Stanford Exploration Project, Report 117, October 23, 2004, pages 1–174

Bounds on geomechanical constants for a model of heterogeneous reservoirs

James G. Berryman[1]

ABSTRACT

A well-known result due to Hill provides an exact expression for the bulk modulus of any multicomponent elastic composite whenever the constituents are isotropic and the shear modulus is uniform throughout. Although no precise analog of Hill's result is available for the opposite case of uniform bulk modulus and varying shear modulus, it is shown here that some similar statements can be made for shear behavior of random polycrystals composed of laminates of isotropic materials. This model is intended to incorporate characteristics that mimic geomechanical properties of heterogeneous earth reservoirs, including local layering due to sedimentary processes. In particular, the Hashin-Shtrikman-type bounds of Peselnick, Meister, and Watt for random polycrystals composed of hexagonal (transversely isotropic) grains are applied to our model of polycrystals of laminates. An exact product formula relating the Reuss estimate of bulk modulus and an effective shear modulus (of laminated grains composing the system) to products of the eigenvalues for quasi-compressional and quasi-uniaxial shear eigenvectors also plays an important role in the analysis of the overall shear behavior of the random polycrystal. When the bulk modulus is uniform in such a system, the equations are shown to reduce to a simple form that depends prominently on the uniaxial shear eigenvalue — as expected from physical arguments concerning the importance of uniaxial shear in these systems. Applications of the analytical results presented here include benchmarking of numerical procedures used for studying elastic behavior of complex composites, and estimating coefficients needed in up-scaled equations for elasticity and/or poroelasticity of heterogeneous reservoirs.

INTRODUCTION

In the course of analyzing a problem on fluid-dependence of shear modulus in poroelastic systems, the author (Berryman, 2004a) uncovered an unanticipated identity in elasticity that appears to have wider implications for many elastic systems and/or composites. The basic result states that for *any* hexagonal (or transversely isotropic) elastic system there is an exact product formula, namely, $6K_RG^V_{\text{eff}} = \omega_+\omega_-$, relating the Reuss estimate K_R of the bulk modulus times the Voigt estimate G^V_{eff} of the uniaxial part of the shear modulus to the product of the two system eigenvalues $\omega_\pm$ for quasi-compressional and quasi-shear modes. There is also

[1]**email:** berryman@sep.stanford.edu

a second product formula with the roles of the Reuss and Voigt averages reversed, but this second identity is somewhat less important as we shall see.

Our goal here will be to show how these facts help to remove in part (although only in one special, but nevertheless interesting, case) the asymmetry in the analysis of elastic composites resulting from the existence of Hill's well-known formula (Hill, 1963, 1964; Milton, 2002) for arbitrary elastic composites, showing that

$$K^* = \left[\sum_{n=1}^{N} \frac{f_n}{K_n + 4\mu/3}\right]^{-1} - 4\mu/3. \tag{1}$$

Here the bulk modulus of the n-th constituent is K_n, the shear modulus takes the same value $\mu_n = \mu$ for all $n = 1, \dots, N$, and the overall effective bulk modulus is K^*. The volume fractions f_n are all nonnegative, and add up to unity. In general there is in fact no corresponding relationship for the overall shear modulus μ^*, when instead the system has constant bulk modulus $K_n = K$ for all N constituents. But, nevertheless, the existence of formulas quite analogous to (1) for shear will be demonstrated for a model random polycrystal composed of laminated grains.

As always in the theory of composites, there are several clear limitations to the use of the analysis in practice: (a) the continuum hypothesis, (b) the implicit assumption of adequate separation of scales between sizes of grains and of the overall composite, and (c) an assumption of negligible porosity. The continuum hypothesis will clearly be violated if the grain sizes are too small, approaching nanometer sizes and below. The deviations expected in our case are similar to those observed in deviations from the Hall-Petch effect (Hall, 1951; Petch, 1953; Schiötz, 1998), *i.e.*, a softening of the composite as a function of decreasing grain size once the size is below some threshold. This effect is caused in part by a significant increase in grain-to-grain interface area (which is not accounted for by the present theory) in composites when the grains become too small. At still smaller grain sizes, atomic scale effects become important and the continuum theory must clearly fail. At the other extreme, if the grains are too large, then there may not be sufficient numbers of particles in the sample for the separation of scales between composite and grains to be adequate. This issue is related to the question of what is an adequate REV (representative elementary volume) (Bear, 1972; Bourbié, 1987; Drugan and Willis, 1996). If the grains are too large and, therefore, too few, the entire sample may not be large enough to serve as an adequate REV. Finally, when a polycrystal is constructed by assembling many crystalline grains, it is also important that very little porosity remain in the resulting polycrystal. It has been estimated (Berryman, 1994) that as little as 0.5% porosity in a composite is sufficient to make it important to include the porosity in the model. But, except to exclude it thus from consideration, porosity is not discussed here.

