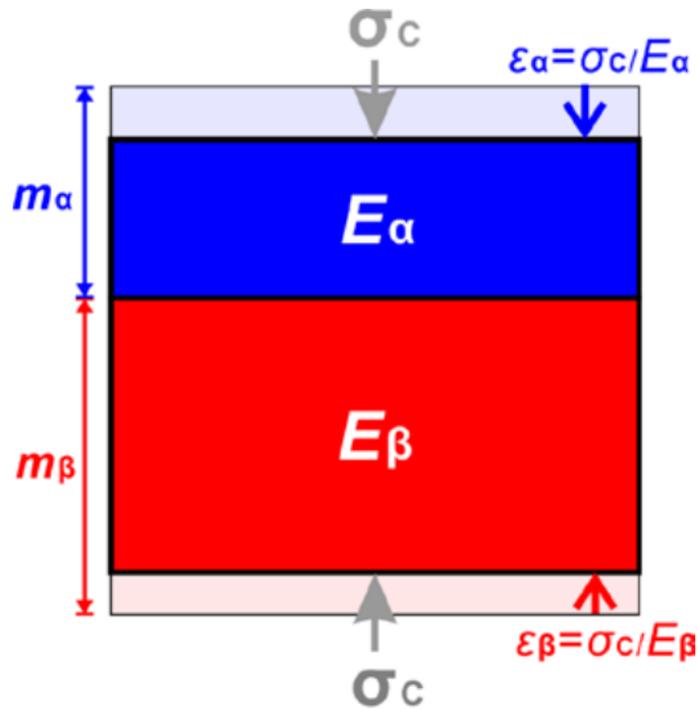


Fig. 2. Schematic representation of the mixture of solid α and solid β in serial. m_α is the volume fraction of solid α and m_β is the volume fraction of solid β . ε_α is the strain applied on solid α , and ε_β is the one on solid β . σ_C is the stress underwent by both the solids.

Using Hooke's law, the definition of the averaged strain on the composite material, and some algebra it is possible to obtain the Reuss average of the elastic constant of a composite material. With Hooke's law (Eq. 2.7.1) it is possible to express the strain experienced by every material in the

composite solid as a function of its elastic constant and of the stress applied to the composite solid, obtaining:

$$\varepsilon_\alpha = \frac{\sigma_C}{E_\alpha} \quad (2.7.7)$$

$$\varepsilon_\beta = \frac{\sigma_C}{E_\beta} \quad (2.7.8)$$

where ε_α is the strain on phase α and ε_β is the strain on phase β , E_α is the elastic constant of phase α and E_β is the elastic constant of phase β , and σ_C is the stress experienced by the composite material. By the basic assumption of the Reuss average $\varepsilon_\alpha \neq \varepsilon_\beta$, $E_\alpha \neq E_\beta$, and $\sigma_\alpha = \sigma_\beta = \sigma_C$. In the configuration of the serially aligned materials the average strain experienced by the composite solid is nothing but the weighted average of the strains experienced by phase α and phase β :

$$\varepsilon_R = \varepsilon_\alpha m_\alpha + \varepsilon_\beta m_\beta \quad (2.7.9)$$

where ε_R is the average strain on the composite material, which is different from the strain on phase α and on phase β ($\varepsilon_R \neq \varepsilon_\alpha \neq \varepsilon_\beta$), m_α is the volume fraction of phase α and m_β is the volume fraction of phase β , with $m_\alpha + m_\beta = 1$. Now, by substituting Eq. 2.7.7 and 2.7.8 into Eq. 2.7.9, the average strain is expressed as a function of the stress on the composite solid and of the elastic constants of phase α and β :

$$\varepsilon_R = m_\alpha \frac{\sigma_C}{E_\alpha} + m_\beta \frac{\sigma_C}{E_\beta} = \left[\frac{m_\alpha}{E_\alpha} + \frac{m_\beta}{E_\beta} \right] \sigma_C \quad (2.7.10)$$

Then, using Hooke's law together with Eq. 2.7.10 the average elastic constant can be expressed as a function of the stress and the strain:

$$\frac{1}{E_R} = \frac{\varepsilon_R}{\sigma_C} = \left[\frac{m_\alpha}{E_\alpha} + \frac{m_\beta}{E_\beta} \right] \sigma_C \sigma_C^{-1} = \frac{m_\alpha}{E_\alpha} + \frac{m_\beta}{E_\beta} \quad (2.7.11)$$

where E_R is the elastic constant of the composite material.

