Combining Analysis of Random Elastic Polycrystals with Poroelasticity for Granular Composites having Porous Grains and Fluid-Filled Pores

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Abstract

Analysis of random polycrystals has typically been applied to solid grains of anisotropic elastic materials. Poroelastic analysis has typically been applied to otherwise isotropic systems with pores having a variety of shapes and filled with fluids. Present effort is focused on combining these two types of geomechanical analyses by treating anisotropic poroelastic grains jumbled together to form an overall polycrystalline poroelastic material. This problem is approximately twice as difficult to solve as the typical elastic polycrystal problem because the polycrystal analysis must be carried through twice: once for the drained (pore-fluid free to escape) constants, and again for the undrained (pore-fluid trapped) poroelastic constants.

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1. Introduction

Poroelastic analysis [1–7] considers the range of responses possible in fluid-saturated porous earth materials when mechanical, seismic, acoustical, ultrasonic or other types of applied stresses are acting on such systems. The inherent symmetries of pertinent poroelastic systems are often transversely isotropic if the entire sample or region to be studied is layered; or they could be more complicated due to various geological processes, in which case one of the most general cases often considered for analysis purposes could be that of orthotropic symmetry [7].

While the well-known Voigt [8] and Reuss [9] bounds, and the Voigt-Reuss-Hill [10] elastic constant estimators for random polycrystals are all easily calculated once the elastic constants of anisotropic crystals are known, the Hashin-Shtrikman bounds [11] and related self-consistent [12] estimators for the same constants are comparatively more difficult to compute. Some recent work [13,14] has shown how to simplify these harder to compute estimators to some extent. The present discussion gives an overview with the main new point being to show how this extra work does provide added value, since — in particular — the well-known Voigt-Reuss-Hill estimators often do *not* fall within the Hashin-Shtrikman bounds, but the self-consistent estimators (for good reasons [15]) have always been found to do so.

Estimators termed "self-consistent" can take a variety of forms, and not all of these forms are equivalent or equally valid. In particular, Hill's version of self-consistency is not the same as the ones that are based on physical arguments and scatterng theory such as the ones that are sometimes called the "coherent potential approximation," including Soven [16], Taylor [17], Gubernatis and Krumhansl [18], Berryman [19], and Olsen and Avellaneda [20]. This class of approximations is one considered specifically by Willis [15], and is one that seems to give reliable results – by which statement we mean to imply in part that the results have been found to be consistent with rigorous bounds. A related class of approximations, also called "self-consistent," is discussed by Kanaun and Levin [21].

Earlier work on Hashin-Shtrikman bounds or on self-consistent estimators has concentrated mostly on one or the other of these approaches, without making an effort to compare, contrast, and/or mutually validate them. Some recent work of the author [13,14] has addressed some of these issues, including the orthorhombic case that will be the main emphasis

here.

In outline, the paper first introduces the poroelastic analysis and then the polycrystal problem. Section 2 treats the poroelastic analysis. Sections 3 and 4 emphasize the drained (fluid freely flowing) and undrained (trapped fluid) constants. Section 5 then introduces the orthotropic polycrystal problem. Section 6 presents the mathematical formulation needed to analyze the bounds and estimators for the polycrystal problems. Section 7 presents an overview of the polycrystal results including results for seven examples, and also some comparisons among both the rigorous and the approximate methods. Section 8 then makes use of the self-consistent polycrystal results by treating these bulk and shear modulus values as effective grain constants. Using these results, it is straightforward to estimate drained constants for specific materials when some assumption is made about shapes and density of cracks within these average grains. Then, it is also possible to estimate undrained constants. Section 9 gives an overview of the various results obtained here, and finally summarizes our conclusions.

2. Analysis of Anisotropic Poroelastic Grains

Consider that each poroelastic grain is anisotropic due to some nonrandom alignment of the solid constituents and/or to the presence of oriented pores or fractures. We consider the orthorhombic anisotropic version of the poroelastic equations:

$$\begin{pmatrix} e_{11} \\ e_{22} \\ e_{33} \\ -\zeta \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} & -\beta_1 \\ S_{12} & S_{22} & S_{23} & -\beta_2 \\ S_{13} & S_{23} & S_{33} & -\beta_3 \\ -\beta_1 & -\beta_2 & -\beta_3 & \gamma \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ -p_f \end{pmatrix}. \tag{1}$$