The next section introduces the notation and basic results used in the rest of the paper. The third section considers the case of constant bulk modulus, and shows that the Voigt and Reuss averages for shear modulus, although differing in their numerical values, nevertheless depend on simple averages of the shear modulus plus another average comparable to (1). The fourth section considers the general problem for bounds on the moduli of random polycrystals of laminates, with special emphasis on the Peselnick-Meister-Watt bounds (Peselnick and Meister, 1965; Watt and Peselnick, 1980). The discussion of the fifth section summarizes some practical conclusions about the analysis and also makes a comparison with a "self-consistent" estimate related to the bounds. Two technical Appendices summarize results used in the main text.

ELASTICITY OF LAYERED MATERIALS

We assume that a typical building block of the random system is a small grain of laminate material whose elastic response for such a transversely isotropic (hexagonal) system can be described by:

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & & & \\ c_{12} & c_{11} & c_{13} & & & \\ c_{13} & c_{13} & c_{33} & & & \\ & & & 2c_{44} & & \\ & & & & 2c_{44} & \\ & & & & & 2c_{66} \end{pmatrix} \begin{pmatrix} e_{11} \\ e_{22} \\ e_{33} \\ e_{23} \\ e_{31} \\ e_{12} \end{pmatrix}, \tag{2}$$

where σ_{ij} are the usual stress components for $i, j = 1-3$ in Cartesian coordinates, with 3 (or z) being the axis of symmetry (the lamination direction for such a layered material). Displacement u_i is then related to strain component e_{ij} by $e_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$. This choice of definition introduces some convenient factors of two into the $44, 55, 66$ components of the stiffness matrix shown in (2).

Although some of the results presented here are more general, we will assume for definiteness that this stiffness matrix in (2) arises from the lamination of N isotropic constituents having bulk and shear moduli K_n, μ_n, in the $N > 1$ layers present in each building block. It is important that the thicknesses d_n always be in the same proportion in each of these laminated blocks, so that $f_n = d_n/\sum_{n'} d_{n'}$. But it is not important what order the layers were added to the blocks, as Backus's formulas (Backus, 1962) for the constants show. For the overall behavior for the quasistatic (long wavelength) behavior of the system we are studying, Backus's results [also see Postma (1955) and Milton (2002)] state that

$$\begin{aligned} c_{33} &= \left\langle \frac{1}{K+4\mu/3} \right\rangle^{-1}, & c_{13} &= c_{33}\left\langle \frac{K-2\mu/3}{K+4\mu/3} \right\rangle, \\ c_{44} &= \left\langle \frac{1}{\mu} \right\rangle^{-1}, & c_{66} &= \langle \mu \rangle, \\ c_{11} &= \frac{c_{13}^2}{c_{33}} + 4c_{66} - 4\left\langle \frac{\mu^2}{K+4\mu/3} \right\rangle, & c_{12} &= c_{11} - 2c_{66}. \end{aligned} \tag{3}$$

This bracket notation can be correctly viewed: (a) as a volume average, (b) as a line integral along the symmetry axis x_3, or (c) as a weighted summation $\langle Q \rangle = \sum_n f_n Q_n$ over any relevant physical quantity Q taking a constant value Q_n in the n-th layer.

The bulk modulus for each such building block (or crystalline grain if you like) is that given by the compressional Reuss average K_R of the corresponding compliance matrix s_{ij} [the inverse of the usual stiffness matrix c_{ij}, whose nonzero components are shown in (2)].

The well-known result is $e = e_{11} + e_{22} + e_{33} = \sigma/K_{\text{eff}}$, where $1/K_{\text{eff}} = 1/K_R = 2s_{11} + 2s_{12} + 4s_{13} + s_{33}$. This quantity can be expressed in terms of the stiffness elements as

$$\frac{1}{K_R - c_{13}} = \frac{1}{c_{11} - c_{66} - c_{13}} + \frac{1}{c_{33} - c_{13}}. \tag{4}$$

When μ_n =const, it is easy to show that (4) implies (1).

