Elastic Behavior of Random Polycrystals Composed of Anisotropic α -Quartz (SiO_2) under Pressure

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Abstract

This work presents several sets of results for granular media all composed of quartz (SiO_2) and all having grains with trigonal (six constant) elastic symmetry. In some cases, the samples had significant amounts of external pressure (up to 20 GPa) applied to the quartz samples while the elastic constants were being either measured or simulated. In other examples, the temperatures ranged from room temperature down to values approaching absolute zero. In addition to the traditional Voigt and Reuss bounds on effective isotropic bulk and shear moduli, the Hashin-Shtrikman bounds of these elastic moduli have also been computed in all these examples. We find that the Hashin-Shtrikman bounds provide a significant tightening of the traditional bounds on the moduli in most cases. Rarely, the Hashin-Shtrikman upper bounds for shear modulus may coincide with Voigt estimates of the shear modulus. More typically we find the HS bounds on both shear and bulk modulus are so close that their averaged values (called here the “self-consistent average” estimates) for both bulk and shear modulus values are tightly constrained by the HS bounds themselves. In contrast, the traditional VRH (Voigt-Reuss-Hill) estimates of the moduli often lie outside of the HS bounds, thus giving reasons for doubting the accuracy of VRH estimates in general – and especially for pressurized samples. Of the eight scenarios considered in the paper, four have substantial confining pressures (10 or 20 GPa), and four have zero confining pressure. One general distinction arising in these particular data sets is observed: when the confining pressure is negligible, the VRH estimates are found always to lie inside the Hashin-Shtrikman bounds. In contrast, when the confining pressure is $P = 10$ GPa or higher the VRH estimates of bulk and shear moduli both lie outside the Hashin-Shtrikman bounds.

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1. Introduction

Massive blocks of crystalline quartz have well-defined, and fairly straightforwardly measurable elastic constants (often obtained using acoustic wave measurements) in a laboratory setting. Examples of data on trigonal α -quartz are included in work by McSkimin *et al.* (1965) and Kimizuka *et al.* (2007). However, for many applications to the earth sciences and mining engineering, including oil and mineral exploration, tunneling, and underground sequestration of unwanted solid waste and fluids, it is useful to know what the effective average mechanical properties might be when anisotropic grains of such rocks are randomly jumbled together to form an effectively isotropic composite medium underground. This problem is the main one to be addressed in the present work.

For our purposes, the most commonly used estimators are still the Voigt (1928) and Reuss (1929) bulk and shear modulus estimators (being rigorous upper and lower bounds respectively) on the bulk and shear moduli for presumed effectively isotropic jumbles of such grains. Since the suggestion of Hill (1952), the modulus estimators most often used are the Voigt-Reuss-Hill (VRH) averages (either arithmetic or geometric means of the Voigt and Reuss values, both choices for averaging the upper and lower bounds giving very comparable results in most cases).

However, since the work of Hashin and Shtrikman (1962), significantly better (*i.e.*, based on the tighter bounds) estimators have become available. It is true that they are somewhat harder to compute than the VRH averages of the bounds, which can easily be computed using a hand calculator. But with modern computing capabilities, it is not very hard to obtain these better HS bounds (or the estimators derived from them), which result in (usually) tighter bounds and therefore more precise estimates of the isotropic average constants. It has also been shown to be possible to construct a different type of self-consistent average values from the Hashin-Shtrikman formulas directly (Berryman, 2005), but it is also true that the HS bounds are often so close together that their average values produce results within both the Voigt-Reuss bounds and the Hashin-Shtrikman bounds. In contrast the VRH average values frequently lie outside the Hashin-Shtrikman bounds, therefore suggesting that the HS bounds and corresponding self-consistent average estimates are likely to provide more accurate estimates in such cases. One goal of the present work is to clarify what types of results might be expected to occur and under what circumstances.