The e_{ii} (no summation over repeated indices) are strains in the $i = 1, 2, 3$ directions. The σ_{ii} are the corresponding stresses. The fluid pressure is p_f. The increment of fluid content is ζ, which (like the strains) is dimensionless. The drained (fluid is not trapped) compliances are $S^d_{ij} \equiv S_{ij}$. The drained Reuss average bulk modulus [9] is defined via

$$\frac{1}{K^d_R} \equiv \sum_{ij=1,2,3} S^d_{ij}, \tag{2}$$

a quantity which is what one commonly takes to be the definition of the bulk modulus of such a simple (non-heterogeneous) anisotropic system. The corresponding undrained

compliances will be symbolized by S^u_{ij}. For the Reuss average undrained bulk modulus K^u_R, we have drained compliances replaced by undrained compliances in a formula otherwise identical in form to (2). Off-diagonal coefficients $\beta_i = S_{i1} + S_{i2} + S_{i3} - 1/3K^g_R$, where K^g_R is again the Reuss average modulus of the grains, *i.e.*, simply replace d's with g's in (2) to determine K^g_R. The alternative Voigt [8] average (also see Hill [10]) of the stiffnesses will play no role in this discussion. And, finally, coefficient $\gamma = \sum_{i=1-3} \beta_i/B$ in (1), where B is the second Skempton [2] coefficient, which will be defined shortly.

The shear terms due to twisting motions (*i.e.*, strains e_{23}, e_{31}, e_{12} and stresses σ_{23}, σ_{31}, σ_{12}) are excluded from this part of the presention because they typically do not couple to the modes of interest for anisotropic systems having orthotropic symmetry, or to more symmetric systems such as those having transversely isotropic or isotropic symmetry.

Summing the off-diagonal coefficients β_i, we find

$$\beta_1 + \beta_2 + \beta_3 = \frac{1}{K^d_R} - \frac{1}{K^g_R} = \frac{\alpha_R}{K^d_R}, \tag{3}$$

where we introduce (similar to the isotropic case) a Reuss effective stress coefficient: $\alpha_R \equiv 1 - K^d_R/K^g_R$. Furthermore, we have

$$\gamma = \frac{\beta_1 + \beta_2 + \beta_3}{B} = \frac{\alpha_R}{K^d_R} + \phi\left(\frac{1}{K_f} - \frac{1}{K^g_R}\right), \tag{4}$$

since a rigorous definition in this notation by Berryman [7] for the Skempton [2] B coefficient is given by

$$B \equiv \frac{1 - K^d_R/K^u_R}{1 - K^d_R/K^g_R} = \frac{\alpha_R/K^d_R}{\alpha_R/K^d_R + \phi(1/K_f - 1/K^g_R)}. \tag{5}$$

Another related formula that will prove very useful to us later is:

$$K^u_R = \frac{K^d_R}{1 - \alpha_R B}, \tag{6}$$

for undrained modulus.

More general versions [4] of the B definition include another bulk modulus for pore response that differs from the grain response if the medium consists of a more heterogeneous collection of grains and/or pores, not being included within our current scope. (But see Brown and Korringa [4] for a thorough discussion of this point. We will also return briefly to this issue in the final technical section of the paper.) With this one caveat, all these formulas presented are rigorous statements based on anisotropic analysis. Appearances of Reuss average quantities K^d_R and α_R are rigorous statements, not approximations (except

for already noted limitations). The specific choices of notation made will also help us to emphasize the similarity between rigorous anisotropic and isotropic formulas, such as those of Gassmann [1].

3. Off-Diagonal Poroelastic Coefficients β_i

Results follow for the off-diagonal β_i coefficients. Then, a general proof of their correctness is presented. The coefficients β_i are determined by

$$\beta_i = S^d_{i1} + S^d_{i2} + S^d_{i3} - \frac{1}{3K^g_R}, \tag{7}$$

where K^g_R is the Reuss average of the grain modulus. Equation (7) holds for homogeneous grains, such that $K^g_R = K^g$. However, when the grains themselves are anisotropic, we also need to allow for this possibility by defining three directional grain bulk moduli determined using:

$$\frac{1}{3\overline{K}^g_i} \equiv S^g_{i1} + S^g_{i2} + S^g_{i3} = S^g_{1i} + S^g_{2i} + S^g_{3i}, \tag{8}$$

for $i = 1, 2, 3$. The second equality follows from symmetry of the compliance matrix. We call these quantities in (8) the partial grain-compliance sums, and the $\overline{K}^g_i$ are pertinent directional grain bulk moduli. Then, the formula in (7) may be replaced by

$$\beta_i = S^d_{i1} + S^d_{i2} + S^d_{i3} - \frac{1}{3\overline{K}^g_i}. \tag{9}$$

The preceding results are for perfectly aligned grains. If the grains are instead perfectly randomly oriented, then it is clear that the formulas in (7) hold as before, but now the definition of the Reuss average grain bulk modulus K^g_R must be reformulated in analogy to (2).