Even though K_{eff} is the same for every grain, since the grains themselves are not isotropic, the overall bulk modulus K^* of the random polycrystal is not necessarily the same as K_{eff} for the individual grains (Hill, 1952). Hashin-Shtrikman bounds on K^* for random polycrystals whose grains have hexagonal symmetry (Peselnick and Meister, 1965; Watt and Peselnick, 1980) show in fact that the value K_R lies outside the bounds in many situations. We will say more about this in the fourth section.

In general an upper bound on the overall shear modulus of an isotropic polycrystal (Hill, 1952) is given by the Voigt average over shear of the stiffness matrix, which may be written as

$$\mu_V = \frac{1}{5}\left(G^V_{\text{eff}} + 2c_{44} + 2c_{66}\right). \tag{5}$$

This expression can be taken as the definition of G^V_{eff}. Eq. (5) implies that $G^V_{\text{eff}} = (c_{11} + c_{33} - 2c_{13} - c_{66})/3$. G^V_{eff} is the energy per unit volume in a grain when a pure uniaxial shear strain of unit magnitude is applied to the grain along its axis of symmetry (Berryman, 2004a).

CONSTANT BULK MODULUS

As a first result, consider a laminated grain composed of isotropic constituents, all having the same bulk modulus K in each layer, but differing shear moduli. Then, if we define the function [compare (1)]

$$g(\zeta) = \left[\sum_{n=1}^{N} \frac{f_n}{\mu_n + \zeta}\right]^{-1} - \zeta, \tag{6}$$

we find from (3) that $G^V_{\text{eff}} = g(\zeta)$ with $\zeta = 3K/4$. This function $g(\zeta)$ has the interesting and useful properties that

$$c_{44} = \langle 1/\mu \rangle^{-1} \equiv g_- \le g(\zeta) \le g_+ \equiv \langle \mu \rangle = c_{66}. \tag{7}$$

Furthermore, $g(\zeta)$ is a monotonic function, achieving its lower bound when $\zeta = 0$ and approaching its upper bound as $\zeta \to \infty$. This formula shows in an elementary way how $G^V_{\text{eff}} = g(3K/4)$ — and therefore μ_V — depends on the constant bulk modulus of the system, and also that this component of the Voigt bound on the overall shear modulus increases with increasing magnitude of the bulk modulus. The overall Voigt bound/estimate (5) for shear therefore has very similar character, but the magnitude of the effect is reduced by a factor of 5, since this is only one of the five distinct contributors to the overall shear behavior of the system. So the largest change in the Voigt shear modulus that variations in bulk modulus can ever induce are expected to be on the order of 20% (or less) of the difference $c_{66} - c_{44}$.

Similarly, the Reuss average for shear is

$$\mu_R = \left[\frac{1}{5}\left(\frac{1}{G^R_{\text{eff}}} + \frac{2}{c_{44}} + \frac{2}{c_{66}}\right)\right]^{-1}, \tag{8}$$

which is also a rigorous lower bound on the overall shear modulus of the polycrystal (Hill, 1952). For each hexagonal grain, the product formulas $3K_R G^V_{\text{eff}} = 3K_V G^R_{\text{eff}} = \omega_+\omega_-/2 = c_{33}(c_{11} - c_{66}) - c^2_{13}$ are valid. The symbols $\omega_\pm$ stand for the quasi-compressional and quasi-uniaxial shear eigenvalues for all the grains (Berryman, 2004). The product formulas show immediately that $G^R_{\text{eff}} = G^V_{\text{eff}} K_R/K_V = G^V_{\text{eff}}$, since $K_R = K_V = K$. Thus, for this relatively simple system, pure compression or tension ($e_{11} = e_{22} = e_{33}$) is an eigenvector corresponding to stiffness eigenvalue $3K$. Uniaxial shear strain ($e_{33} = -2e_{11} = -2e_{22}$) is also an eigenvector and $2G^V_{\text{eff}} = 2G^R_{\text{eff}}$ is the corresponding eigenvalue.