From Eq. 2.7.11 it is obtained the definition of the Reuss average (or Reuss bound), in which the reciprocal of the averaged elastic constant is the sum of the ratios of the volume fraction of the composing solids by their elastic constants. The Reuss average represents the lower bound for the elastic constants of a composite material.

Using the elastic constants calculated by the Voigt and Reuss averages, the Hill average can be defined as the simple arithmetic average of the elastic constants:

$$E_{Hill} = \frac{E_V + E_R}{2} \quad (2.7.12)$$

where E_{Hill} is the elastic constant of the composite solid obtained by the Hill average, and E_V and E_R are the elastic constant obtained from the Voigt and Reuss average respectively.

7.4 Hashin-Shtrikman bounds

The Hashin-Shtrikman bounds are the best bounds for calculating the average elastic constants of a composite material without the need to specify the grain size or the texture of the fabric. These bounds have been derived by Hashin and Shtrikman in 1963 using a variational approach involving the elastic polarization tensor. The results they obtained are some very tight bounds that allow the elastic constant

of the composite material to be calculated with a high precision. The formulation they obtained for an [isotropic material](#) is the following:

$$K^{HS\pm} = K_{\alpha} + \frac{f_{\beta}}{(K_{\beta} - K_{\alpha})^{-1} + f_{\alpha} \left(K_{\alpha} + \frac{4}{3} \mu_{\alpha} \right)^{-1}} \quad (2.7.13)$$

$$\mu^{HS\pm} = \mu_{\alpha} + \frac{f_{\beta}}{(\mu_{\beta} - \mu_{\alpha})^{-1} + \frac{2f_{\alpha}(K_{\alpha} + 2\mu_{\alpha})}{5\mu_{\alpha} \left(K_{\alpha} + \frac{4}{3} \mu_{\alpha} \right)}} \quad (2.7.14)$$

where α and β are the two phases composing the solid, K is the [bulk modulus](#), μ is the [shear modulus](#), and f indicates the volume fraction of the phases. The upper bound for these two equations is given if phase α is [stiffer](#) than phase β , to calculate the lower bound we must swap the α and β indices in the equations.

It has been proven that the upper bound obtained from Equation 2.7.13 is the exact value of the bulk modulus of a material made of a [matrix](#) of phase α with spherical inclusions of phase β distributed inside of it, while the lower bound reflects the opposite case of a matrix of phase β with spherical inclusions of phase α .

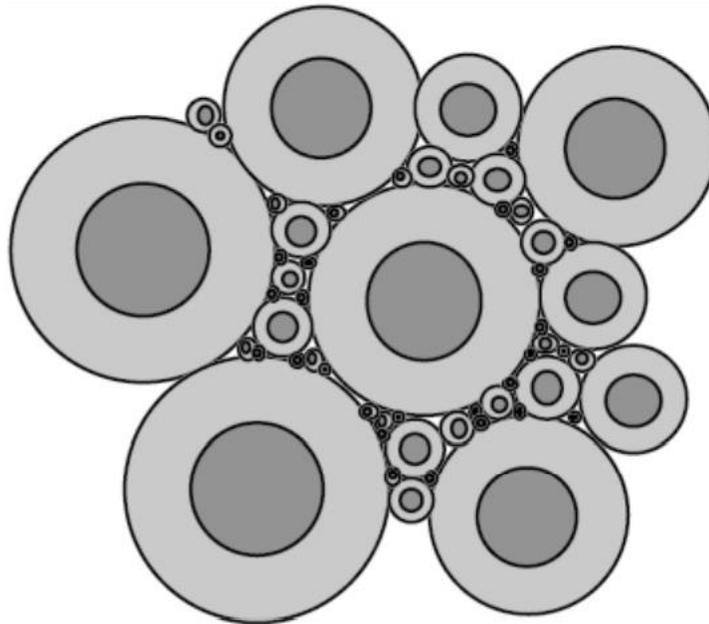


Fig. 3. Schematic representation of the composite material described in the formulation of the Hashin-Shtrikman bounds, where spheres of one material (dark grey) with some elastic constants are surrounded by shells of a different material (light grey) with different elastic constants.