All of these statements about the β_i's are easily proven by considering a particular combination of the applied stresses, such that $\sigma_{11} = \sigma_{22} = \sigma_{33} = -p_c = -p_f$. Then, from (1), we have:

$$\begin{aligned} -e_{ii} &= \left(S^d_{i1} + S^d_{i2} + S^d_{i3}\right) p_c + \beta_i(-p_f) \\ &= \left(S^g_{i1} + S^g_{i2} + S^g_{i3}\right) p_f \equiv \tfrac{p_f}{3\overline{K}^g_i} \end{aligned}, \tag{10}$$

in the most general of the cases to be discussed. This result holds true for each value of $i = 1, 2, 3$. This statement about the strain e_{ii} (no sum over i) would always hold in the situation considered, as it must be the same if these anisotropic (or inhomogeneous) grains

are immersed in fluid, while measurements are taken of strains observed in each of the three directions $i = 1, 2, 3$, during variations of this uniformly applied pressure p_f. This argument is analogous to ones given by Biot and Willis [3] for isotropic, homogeneous examples.

The relationship of coefficient γ to the other coefficients is easily established because the main issue involves determining the role of the various other constants contained in the definition of Skempton's coefficient [2] B. Again, from (1), we find that

$$-\zeta = 0 = -\left(\beta_1 + \beta_2 + \beta_3\right)\sigma_c - \gamma p_f, \tag{11}$$

for undrained boundary conditions. We find that

$$\frac{p_f}{p_c} \equiv B = \frac{\beta_1 + \beta_2 + \beta_3}{\gamma}, \tag{12}$$

where $p_c = -\sigma_c$ is the external confining pressure. Thus, the scalar coefficient γ is determined uniquely, and given by

$$\gamma = \frac{\beta_1 + \beta_2 + \beta_3}{B} = \frac{\alpha_R / K_R^d}{B} = \alpha_R / K_R^d + \phi\left(\frac{1}{K_f} - \frac{1}{K_R^g}\right). \tag{13}$$

This formula also provides an alternative (but nevertheless equivalent) definition of Skempton's second coefficient:

$$B = \frac{\alpha_R}{\gamma K_R^d}, \tag{14}$$

although this special result is limited to systems having homogeneous grains.

4. Undrained Compliance Matrix S_{ij}^u

The undrained compliance matrix S_{ij}^u can be determined easily now. A general condition for undrained behavior is given by:

$$-\zeta = 0 = -(\beta_1\sigma_{11} + \beta_2\sigma_{22} + \beta_3\sigma_{33}) - \gamma p_f, \tag{15}$$

which relates the undrained p_f to all the values of the applied external stresses σ_{11}, σ_{22}, and σ_{33}. Then, (1) is replaced by

$$\begin{pmatrix} e_{11} \\ e_{22} \\ e_{33} \end{pmatrix} = \begin{pmatrix} S_{11}^d & S_{12}^d & S_{13}^d & -\beta_1 \\ S_{12}^d & S_{22}^d & S_{23}^d & -\beta_2 \\ S_{13}^d & S_{23}^d & S_{33}^d & -\beta_3 \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ -p_f \end{pmatrix}, \tag{16}$$

where $p_f = -(\beta_1\sigma_{11} + \beta_2\sigma_{22} + \beta_3\sigma_{33})/\gamma$ from (15). Rewriting this expression in its most intuitive form gives:

$$\begin{pmatrix} e_{11} \\ e_{22} \\ e_{33} \end{pmatrix} = \begin{pmatrix} S^u_{11} & S^u_{12} & S^u_{13} \\ S^u_{12} & S^u_{22} & S^u_{23} \\ S^u_{13} & S^u_{23} & S^u_{33} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \end{pmatrix}, \tag{17}$$

where

$$S^u_{ij} = S^d_{ij} - \frac{\beta_i\beta_j}{\gamma}. \tag{18}$$

To distinguish drained (d) and undrained (u) compliances, we have added superscripts accordingly. Compliances without superscripts are always assumed to be drained, so $S_{ij} = S^d_{ij}$.