MODEL OF HETEROGENEOUS RESERVOIRS

Returning to the general problem for arbitrary K_n, suppose we construct a random polycrystal by packing small bits of this laminate material into a large container in a way so that the axis of symmetry appears randomly over all possible orientations and also such that no empty volume (porosity) is left in the resulting composite. If the ratio of grain size to overall composite is small enough so the usual implicit assumption of scale separation applies to the composite — but not so small that we are violating the continuum hypothesis — then we have an example of the type of material we want to study.

For each individual grain in this polycrystal, Eqs. (3) are valid locally (*i.e.*, for locally defined coordinates), and the grain bulk modulus K_R is given by (4) for all the grains. The factors $3K_R$ and $2G^V_{\text{eff}}$ are not necessarily eigenvalues of elastic stiffness for individual grains. The Voigt average for shear is again given by (5), which is an upper bound on the isotropic shear modulus of the random polycrystal (Hill, 1952).

The advantage of studying polycrystals of laminates is that we have available an array of theoretical results from which to choose. For example, since each grain is composed of isotropic constitutents, standard Voigt and Reuss bounds (Hill, 1952), as well as the more restrictive Hashin-Shtrikman bounds (Hashin and Shtrikman, 1962; 1963) on composites made up of isotropic constituents are all available. Then, we can instead, or in addition, consider Voigt and Reuss bounds on the laminated grain materials. Formulas for these bounds have already been given here in Eqs. (4), (5), and (8), respectively for K_R, μ_V, and μ_R. The remaining formula is well-known to be

$$K_V = [2(c_{11} + c_{12}) + 4c_{13} + c_{33}]/9. \tag{9}$$

Then, it is useful to distinguish between "correlated" and "uncorrelated" bounds. For example, the most familiar bounds — after the uncorrelated Voigt and Reuss bounds (*i.e.*, the volume

Figure 1: Various bulk modulus bounds: The outer most bounds (blue dot-dash lines) are the standard Hashin-Shtrikman bounds (HS) based only on information about the layer constituents and their volume fractions. The black solid lines are the Voigt and Reuss bounds (XV,XR) obtained from appropriate averages of laminate constants in (3). The inner most bounds (also blue dot-dash lines) are the Peselnick-Meister bounds (PM) for hexagonal polycrystals. For contrast, the Dederich-Zeller bounds (DZ) (see Appendix B) are also shown (dashed red lines). jim2-K4bounds [NR]

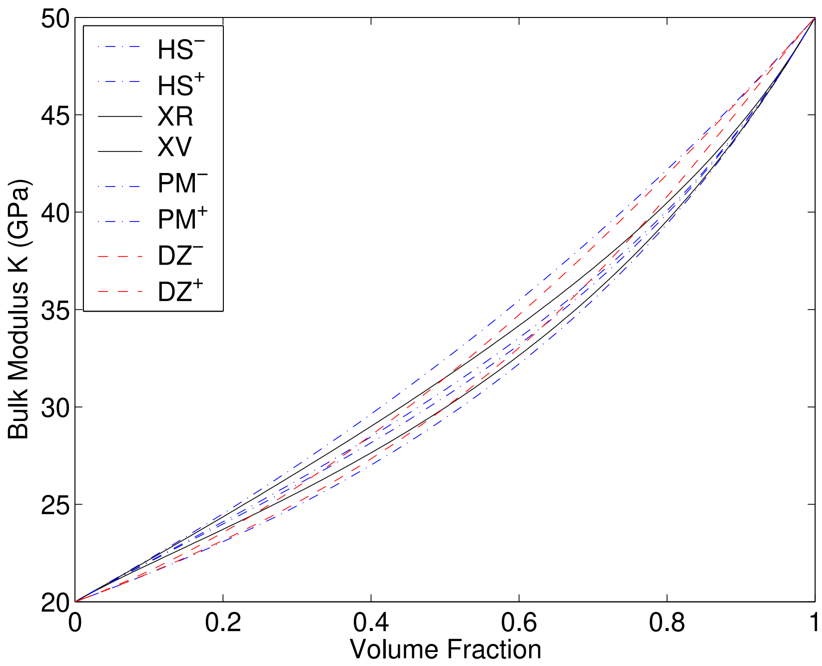
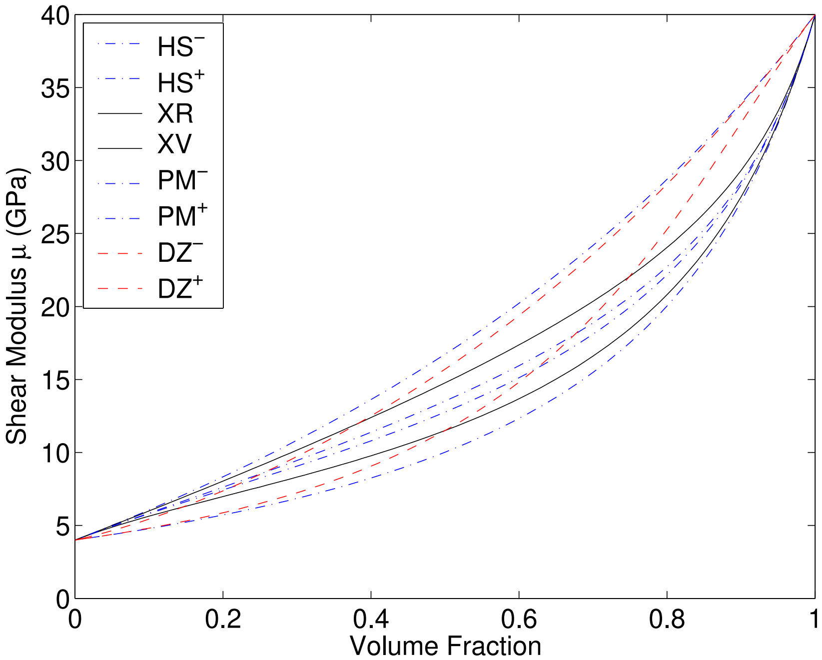