The examples that follow are intended to be illustrative, based in part on the elastic constant results presented in the paper concerning pressure dependence by Kimizuka *et al.* (2007), while some earlier data on temperature dependence of McSkimin *et al.* (1965) has been used here as well for quantitative and qualitative checks on the more recent work. Applied pressures considered in the GPa range are most likely to be present in a high-pressure laboratory setting. For applications to the subsurface, based on the density of quartz and the earth's surface gravity of 9.8 m/s^2 , we should not expect overburden pressures to exceed about 26 MPa per km of depth.

For such applications 200 km depth corresponds to about 5 GPa of overburden (by comparison, Earth's radius is about 6400 km). Note: This estimate has not taken into account the changes (typically being reduction, but there are also local fluctuations) in gravitation constant with depth due to opposing gravitational forces from solid materials both above and below each point considered at any given depth, which will also tend to reduce these effects. Such counterbalancing effects will be very small at shallow depths, but increasingly significant at greater and greater depths. See Symon (1960) for the physics related reasons (*i.e.*, potential theory) for these changes with depth. Lay and Wallace (1995) present tabulated values of earth's actual gravity field with depth due to measured nonuniform density distribution, and a selection of these results is shown here in Table G.

2. Methodology

Our examples are limited here to α -quartz having trigonal symmetry with six independent constants, since $C_{25} = 0$ and $C_{66} = (C_{11} - C_{12})/2$. The pertinent stress-strain relations are given by

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & & \\ & C_{12} & C_{11} & C_{13} & -C_{14} & \\ & C_{13} & C_{13} & C_{33} & & \\ & C_{14} & -C_{14} & & C_{44} & \\ & & & & C_{44} & C_{14} \\ & & & & C_{14} & C_{66} \end{pmatrix} \begin{pmatrix} e_{11} \\ e_{22} \\ e_{33} \\ e_{23} \\ e_{31} \\ e_{12} \end{pmatrix}, \quad (1)$$

where σ_{ij} , for $i, j = 1, 2, 3$ (representing the x, y, z directions respectively), are the stresses, and e_{ij} , for $i, j = 1, 2, 3$, are the strains. See Nye (1985) for a full explanation of the various

symmetries and restrictions on elastic constants C_{ij} that are possible and typically found in nature.

The calculations performed here make use of the methods of Voigt (1928), Reuss (1929), Hill (1952), Hashin-and Shtrikman (1962), Peselnick and Meister (1965), Watt and Peselnick (1980), and Watt (1986), as well as some earlier work of the author (Berryman, 2005). Data used include laboratory measurements of McSkimin *et al.* (1965), and simulations of Kimizuka *et al.* (2007).

3. Birch Coefficients for effective elastic constants of crystals under pressure

If C_{ijkl} are the elastic constants using the common four index subscript notation, then Birch (1947, 1952), Wallace (1965), and Barron and Klein (1965) show that the Birch coefficients, required for analysis of crystals under pressure are given by

$$B_{ijkl} = C_{ijkl} + P(\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}), \quad (2)$$

where P is the applied hydrostatic pressure and δ_{ij} is the Kronecker delta.

For the trigonal case, this formula implies – when presented instead using the popular two index notation – that:

$$B_{11} = C_{11} - P, B_{33} = C_{33} - P, B_{44} = C_{44} - P, B_{66} = C_{66} - P, \quad (3)$$

for the diagonal components, and

$$B_{12} = C_{12} + P, B_{13} = C_{13} + P, B_{14} = C_{14} + 0, \quad (4)$$

for the off-diagonal components. This two index notation is the one used in all the examples that follow.

4. Results

Our results are displayed in 8 Figures and 12 Tables. The first two Figures are based on the McSkimin *et al.* (1965) data and the remaining Figures are based on the Kimizuka *et al.* (2007) simulation results.

All the information used to construct the Figures is from the Tables and is elaborated in the Figure captions.