5. Analysis of Random Polycrystals Composed of Orthotropic Elastic Meterials

Now we briefly review random polycrystal analysis. We use the common convention of reducing elastic tensors to 6×6 matrices using the Voigt prescription:

$$\begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \epsilon_{23} \\ \epsilon_{13} \\ \epsilon_{12} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & S_{13} & & & \\ S_{12} & S_{22} & S_{23} & & & \\ S_{13} & S_{23} & S_{33} & & & \\ & & & S_{44} & & \\ & & & & S_{55} & \\ & & & & & S_{66} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix}. \tag{19}$$

Again, the σ_{ij}'s are the stresses, and the ϵ_{ij}'s are the strains, for $i, j = 1, 2, 3$, corresponding respectively to spatial axes x, y, z. Compliances are symmetric, so $S_{21} = S_{12}$, etc. And we consider orthotropic symmetry, which is not the most general case, but one case frequently treated in practice. The elastic compliances S_{44}, S_{55}, S_{66} are those for the twisting shear strains: ϵ_{23}, ϵ_{13}, ϵ_{12}, and their related stresses. For isotropic elastic materials, the stiffness (inverse of compliance) moduli satisfy $C_{11} = C_{22} = C_{33} = \lambda + 2\mu$, $C_{44} = C_{55} = C_{66} = \mu$, and $C_{12} = C_{13} = C_{23} = \lambda$, where λ and μ are the two Lamé constants, and the isotropic bulk and shear moduli are given (but only in the isotropic case) by $K = \lambda + 2\mu/3$ and $G = \mu$, respectively.

It is well-understood that, for such orthorhombic media, there are typically only three simple eigenvectors and eigenvalues, and these are the ones associated again with the twisting

shear modes and the compliances, namely S_{44}, S_{55}, and S_{66}, corresponding to rotations about spatial axes x, y, z, respectively. There are also three eigenmodes associated with the 3×3 submatrix in the upper lefthand corner of the full elastic matrix. However, these modes are not related in any simple way either to pure compression/extension or to pure shear modes. It follows that our analysis of effective moduli such as effective bulk and shear modulus of polycrystals requires understanding a rather complex relationship between the simpler ideas of a bulk modulus for pure compression or extension, and a shear modulus for one of the five potentially distinct shear modes of any elastic material. The resulting mixing of the modes is the main cause of any difficulties we may have when analyzing the average modal behavior of (by assumption) perfectly isotropic polycrystals (on average), and therefore makes use of the comparatively tedious methods under discussion. Most studies of such systems are aimed at quantifying the behavior of random polycrystals — where the word "random" as used in this context usually implies that the polycrystals are composed of a large number of small crystallites typically oriented arbitrarily in space so the overall polycrystalline behavior is either isotropic or sufficiently close to isotropic for most purposes. The resulting effective isotropic constants can then be chosen to be effective bulk K and shear G moduli.

The main goal of the rest of this paper will therefore be to find ways of estimating these bulk and shear moduli of such an overall isotropic average medium. The means we use to quantify these constants are rigorous bounds, and approximate theoretical estimators.

6. Bounds and Estimators

Results of Watt [22] for bounds on bulk modulus bounds $K_{HS}^{\pm}$ and those of Middya and Basu [23] for self-consistent estimates K_{SC}^{*} of bulk modulus can both be written in virtually the same form:

$$K_{HS}^{\pm} = K_{\pm} + \frac{3B_1^{\pm} + 2B_2^{\pm}}{3 + \alpha^{\pm}(3B_1^{\pm} + 2B_2^{\pm})}, \tag{20}$$

where

$$3B_1^{\pm} + 2B_2^{\pm} = \frac{9(K_V - K_{\pm}) + 2\beta_{\pm}(d^{\pm} + e^{\pm} - c^{\pm}) + 3\beta_{\pm}^2\Omega^{\pm}}{1 - a^{\pm}\beta_{\pm} - 9\gamma_{\pm}(K_V - K_{\pm}) + D_{\pm}}. \tag{21}$$

The coefficients $a_{\pm}$, $b_{\pm}$, $c_{\pm}$, $d_{\pm}$, $e_{\pm}$ are defined here (see the Appendix). The coefficients $\alpha_{\pm}$, $\beta_{\pm}$, $\gamma_{\pm}$ are defined below following Eq. (28). $\Omega^{\pm}$ is defined in (34) and (35). For self-consistency, simply replace the subscripts or superscripts $\pm$ with either $*$'s or SC symbols as desired, while also removing the HS (and/or PM) subscripts.