7.5 Difference between the upper and lower bounds of two mineral mixtures

The Hashin-Shtrikman bounds represent a better tool to calculate the average elastic moduli of a mixture of materials than the Reuss and Voigt averages. To prove this point let's take a mixture of two

materials and let's evaluate both the Reuss and Voigt averages, and the Hashin-Shtrikman upper and lower bounds. The mixture is made of two materials: α , which has a bulk modulus $K_{S\alpha} = 240$ GPa, and β , with a bulk modulus $K_{S\beta} = 160$ GPa. The average bulk modulus of the mixture has been calculated for a fraction of phase β going from 0 (monophasic material of phase α) to 1 (monophasic material of phase β), obviously all the averages give the exact (and the same) results when the fraction of phase β is 0 ($K_s = K_{S\alpha} = 240$ GPa) and 1 ($K_s = K_{S\beta} = 160$ GPa). It is clear from Fig. 4 that for all the fractions of phase β (except for 0 and 1) the Hashin-Shtrikman bound are tighter than the Reuss and Voigt averages, with the difference between the upper and lower Hashin-Shtrikman bounds going up to 0.4 GPa, which is a negligible amount, while the difference between the Voigt and Reuss averages goes up to 8 GPa, which is an important and non-negligible difference when calculating the elastic properties of a composite material.