In order to keep the Figures as uncluttered as possible, the only lines inside the Figures are those connecting the end points for the VR bounds, which are (K_R, G_R) and (K_V, G_V) , and those connecting the end points of the HS bounds which are (K_{HS}^-, G_{HS}^-) and (K_{HS}^+, G_{HS}^+) . In most cases, the bounding rectangle for the VR bounds is very close to the same as the bounds of the Figure itself. In each case, the rectangle in question (but not actually shown here) involves vertical lines through the two VR end points (squares), and also horizontal lines through the same two end points. Similarly, the bounding rectangle for the HS bounds is constructed with similar vertical and horizontal lines through the two corresponding HS end points (asterisks).

In the first three Figures, the HS line between the end points actually passes through the VR line, and in all these cases the VRH point falls easily within the HS bounding rectangle. The same result is also found (and for the same reasons) in Figure 6. In the remaining four cases, which are Figures 4, 5, 7, and 8, the line connecting the HS bounds does not cross the VR line, while the relative displacement is also great enough that the VRH estimates cannot fall inside the HS bounding rectangle. While the data set presented is clearly limited, the results are nevertheless suggestive of a general rule that may apply such that higher pressure environments might be expected to result in effective constants that frequently differ from those of the traditional VRH estimates.

5. Discussion

When checking the stated experimental errors in the elastic constant measurements, the freedom allowed by the traditional Voigt and Reuss bounds and the VRH average estimators tend to be about an order of magnitude larger than the experimental uncertainties as quoted. In contrast, the Hashin-Shtrikman bounds and estimators provide a range of permitted values found to be very comparable in magnitude to those of the experimental numbers in many cases. Comparisons show therefore that the Voigt and Reuss bounding estimates are often too crude to take advantage of the precision of high quality laboratory measurements, while the Hashin-Shtrikman bounds and estimators have very comparable precision and uncertainties to those of such laboratory data whenever available.

In the eight examples considered here, four had external pressure applied during the lab measurements or computer simulations. In all four of these high pressure experiments the VRH estimates were found to lie outside the Hashin-Shtrikman bounding rectangles. In contrast, all four of the examples with no external pressure (and regardless of the difference in temperature changes) the VRH estimates did lie within the HS bounding rectangles. How general these results might be is surely a subject for further study.

The methods developed and discussed here can easily be applied to other granular systems composed of anisotropic grains having trigonal elastic symmetry, and — with some known technical modifications — also to those having other types of elastic symmetry as well.

TABLE G. Examples of known changes in gravitational acceleration g at depth in the earth. All data from Lay and Wallace (1995).

Depth (km)	g (m/s ²)
0	9.82
150	9.94
600	10.00
2891	10.68
5371	3.62

TABLE 1. Values of the measured single crystal constants for two examples of trigonal (6 constant) α -quartz (SiO₂), where $C_{66} = \frac{1}{2}(C_{11} - C_{12})$. All elastic constants are in units of GPa (gigapascal). Data from McSkimin *et al.* (1965).

T	C_{11}	C_{33}	C_{44}	C_{12}	C_{13}	C_{14}	C_{66}
25° C	86.8	105.8	58.2	7.04	11.9	-18.0	39.9
- 195.8° C	87.3	109.2	59.7	9.90	13.0	-17.7	38.7

TABLE 2A. Values of auxiliary constants computed in the geomechanical analysis (13), (8), (7), and (12), for trigonal α -quartz. All source elastic constants are in units of GPa (gigapascal) from the work of McSkimin *et al.* (1965). Note that the four constants shown are always well-ordered in both cases, from lowest to highest.

T	μ_-	G_{eff}^r	G_{eff}^v	μ_+
25° C	28.9	42.4	43.0	69.2
-195.8° C	28.6	43.3	43.9	69.8

TABLE 2B. Values of the Voigt and Reuss shear and bulk moduli computed in the geomechanical analysis: for two examples of trigonal α -quartz. All source elastic constants are in units of GPa (gigapascal) from the work of McSkimin *et al.* (1965).