The denominator of expression (21) is the same as the denominator of the first term in

$$\begin{aligned} 15B_2^{\pm} &= \tfrac{a^{\pm}-b^{\pm}+\beta_{\pm}(2d^{\pm}-2c^{\pm}-e^{\pm})+3\gamma_{\pm}(d^{\pm}-c^{\pm}+e^{\pm})+\alpha_{\pm}\beta_{\pm}\Omega^{\pm}}{1-a^{\pm}\beta_{\pm}-9\gamma_{\pm}(K_V-K_{\pm})+D_{\pm}} \\ &+ 3(G_{\pm}+\zeta_{\pm})^2\left(\tfrac{3}{G_{\pm}+\zeta_{\pm}}-\tfrac{1}{C_{44}+\zeta_{\pm}}-\tfrac{1}{C_{55}+\zeta_{\pm}}-\tfrac{1}{C_{66}+\zeta_{\pm}}\right), \end{aligned} \tag{22}$$

and $D_{\pm}$ is defined in

$$D_{\pm} = \beta_{\pm}(\beta_{\pm}+2\gamma_{\pm})(c^{\pm}-d^{\pm}) - 2e^{\pm}\beta_{\pm}\gamma_{\pm} - \frac{\alpha_{\pm}\beta_{\pm}^2\Omega_{\pm}}{3}. \tag{23}$$

The Voigt average of the bulk modulus is

$$K_V = \frac{1}{9}\left[C_{11}+C_{22}+C_{33}+2(C_{12}+C_{23}+C_{13})\right]. \tag{24}$$

Similarly, the Voigt average of the shear modulus is

$$G_V = \frac{1}{15}\left[C_{11}+C_{22}+C_{33}-C_{12}-C_{23}-C_{13}+3(C_{44}+C_{55}+C_{66})\right]. \tag{25}$$

For completeness, we also note that the corresponding Reuss averages [2] for orthorhombic crystals are given by

$$\frac{1}{K_R} = (S_{11}+S_{22}+S_{33}) + 2\left(S_{23}+S_{31}+S_{12}\right) \tag{26}$$

and

$$\frac{15}{G_R} = 4\left(S_{11}+S_{22}+S_{33}\right) - 4\left(S_{23}+S_{31}+S_{12}\right) + 3\left(S_{44}+S_{55}+S_{66}\right), \tag{27}$$

where the S_{ij}'s are the compliance matrix elements, related to the stiffness matrix elements by the matrix equation $\mathbf{S} = \mathbf{C}^{-1}$.

The equation corresponding to bulk modulus K result (20) for the shear modulus G is given by

$$G_{PM}^{\pm} = G_{\pm} + \frac{B_2^{\pm}}{1+2\beta_{\pm}B_2^{\pm}}, \tag{28}$$

where PM indicates the contribution of Peselnick and Meister [24], who were early evaluators of the pertinent HS bounds. The Hashin-Shtrikman bounds themselves are then given exactly by $K_{HS}^{\pm} \equiv K_{PM}^{\pm}$ and $G_{HS}^{\pm} \equiv G_{PM}^{\pm}$. Again K_V is the Voigt average of bulk modulus. Definitions of another useful shear factor G_{eff}^{v} depend on the specific crystal symmetry under consideration (see Refs. [13, 14] for specifics).

Factor $B_2^{\pm}$ itself was defined in (22).

Parameters $\alpha_\pm$ and $\beta_\pm$ appear repeatedly above and can be related to Eshelby [25] results by rewriting them in the forms:

$$-\frac{1}{\alpha_\pm} = K_\pm + 4G_\pm/3 \tag{29}$$

and

$$-\frac{1}{2\beta_\pm} = G_\pm + \zeta_\pm. \tag{30}$$

Another combination of these two frequently appearing in the formulas is

$$\gamma_\pm \equiv \frac{\alpha_\pm - 3\beta_\pm}{9}. \tag{31}$$

Using these definitions, we find that:

$$\frac{1}{K_{HS}^\pm + 4G_\pm/3} = \frac{1 - (B_1^\pm + 2B_2^\pm/3)/(K_\pm + 4G_\pm/3)}{K_\pm + 4G_\pm/3}, \tag{32}$$

which is valid for orthorhombic and some more symmetric crystal structures, such as hexagonal, tetragonal, and trigonal. Eq. (32) may then be compared to the analogous shear formula given by

$$\frac{1}{G_{PM}^\pm + \zeta_\pm} = \frac{1 - B_2^\pm/(G_\pm + \zeta_\pm)}{G_\pm + \zeta_\pm}, \tag{33}$$

which is valid for the same crystal symmetries, with (32) and (33) being analogous forms respectively for the bulk and shear moduli.