Figure 2: Same as Figure 1 for the various shear modulus bounds. jim2-mu4bounds [NR]



averaged mean and harmonic mean respectively of the consitutents' constants) — are the uncorrelated Hashin-Shtrikman bounds:

$$K_{HS}^{\pm} = \left[\sum_{n=1}^{N} \frac{f_n}{K_n + 4\mu_{\pm}/3} \right]^{-1} - 4\mu_{\pm}/3 \tag{10}$$

and

$$\mu_{HS}^{\pm} = \left[\sum_{n=1}^{N} \frac{f_n}{\mu_n + \zeta_{\pm}} \right]^{-1} - \zeta_{\pm}, \tag{11}$$

where

$$\zeta_{\pm} = \frac{\mu_{\pm}}{6} \left(\frac{9K_{\pm} + 8\mu_{\pm}}{K_{\pm} + 2\mu_{\pm}} \right), \tag{12}$$

with K_+ and K_- being the highest and lowest values of K_n in the system, and similarly μ_+ (μ_-) being the highest (lowest) value of the shear modulus. Milton (1981) presented examples of correlated bounds where the correlations were introduced specifically through spatial correlation functions. But here we introduce correlations instead through the laminated grains. The bounds (4), (5), (8), and (9) are then correlated Voigt and Reuss bounds because of the assumed internal grain-like structure.

We see in Figures 1 and 2 that these bounds (XR and XV) for the polycrystalline case are fairly substantial improvements over the uncorrelated Hashin-Shtrikman bounds (HS$^{\pm}$), which are themselves substantial improvements over the uncorrelated version of the Voigt and Reuss bounds (the Voigt bound is not shown here, but is just a straight line in each plot between the end points of these curves).

A correlated version of the Hashin-Shtrikman bounds can be computed also, as has been shown by Peselnick and Meister (1965) and Watt and Peselnick (1980) (see Appendix A for the details of these formulas, but not their derivation). We see that these bounds are very tight indeed in comparison to all the others considered here. In particular, note that K_R computed from (4) falls outside the correlated Voigt and Reuss bounds (curves XV and XR) of Figure 1.

For contrast, Figures 1 and 2 also plot another set of bounds derived by Dederichs and Zeller (1973) that is also intended for use in uncorrelated systems (see Appendix B for the formulas and a brief discussion). The DZ bounds behave quite differently from those of the correlated bounds XR, XV, PM$^{\pm}$. It is easy to see why this is so. In the laminates, as the volume fractions become small for one constituent at one end of the curves and for the other constituent at the other end, the low volume fraction constituent is approaching a flat disc-like geometry. It is well-known (Milton, 1981) that in this circumstance results for disc-like inclusions tend to dominate the behavior and, therefore, tend to hug the upper Hashin-Shtrikman bound in the lower left-hand limit, and then to hug the lower Hashin-Shtrikman bound in the upper right-hand limit of the Figures. We see that this is so for the correlated bounds XR, XV, PM$^{\pm}$. But the DZ$^{\pm}$ bounds are uncorrelated and do not show this type of behavior at all.