T	G_R	G_V	K_R	K_V
25° C	41.1	47.8	37.4	37.9
- 195.8° C	41.1	48.1	39.0	39.5

TABLE 2C. Values of Hashin-Shtrikman bounds computed for shear and bulk modulus in the geomechanical analysis for two examples of trigonal α -quartz. All source elastic constants are in units of GPa (gigapascal) from the work of McSkimin *et al.* (1965).

T	G_{HS}^-	G_{HS}^+	K_{HS}^-	K_{HS}^+
25° C	43.6	44.8	37.6	37.7
-195.8° C	43.8	45.0	39.2	39.3

TABLE 3. Values of the calculated single crystal constants for three examples of trigonal (6 constant) α -quartz (SiO_2), where $C_{66} = \frac{1}{2}(C_{11} - C_{12})$. Pressure P and all elastic constants are in units of GPa (gigapascal). All data from Kimizuka *et al.* (2007).

P	C_{11}	C_{33}	C_{44}	C_{12}	C_{13}	C_{14}	C_{66}
0	81.1	104.8	49.7	8.3	7.5	23.3	36.4
10	132.6	233.4	67.0	56.0	49.6	-4.1	38.3
20	176.4	294.9	69.6	61.4	69.5	-19.9	57.5

TABLE 4A. Values of auxiliary constants computed in the geomechanical analysis (13), (8), (7), and (12), for trigonal α -quartz. All source elastic constants are in units of GPa (gigapascal) from the work of Kimizuka *et al.* (2007). Note that the four constants are *not* always well-ordered in these three cases, from lowest to highest. $P = 10$ GPa and $P = 20$ GPa are two examples of well-ordered constants.

P	μ_-	μ_+	G_{eff}^r	G_{eff}^v
0	18.8	67.3	44.3	44.8
10	37.7	67.6	72.5	76.2
20	42.8	84.3	86.5	91.6

TABLE 4B. Values of the Reuss and Voigt shear and bulk moduli from the geomechanical analysis for trigonal α -quartz under three values of applied pressure P . All source elastic constants are in units of GPa (gigapascal) from the work of Kimizuka *et al.* (2007).

P	G_R	G_V	K_R	K_V
0	31.5	43.4	34.4	34.8
10	47.5	57.4	85.6	96.1
20	61.0	70.2	103.9	116.5

TABLE 4C. Values of the Hashin-Shtrikman bulk and shear modulus bounds computed in the geomechanical analysis for trigonal α -quartz under three values of applied pressure P . All effective constants are in units of GPa (gigapascal) based on the work of Kimizuka *et al.* (2007).

P	G_{HS}^-	G_{HS}^+	K_{HS}^-	K_{HS}^+
0	35.6	38.6	34.5	34.7
10	54.4	55.2	87.1	87.5
20	64.6	66.1	112.3	112.8

TABLE 5. Values of the calculated Birch effective elastic constants for three examples of trigonal (6 constant) α -quartz (SiO_2), where $B_{66} = \frac{1}{2}(B_{11} - B_{12})$. Pressure P and all elastic constants are in units of GPa (gigapascal). Data from Kimizuka *et al.* (2007).

P	B_{11}	B_{33}	B_{44}	B_{12}	B_{13}	B_{14}	B_{66}
0	81.1	104.8	49.7	8.3	7.5	23.3	36.4
10	122.6	223.4	57.0	66.0	59.6	-4.1	28.3
20	156.4	274.9	49.6	81.4	89.5	-19.9	37.5

TABLE 6A. Values of auxiliary constants computed in the geomechanical analysis (13), (8), (7), and (12), for trigonal α -quartz based on the Birch effective elastic constants under applied pressure P . All source elastic constants are in units of GPa (gigapascal) from the work of Kimizuka *et al.* (2007). Note that the four constants are *not* always well-ordered

in these three cases, from lowest to highest. $P = 10$ GPa and $P = 20$ GPa are two examples of well-ordered constants.