As previously noted, these equations are for the upper and lower bounds $K_{HS}^\pm$ on the bulk modulus. Resulting bounds are obtained when the constraints are optimal. Then the determinant of the matrix $X^\pm$ is given by

$$\Omega^\pm \equiv \det\left(X^\pm\right) = X_{11}^\pm X_{22}^\pm X_{33}^\pm + 2X_{12}^\pm X_{23}^\pm X_{13}^\pm - X_{11}^\pm \left(X_{23}^\pm\right)^2 - X_{22}^\pm \left(X_{13}^\pm\right)^2 - X_{33}^\pm \left(X_{12}^\pm\right)^2, \tag{34}$$

and we must have $\Omega^\pm = \det(X^\pm) \equiv 0$. Here $X^\pm$ is a 3×3 positive- or negative-semi-definite matrix, as defined by

$$\begin{aligned} X_{11}^\pm &= C_{11} - K_\pm - \tfrac{4}{3}G_\pm,\ X_{12}^\pm = C_{12} - K_\pm + \tfrac{2}{3}G_\pm, \\ X_{22}^\pm &= C_{22} - K_\pm - \tfrac{4}{3}G_\pm,\ X_{13}^\pm = C_{13} - K_\pm + \tfrac{2}{3}G_\pm, \\ X_{33}^\pm &= C_{33} - K_\pm - \tfrac{4}{3}G_\pm,\ X_{23}^\pm = C_{23} - K_\pm + \tfrac{2}{3}G_\pm. \end{aligned} \tag{35}$$

Vanishing of $\det(X)$ is a necessary requirement because then, and only then, have we found either the greatest lower bound, or the smallest upper bound.

Middya and Basu [23] have already shown these same equations can be used to determine self-consistent estimates, as well as the bounds. Self-consistent values are determined specifically by considering two conditions: $B_2 = 0$ and $3B_1 + 2B_2 = 0$. Both conditions must apply simultaneously if the self-consistency conditions are to be satisfied. And so, it follows that $B_1 = 0$; but we never need to impose this condition on B_1 separately. The self-consistency conditions are therefore (obviously) given by:

$$K_{SC} = K^* \qquad \text{and} \qquad G_{SC} = G^*, \tag{36}$$

where the conditions that determine the values of K^* and G^* are exactly the ones that guarantee the two factors B_1 and B_2 to vanish simultaneously. Although this simultaneity condition might sound hard to achieve, it has been found in practice to be very easy to satisfy by applying an iterative process wherein some initial K_0 and G_0 values are first chosen and substituted into (32) and (28) for the $K_\pm$ and $G_\pm$ values. The results that are next obtained for the left-hand-sides of both these equations then become the new trial values for K_0 and G_0. Repeating this process has always been found to converge quickly as long as some reasonably intelligent choices are made for the initial values of K_0 and G_0. So this part of the overall search procedure is not difficult to implement in practice.

Determining the HS bounds from this same set of equations is harder by comparison, but some tricks were developed in previous work of the author [14] that made the computational process more efficient. This work will be only briefly elaborated. In particular, a useful "shooting method of optimization" (which makes use of the computed values of the self-consistent estimates in order to speed up the search for HS bounds) was developed previously to streamline the algorithm used to produce the Hashin-Shtrikman bounds [11, 13, 14, 22]. We refer the interested reader in particular to Ref. [14] for more details of this approach. The basic outline is this: Having already computed the pertinent self-consistent values, and knowing the Reuss and Voigt bounds on both K and G, we scan from the simple bounding values towards the SC point. We then take care to observe where sign changes in these functionals occur. In this way, the optimal bounds (those closest) to the SC estimates can be quickly determined.

7. Discussion of Bounds and Estimators

A variety of other bounds and estimators are found in the literature [27-30] in addition to the ones that we discuss here in detail.

Although we consider (in this section) only seven specific examples in the following analysis of the bounds and estimates, we are nevertheless able to show that a number of rather plausible hypotheses about possible relationships between and among the various bounds and estimates can be quickly excluded via specific counterexamples. The numerical values of the various bounds and estimates for the cases considered are summarized in Table 1.

First, we correctly anticipate that the self-consistent (SC) estimates always lie inside the Hashin-Shtrikman (HS) bounds. This expectation follows from the form of the equations for the self-consistent approximation, being based as they are — here for orthorhombic materials only — on essentially the same equations as those for the HS bounds. However, a further hypothesis (which might have seemed reasonable) that the SC estimates could always lie at or near the center of the HS bounding region is quickly disproven. Of these seven orthorhombic examples considered, six produce results close to an edge of the HS bounding box. Only for Danburite among the examples computed do the SC estimates appear to be nearly centered in the HS bounding box. In all six of the remaining cases, the SC estimates lie either on or very near to a point on the boundary of the HS bounding box.