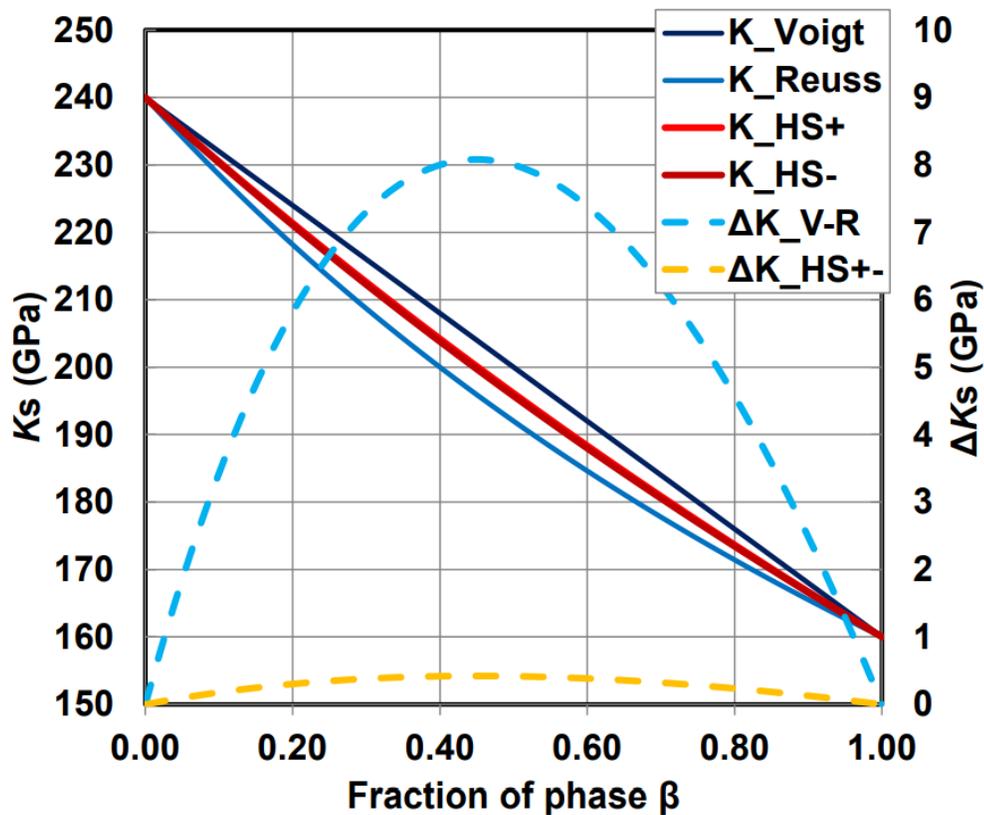


Fig. 4. Representation of the average bulk modulus of a mixture of phase α and β as a function of the fraction of phase β . The dark blue line represents the bulk modulus calculated using the Voigt average, the blue line represents the one calculated using the Reuss average, the orange line represents the bulk modulus calculated using the upper Hashin-Shtrikman bound, and the red line is the result obtained from the lower Hashin-Shtrikman bound. The dashed light blue line is the difference between the average bulk modulus calculated with the Voigt average and the one obtained from the Reuss average. The dashed yellow line represents the difference between the average bulk modulus obtained from the Hashin-Shtrikman upper and lower bounds.

7.6 Evaluation of elasticity of mineral aggregate with pore

If the elastic properties of the composing phases are very different it is very hard to predict the average elastic properties of the composite material. Let's consider a composite material made of a

mixture of phase α and β where $Ks_{\alpha} = 130$ GPa (an analogue of [olivine](#)) and $Ks_{\beta} = 10$ MPa (analogue to a fluid phase inside the [pores](#) of the material). The average bulk modulus has been calculated for a fraction of pores (corresponding to a fraction of phase β) going from 0 to 0.05 (0 to 5%). In this case the average bulk modulus calculated with the Reuss average and with the Hashin-Shtrikman lower bound overlap and show a value very close to Ks_{β} , even only 1% of pores makes the average bulk modulus almost 1/10. On the other hand, the bulk modulus calculated using the Voigt average and the Hashin-Shtrikman upper bound, while not overlapping, are very close to Ks_{α} . The results obtained from the calculations are therefore useless in estimating the elastic properties of the porous material.