P	μ_-	μ_+	G_{eff}^r	G_{eff}^v
0	18.8	67.3	44.3	44.8
10	27.7	57.6	62.6	66.2
20	22.8	64.3	66.8	71.6

TABLE 6B. Values of the Voigt and Reuss shear and bulk moduli computed in the geomechanical analysis for trigonal α -quartz based on the Birch effective elastic constants under applied pressure P . All source elastic constants are in units of GPa (gigapascal) from the work of Kimizuka *et al.* (2007).

P	G_R	G_V	K_R	K_V
0	31.5	43.4	34.4	34.8
10	34.0	47.4	88.2	93.2
20	37.4	49.2	114.9	122.8

TABLE 6C. Values of Hashin-Shtrikman bounds computed for shear and bulk modulus in the geomechanical analysis for trigonal α -quartz based on the Birch effective elastic constants under applied pressure P . All effective constants are in units of GPa (gigapascal) from the work of Kimizuka *et al.* (2007).

P	G_{HS}^-	G_{HS}^+	K_{HS}^-	K_{HS}^+
0	35.6	38.6	34.5	34.7
10	43.6	44.7	89.9	90.5
20	42.1	44.6	117.2	118.5

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FIG. 1: Voigt and Reuss bounds and Hashin-Shtrikman bounds on bulk and shear moduli for McSkimin *et al.* (1965) $T = 25^\circ$ C laboratory data. VRH estimates both lie inside the HS bounding rectangle.

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FIG. 2: Voigt and Reuss bounds and Hashin-Strikman bounds on bulk and shear moduli for McSkimin *et al.* (1965) $T = -196^\circ\text{C}$ laboratory data. VRH estimates both lie inside the HS bounding rectangle.

Appendix: The Peselnick-Meister-Watt algorithm [Peselnick and Meister (1965), Watt and Peselnick (1980)] for computing the Hashin-Shtrikman bounds of granular systems having grains with trigonal elastic symmetry

The Voigt (1928) and Reuss (1929) averages for bulk and shear modulus of composites formed from trigonal symmetry grains are:

$$K_V = [2(C_{11} + C_{12}) + 4C_{13} + C_{33}] / 9, \quad (5)$$

FIG. 3: Voigt and Reuss bounds and Hashin-Strikman bounds on bulk and shear moduli for Kimizuka *et al.* (2007) $P = 0$ GPa simulation data on B constants. VRH estimates both lie inside the HS bounding rectangle.

and

$$K_R = \frac{[C_{33}(C_{11} - C_{66}) - C_{13}^2]}{3G_{eff}^v}, \quad (6)$$

where

$$G_{eff}^v = (C_{11} + C_{33} - 2C_{13} - C_{66})/3, \quad (7)$$

and

$$G_{eff}^r = \frac{[C_{33}(C_{11} - C_{66}) - C_{13}^2]}{3K_V}. \quad (8)$$

FIG. 4: Voigt and Reuss bounds and Hashin-Shtrikman bounds on bulk and shear moduli for Kimizuka *et al.* (2007) $P = 10$ GPa simulation data on B constants. VRH estimates both lie outside the HS bounding rectangle.

Note that an identity apparent from the formulas in (6) and (8) is given by

$$K_R G_{eff}^v = K_V G_{eff}^r \quad (9)$$

also holds and is sometimes useful in simplifying the analysis.

The shear moduli G_{eff}^r and G_{eff}^v are two of the four moduli we call the auxiliary shear constants. To show their importance, first consider their roles in the definitions of the Voigt and Reuss averages for effective shear modulus. We have

$$G_V = \frac{1}{5}(G_{eff}^v + 2\mu_- + 2\mu_+) \quad (10)$$

FIG. 5: Voigt and Reuss bounds and Hashin-Strikman bounds on bulk and shear moduli for Kimizuka *et al.* (2007) $P = 20$ GPa simulation data on B constants. VRH estimates both lie outside the HS bounding rectangle.

and

$$G_R = \left[\frac{1}{5} \left(\frac{1}{G_{eff}^r} + \frac{2}{\mu_-} + \frac{2}{\mu_+} \right) \right]^{-1}. \quad (11)$$

Because of the suggestive forms of the two preceding equations, (*i.e.*, being Voigt- and Reuss-like averages of four shear effective moduli), it seems natural to think of these four constants G_{eff}^v , G_{eff}^r , μ_+ , and μ_- as *effective component shear moduli* of the overall isotropic granular material. We term these four constants collectively the four “auxiliary constants,” and they appear repeatedly in the analysis that follows.