Another general observation is that the *relative differences* between the SC estimates and the VRH estimates for these five orthorhombic materials are quantitatively small, *i.e.*, typically being fractions of 1%. This fact suggests that, for applications not requiring very high precision estimates, the VRH estimates will continue to be of some value.

Among all the cases considered here, only Danburite has the SC point well-centered within the HS bounding box.

8. Drained and Undrained Constants for Fractured Poroelastic Polycrystalline Systems

In order to complete our generalization of the polycrystalline analysis to poroelastic systems, we need to find ways to compute both drained and undrained constants for these systems. Similarly, Berryman and Grechka [36] discuss related issues for fractured systems

without fluids, which case is essentially the same as that for drained poroelastic systems. If G^g and K^g are the bulk and shear grain moduli for the nonporous (polycrystalline) system (in our examples these would correspond to the self-consistent values of G and K [37-39]), and G^d and K^d are the effective isotropic drained moduli when cracks or pores are present. Then we have respectively

$$\frac{1}{G^d} - \frac{1}{G^g} \simeq \frac{4\rho}{3}\eta_2 \tag{37}$$

and

$$\frac{1}{K^d} - \frac{1}{K^g} \simeq 2\rho\eta_2. \tag{38}$$

Here we have kept only the contributions from the second crack parameter η_2 in the pertinent expansions, because it is known that η_1 normally contributes less than a 5 percent correction, and η_3 and higher terms produce still smaller corrections.

The most significant factor η_2 itself can be determined independently within the noninteraction approximation (NIA) by

$$\eta_2 = \frac{8(1-\nu_0)(5-\nu_0)}{15G_0(2-\nu_0)}, \tag{39}$$

where $\nu_0 = (3K_0 - 2G_0)/2(3K_0 + G_0)$ is the pertinent value of Poisson's ratio. For this problem, the nonporous values obtained using the self-consistent method are the preferred numerical values that should be used.

Results for drained, undrained, and nonporous values are shown in Table 2. For easy reference, the values of η_2 used in producing Table 2 are displayed in Table 3.

The final step in the process of finding all the pertinent parameters for granular poroelastic systems is the one where we obtain the undrained constants from the drained constants. The formula for doing this is well-known to be:

$$K_R^u = \frac{K_R^d}{1 - \alpha_R B}, \tag{40}$$

where α_R is the Biot-Willis coefficient (4), B is Skempton's second coefficient (5), and K_R^d is the drained bulk modulus, which we have calculated above for these various materials in the preceding section. For a crack density $\rho = na^3$, we need to multiply by $(4\pi/3)\times$(aspect ratio) to determine the pertinent porosity. For $\rho = 0.1$, we find porosity $\phi \simeq 0.04$ for an aspect ratio of 0.1. We assume here that the pore-fluid is water, so $K_f = 2.25$ GPa.

In Table 2, we also display the ratio of the differences: drained to undrained over those from drained to nonporous. Results show that there are significant differences in these ratios,

both when comparing rsults for shear and bulk moduli for the same material, and also when comparing the results for different elastic materials.

9. Overview and Conclusions

To summarize: Once the full set of elastic constants for an orthorhombic material constituting the random elements of the composite is known, the easiest isotropic estimators to compute are always the Voigt and Reuss averages for both bulk and shear moduli. Among the typical estimators most workers might consider computing, the next easiest and most useful quantities to compute are the self-consistent estimates. These SC estimates can also be used to speed up the computation of the Hashin-Shtrikman bounds as shown previously [14], and observed again here. The self-consistent estimators themselves are very closely related to the HS bounds, and knowledge of the SC values is therefore useful in pinning down the optimal zeroes of the functionals needed to determine these HS bounds.

It is also possible to redo some of the analysis presented here using the popular differential scheme [39,40]. However, for the polycrystal analysis, it seems that Hashin-Shtrikman bounds and self-consistent estimates are very closely related estimators, and also somewhat easier to compute than differential scheme results. So the main reason to switch to a differential-scheme-based approach is likely to be in situations where it is known that the microstructure (of the actual materials to be studied) is better represented by the implicit microstructure of the differential scheme. With modern microtomography methods now being applied to rocks, such circumstances could easily arise in the near future [42].