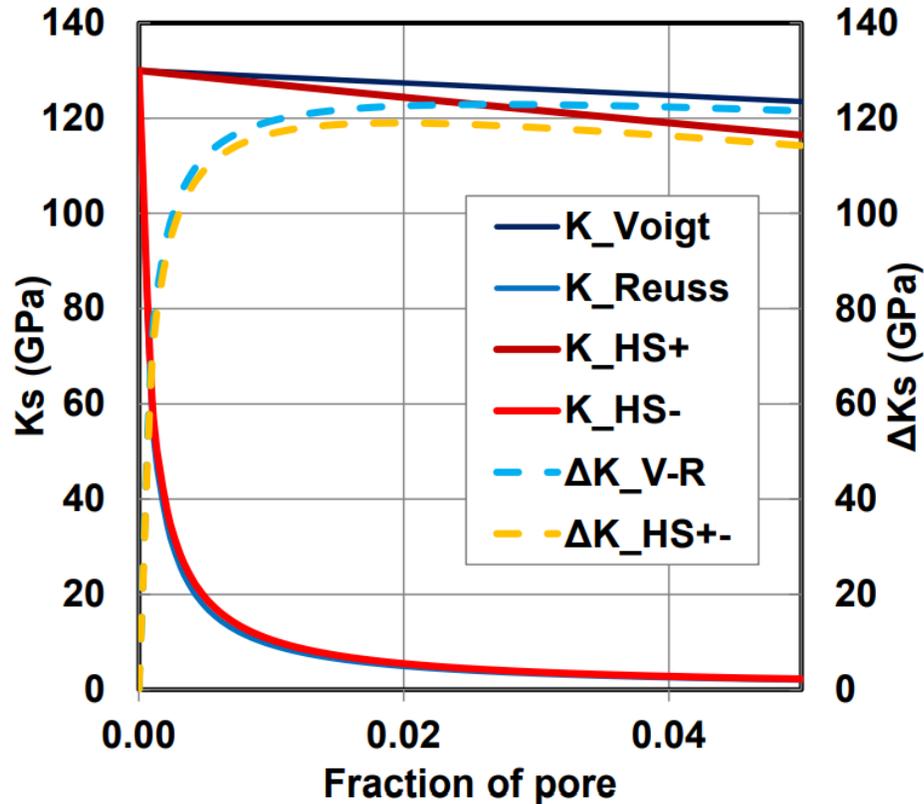


Fig. 5. Representation of the average bulk modulus of a mixture of phase α (olivine analogue) and β (fluid in pore analogue) as a function of the fraction of pores, from 0 to 5%. The dark blue line represents the bulk modulus calculated using the Voigt average, the blue line represents the one calculated using the Reuss average, the dark red line represents the bulk modulus calculated using the upper Hashin-Shtrikman bound, and the red line is the result obtained from the lower Hashin-Shtrikman bound. The dashed light blue line is the difference between the average bulk modulus calculated with the Voigt average and the one obtained from the Reuss average. The dashed yellow line represents the difference between the average bulk modulus obtained from the Hashin-Shtrikman upper and lower bounds.

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

For a composite material made of [anisotropic](#) phases the Reuss average of the bulk modulus is computed starting from the assumption of [hydrostatic pressure](#). As already stated in section 7.3, when calculating the Reuss average we assume that the stresses are identical on the different phases. Let's

consider crystals under hydrostatic pressure conditions, the stresses (expressed using the Voigt notation) are:

$$\sigma_1 = \sigma_2 = \sigma_3 = -\Delta P \quad (2.7.15)$$

$$\sigma_4 = \sigma_5 = \sigma_6 = 0 \quad (2.7.16)$$

where σ is the stress and P is the pressure.

It is possible to derive the bulk modulus of an anisotropic material using Reuss average coupled with the compliance tensor (S). Now let's use the generalized Hooke's law in its inverse expression to write the strain (ε) as a function of the stress and the compliance tensor:

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} & S_{15} & S_{16} \\ S_{21} & S_{22} & S_{23} & S_{24} & S_{25} & S_{26} \\ S_{31} & S_{32} & S_{33} & S_{34} & S_{35} & S_{36} \\ S_{41} & S_{42} & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & S_{53} & S_{54} & S_{55} & S_{56} \\ S_{61} & S_{62} & S_{63} & S_{64} & S_{65} & S_{66} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = [S_{ij}] \begin{bmatrix} -\Delta P \\ -\Delta P \\ -\Delta P \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (2.7.17)$$

By doing the calculations of Eq. 2.7.17, the strains can be expressed as a function of the pressures and the components of the compliance tensor as:

$$\varepsilon_1 = S_{11}\sigma_1 + S_{12}\sigma_2 + S_{13}\sigma_3 = -\Delta P(S_{11} + S_{12} + S_{13}) \quad (2.7.18)$$

$$\varepsilon_2 = S_{21}\sigma_1 + S_{22}\sigma_2 + S_{23}\sigma_3 = -\Delta P(S_{21} + S_{22} + S_{23}) \quad (2.7.19)$$

...

$$\varepsilon_6 = S_{61}\sigma_1 + S_{62}\sigma_2 + S_{63}\sigma_3 = -\Delta P(S_{61} + S_{62} + S_{63}) \quad (2.7.20)$$

The volume change is $\Delta V/V$ and therefore, using Hooke's law, it can be calculated from the stresses and the elastic constants as:

$$\frac{\Delta V}{V} = \sum_{k=1}^3 \varepsilon_k = \sum_{i=1}^3 \sum_{j=1}^3 S_{ij} \sigma_i = -\Delta P \sum_{i=1}^3 \sum_{j=1}^3 S_{ij} \quad (2.7.21)$$

Since the bulk modulus (K) is defined as minus the change in pressure over the volume change ($K = -\frac{\Delta P}{\Delta V/V}$), the reciprocal of the bulk modulus can be written, using Eq 2.7.21 as:

$$\frac{1}{K} = -\frac{\Delta V/V}{\Delta P} = \sum_{i=1}^3 \sum_{j=1}^3 S_{ij} = S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{23} + S_{13}) \quad (2.7.22)$$

where V is the volume. Then, it is obvious that the bulk modulus is nothing but the reciprocal of Eq. 2.7.22, namely:

$$K_{Reuss} = \frac{1}{S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{23} + S_{13})} \quad (2.7.23)$$

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

To calculate the Voigt average of the bulk modulus for a composite material made of anisotropic solids it is assumed that the material is equally compressed in all the three directions. When calculating the Voigt average, it is assumed that all the phases composing the composite body are deformed of the

same amount, as already pointed out in section 7.2. In this case the composite body is compressed equally in all the three dimensions, so the strains are:

$$\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = -\frac{\Delta V}{3V} \quad (2.7.24)$$

$$\varepsilon_4 = \varepsilon_5 = \varepsilon_6 = 0 \quad (2.7.25)$$

where ε is the strain and V is the volume.