The forms of the two remaining auxiliary shear parameters used in (10) and (11) are

FIG. 6: Voigt and Reuss bounds and Hashin-Strikman bounds on bulk and shear moduli for Kimizuka *et al.* (2007) $P = 0$ GPa simulation data on C constants. VRH estimates both lie inside the HS bounding rectangle.

defined by:

$$\mu_+ = \frac{1}{2}[C_{44} + C_{66} + ([C_{44} - C_{66}]^2 + 4C_{14}^2)^{1/2}] \quad (12)$$

and

$$\mu_- = \frac{1}{2}[C_{44} + C_{66} - ([C_{44} - C_{66}]^2 + 4C_{14}^2)^{1/2}]. \quad (13)$$

For isotropic systems, these two constants both reduce to the unique isotropic shear modulus, as do both G_{eff}^r and G_{eff}^v . It is also sometimes useful to recall that for trigonal symmetry there are two general inequalities that are pertinent, which are:

$$\max(C_{44}, C_{66}) \leq \mu_+ \quad (14)$$

FIG. 7: Voigt and Reuss bounds and Hashin-Shtrikman bounds on bulk and shear moduli for Kimizuka *et al.* (2007) $P = 10$ GPa simulation data on C constants. VRH estimates both lie outside the HS bounding rectangle.

and

$$\mu_- \leq \min(C_{44}, C_{66}). \quad (15)$$

Furthermore, we note that sometimes (but only known so far for special cases discussed in other papers of the author — for carbonates) we have the inequalities : $\mu_- \leq G_{eff}^r \leq G_{eff}^v \leq \mu_+$ in particular applications. Such relationships can be useful to our algorithm for evaluating the HS bounds.

Algorithms for determining the HS bounds on bulk and shear moduli for granular composites with grains having trigonal symmetry were originally derived by Peselnick and Meister

FIG. 8: Voigt and Reuss bounds and Hashin-Strikman bounds on bulk and shear moduli for Kimizuka *et al.* (2007) $P = 20$ GPa simulation data on C constants. VRH estimates both lie outside the HS bounding rectangle.

(1965), refined by Watt and Peselnick (1980), and then applied extensively by Watt (1986).

The remaining four parameter types appearing in Section 3 are defined in terms of two pairs of parameters $K_{\pm}$ and $G_{\pm}$ given first by

$$K_{\pm} = \frac{K_V(G_{eff}^r - G_{\pm})}{G_{eff}^v - G_{\pm}}. \quad (16)$$

For trigonal symmetry, we must determine the values of $G_{\pm}$ within the ranges

$$\max(G_{eff}^v, \mu_+) = \mu_+ \leq G_+ \leq \infty, \quad (17)$$

and

$$0 \leq G_- \leq \min(\mu_-, G_{eff}^r) = \mu_- \quad (18)$$

in order to evaluate the HS bounds.

In some of the cases considered here, the lower bound on G_+ as given by maximum relation on the left of (17) can be satisfied by G_{eff}^v . However, when this happens the upper HS bound on the shear modulus is difficult to determine precisely because taking the value $G_+ = G_{eff}^v$ results in a singularity in the usual HS bounding formulas. One possible solution to this problem is to take $G_+ \rightarrow \infty$ instead, which gives a trial result that $G_{HS}^+ \rightarrow G_V$, which is just the Voigt estimate for shear modulus, and therefore the resulting estimate is gives no improvement over Voigt's well-known result. In the cases when this occurs, it nevertheless may often seem to be a reasonable choice since all the values for these shear estimators are then quite close together, while still all well-justified. The better alternative however may be always to make the choice $G_+ \equiv \mu^+$. This substitution removes the singularity while also providing an improvement over the Voigt estimator G_V . Examples presented here where this situation arises include Table 4c for $P = 10$ and 20 GPa, and also Table 6c for $P = 10$ and 20 GPa. However, there is never any corresponiding issue of this type for the bulk modulus upper bound.