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Appendix: Coefficients $a^{\pm} - e^{\pm}$

The remaining constants appearing in (22) are given by

$$\begin{aligned} a^{\pm} &= X^{\pm}_{11} + X^{\pm}_{22} + X^{\pm}_{33}, \qquad b^{\pm} = X^{\pm}_{12} + X^{\pm}_{23} + X^{\pm}_{13}, \\ c^{\pm} &= X^{\pm}_{11}X^{\pm}_{22} + X^{\pm}_{22}X^{\pm}_{33} + X^{\pm}_{33}X^{\pm}_{11}, \qquad d^{\pm} = \left(X^{\pm}_{12}\right)^2 + \left(X^{\pm}_{23}\right)^2 + \left(X^{\pm}_{13}\right)^2, \\ e^{\pm} &= X^{\pm}_{12}X^{\pm}_{13} + X^{\pm}_{13}X^{\pm}_{23} + X^{\pm}_{23}X^{\pm}_{13} - X^{\pm}_{11}X^{\pm}_{23} - X^{\pm}_{22}X^{\pm}_{13} - X^{\pm}_{33}X^{\pm}_{12}, \end{aligned} \tag{41}$$

where the $X^{\pm}$ matrix elements were defined in (35). [Note: The symbol $\pm$ always appears as a subscript for scalar quantities, except for the scalar Hashin-Shtrikman bounds themselves, where the bound label is used as a subscript. The symbol $\pm$ appears as a superscript for all quantities that are themselves matrix elements (therefore having additional subscripts), and for quantities that are combinations only of such matrix elements. For scalar quantities that are themselves combinations of scalars and also quantities derived from matrix elements, the subscript version is again used – except as already noted for the scalar bounds themselves.]

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TABLE 1. Comparisons of bounds and estimates for the bulk (K) and shear moduli (G) of polycrystals (composites of randomly oriented crystals of uniform type) for seven orthorhombic elastic materials: α-Uranium, Aragonite ($CaCO_3$), Danburite ($CaB_2Si_2O_8$), Enstatite ($MgSiO_3$), Forsterite (Mg_2SiO_4), Sulfur (S), and Topaz ($Al_2(F,OH)_2SiO_4$). Estimators shown are: Reuss lower bound (R), Hashin-Shtrikman lower bound (HS^-), Self-consistent estimate (SC^*), Hashin-Shtrikman upper bound (HS^+), and Voigt (V) upper bound, respectively, for both the bulk (K) and shear moduli (G). All effective constants are in units of GPa (gigapascal).

	K, G	R	HS^-	SC^*	HS^+	V
α-Uranium	K	111.3	112.5	112.7	113.1	114.6
	G	80.7	83.6	84.1	84.9	87.9
Aragonite	K	44.71	45.56	46.36	46.41	49.04
	G	36.62	37.56	38.31	38.35	40.41
Danburite	K	90.52	91.37	91.89	92.40	92.89
	G	62.47	63.50	64.27	65.06	65.87
Enstatite	K	107.29	107.65	107.83	107.83	108.29
	G	75.18	75.52	75.70	75.71	76.15
Forsterite	K	127.27	128.49	128.49	128.49	131.67
	G	79.54	80.35	80.35	80.89	82.58
Sulfur	K	17.56	18.76	18.85	18.87	20.60
	G	6.17	6.61	6.64	6.66	7.22
Topaz	K	166.19	167.37	167.46	167.73	168.67
	G	113.54	114.73	115.06	115.09	116.00

TABLE 2. Polycrystal constants for drained, undrained, and nonporous examples in units of GPa (gigapascal). The final column provides a measure of the relative importance of the changes in values from drained to undrained in comparison to those from drained to nonporous.

	K, G	Drained	Undrained	Nonporous (SC*)	$\frac{U-D}{N-D}$
α-Uranium	K	85.7	91.8	112.7	.226
	G	43.4	73.1	84.1	.730
Aragonite	K	36.3	38.4	46.36	.209
	G	16.3	32.6	38.31	.741
Danburite	K	70.2	79.1	91.89	.410
	G	56.1	58.3	64.27	.269
Enstatite	K	81.7	88.9	107.83	.276
	G	65.9	66.7	75.70	.008
Forsterite	K	95.2	104.7	128.49	.285
	G	70.1	71.3	80.35	.117
Sulfur	K	12.10	16.09	18.85	.591
	G	5.87	5.90	6.64	.039
Topaz	K	126.37	141.3	167.46	.339
	G	100.15	103.8	115.06	.245

TABLE 3. Values of η_2 used in computations for Table 2.

	η_2 (GPa^{-1})
α-Uranium	0.014
Aragonite	0.030
Danburite	0.017
Enstatite	0.015
Forsterite	0.014
Sulfur	0.149
Topaz	0.010

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