It is possible to derive the bulk modulus of an anisotropic material using Voigt average coupled with the stiffness tensor (\mathbf{C}). Using the generalized formulation of the Hooke's law, the stresses can be written as a function of the strain and the stiffness tensor:

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix} \begin{bmatrix} -\Delta V/3V \\ -\Delta V/3V \\ -\Delta V/3V \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (2.7.26)$$

The pressure change is defined as minus the average of the normal stresses $(-(\sigma_1 + \sigma_2 + \sigma_3)/3)$, so it can be expressed using Equation 2.7.26 as:

$$-\Delta P = \frac{\sigma_1 + \sigma_2 + \sigma_3}{3} = -\Delta V \frac{C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})}{9V} \quad (2.7.27)$$

So the bulk modulus is:

$$K_{Voigt} = -\frac{\Delta P}{\Delta V/V} = \frac{C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})}{9} \quad (2.7.28)$$

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

The Reuss and Voigt averages are used to calculate the rigidity (G) of a composite material made of orthorhombic crystals. In the Reuss average the stresses are the same between adjacent crystals:

$$G_{Reuss} = \frac{15}{4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{13} + S_{23}) + 3(S_{44} + S_{55} + S_{66})} \quad (2.7.29)$$

where S_{ij} are the components of the compliance tensor. In the Voigt average the strains are the same between adjacent crystals:

$$G_{Voigt} = \frac{(C_{11} + C_{22} + C_{33}) - (C_{12} + C_{13} + C_{23}) + 3(C_{44} + C_{55} + C_{66})}{15} \quad (2.7.30)$$

where C_{ij} are the components of the stiffness tensor.

7.10 Examples of Voigt and Reuss averages of bulk moduli and rigidities

Material	c11	c22	c33	C44	C55	C66	C12	C13	C23	K			K Diff %	G			G Diff %	
										Voigt	Reuss	K Hill		Voigt	Reuss	G Hill		
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

Fig. 6. Table showing various minerals, their values of the stiffness tensor (C_{ij}), the bulk modulus (K) and rigidity (G) calculated using the Voigt, Reuss and Hill average, and the difference between the values of the Voigt and Reuss average expressed as % for both the bulk modulus and the rigidity. In the table are listed only the non-zero, independent components of the stiffness tensor, if a component is left blank in the table, it is because, due to symmetry of the crystal, it is equivalent to another component already stated in the table. Cubic crystals have only three independent components, trigonal crystals have six, and orthorhombic crystals have nine.

Contrary to what could be expected, the difference in the values of the rigidity calculated using Voigt (G_{Voigt}) and Reuss (G_{Reuss}) average for non-isotropic materials does not depend on the symmetry of the material (*i.e.*, highly symmetric crystal not necessarily show a smaller difference between G_{Voigt} and G_{Reuss} than less symmetric crystals). In the table represented in Fig. 6 are listed the components of the stiffness tensor for various minerals with different symmetries. For cubic crystals, which are highly symmetrical, the bulk moduli calculated using the Voigt (K_{Voigt}) and Reuss (K_{Reuss}) average have the same values (*i.e.*, K_{Diff} is 0%), on the other hand, less symmetrical minerals show a $K_{Diff} \neq 0\%$. However, the rigidities are different, the difference between the calculated values of G_{Voigt} and G_{Reuss} does not seem to show any dependence on the symmetry of the material, *e.g.* spinel (cubic) has a G_{Diff} of 8.98%, while enstatite (orthorhombic) shows a G_{Diff} of 0.59%, lower than spinel, even though spinel is highly symmetric with respect to enstatite.