As already mentioned, it is also easy to see that taking $G_+ \rightarrow \infty$ gives $K_+ = K_V$. Similarly, it is not hard to show that taking $G_- \rightarrow 0$ gives $K_- = K_R = K_V G_{eff}^r / G_{eff}^v$. So the desired optimal Hashin-Shtrikman bounds are produced with $G_{\pm}$ values in the mid-range. It is also important to understand that the $K_{\pm}$ are not the actual bounds, but rather parameters needed to compute the bounds on $K_{HS}^{\pm}$ in (23) and (24), which follow.

Values for the various auxiliary parameters pertinent to the trigonal examples being presented are displayed in TABLE 2A, 4A, and 6A.

Then, the remaining parameters dependent on $K_{\pm}$ and $G_{\pm}$ can also be found by first computing the following eight additional parameters:

$$\alpha_{\pm} = \frac{-1}{K_{\pm} + 4G_{\pm}/3}, \quad (19)$$

and

$$\beta_{\pm} = \frac{2\alpha_{\pm}}{15} - \frac{1}{5G_{\pm}} = -\frac{1}{5} \left[\frac{1}{G_{\pm}} + \frac{2}{3K_{\pm} + 4G_{\pm}} \right], \quad (20)$$

and

$$\gamma_{\pm} = \frac{1}{9} (\alpha_{\pm} - 3\beta_{\pm}), \quad (21)$$

and

$$\zeta_{\pm} = \frac{G_{\pm}}{6} \left(\frac{9K_{\pm} + 8G_{\pm}}{K_{\pm} + 2G_{\pm}} \right). \quad (22)$$

The Hashin-Shtrikman bounds for bulk modulus are then given by

$$K_{HS}^{\pm} = \frac{K_V(G_{eff}^r + \zeta_{\pm})}{G_{eff}^v + \zeta_{\pm}}. \quad (23)$$

Similarly, although the formulas are clearly more complicated, the Hashin-Shtrikman bounds for shear modulus are again determined by a formula:

$$\frac{1}{G_{HS}^{\pm} + \zeta_{\pm}} = \frac{1}{5} \left[\frac{1 - \alpha^{\pm}(K_V - K_{\pm})}{G_{eff}^v + \zeta_{\pm} + (\alpha_{\pm}/2\beta_{\pm})(K_V - K_{\pm})} + \frac{2}{\mu_{-} + \zeta_{\pm}} + \frac{2}{\mu_{+} + \zeta_{\pm}} \right]. \quad (24)$$

We have made use of the auxiliary constants μ_{+} and μ_{-} from (12) and (13), as well as the pair of very useful identities (7) and (8) for G_{eff}^v and G_{eff}^r when evaluating (23) and (24).

A self-consistent version of these equations is found approximately (using our present definition) by replacing the $\pm$ expressions everywhere with *sca* (*i.e.*, for self-consistent average) and simply averaging the two Hashin-Shtrikman bounds for bulk modulus, and similarly for the shear modulus. To solve the fully *SC* equations completely (including the coupling to shear modulus) requires an iteration procedure (Berryman, 2005) that could start at either the lower bounds, or the upper bounds, or anywhere in between. As explained here in the main text, this self-consistency procedure may not be necessary however in practice for many problems being considered, because the iterated self-consistent values have generally been found to lie very close (about $\pm 1\%$) to the same values as the arithmetic means of the upper and lower Hashin-Shtrikman bounds, which themselves can be found directly for both the bulk modulus and the shear modulus using definite formulas that therefore do not require either iteration or searching.

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