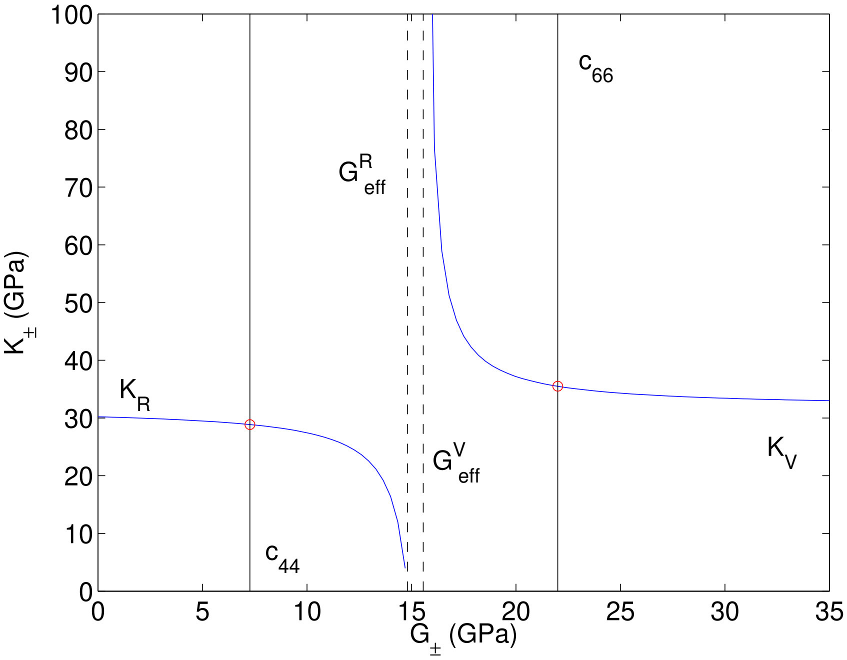


Figure 3: Illustrating the graphical construction leading to the optimum parameters for the comparison material of the lower and upper Peselnick-Meister-Watt bounds: (G_-, K_-), (G_+, K_+), shown as red circles. The case shown is for the middle point of the examples shown in Figures 1 and 2 (volume fraction of 0.50). Values of the constants entering the expressions (see Appendix A) are: $K_V = 30.2162$, $c_{44} = 7.2727$, $c_{66} = 22.0000$, $G^R_{\text{eff}} = 14.8082$, and $G^V_{\text{eff}} = 15.5653$, in units of GPa. The two parts of the blue solid curve are determined by (14) and (16). jim2-PMW [NR]

The best and also most relevant bounds here are obviously the Peselnick-Meister-Watt bounds (Peselnick and Meister, 1965; Watt and Peselnick, 1980), which are presented and briefly discussed in Appendix A. Figure 3 [following some similar figures in Watt and Peselnick (1980)] shows how the parameter sets for the elastic comparison materials are determined. The allowed regions in Figure 3 are the bounded area in the upper right-hand corner, and the similarly bounded area in the lower left-hand corner. The red circles are therefore the points in the $(G_\pm, K_\pm)$-plane that produce the optimum bounds. It is clear that the value of G^V_{eff} plays a very dominant role in the structure of this Figure as the singularity in the blue solid curve occurs exactly at this value.

For the case of constant bulk modulus $K_n = K$, Figure 3 should be contrasted with Figure 4. Obviously, the structure is much simpler, as the singularities in (22) and (24) have disappeared through direct cancelation with the numerator. It is still the case however that the allowed regions in Figure 4 are the bounded areas in upper right-hand corner, and the lower left-hand corner. Again the red circles are the points in the $(G_\pm, K_\pm)$-plane that produce the optimum bounds. However, it is no longer clear from this Figure whether G^V_{eff} is playing any role in the analysis or not.

While attempting to find an answer to this question, the author has spent some effort manipulating the form of the equations for the shear modulus bounds and has found what may be a more enlightening form of these equations. (The derivation will not be given here as it is rather straightforward to find the result again, once the final expression is known.) The resulting simplified formula for the Peselnick-Meister-Watt bounds on overall shear modulus

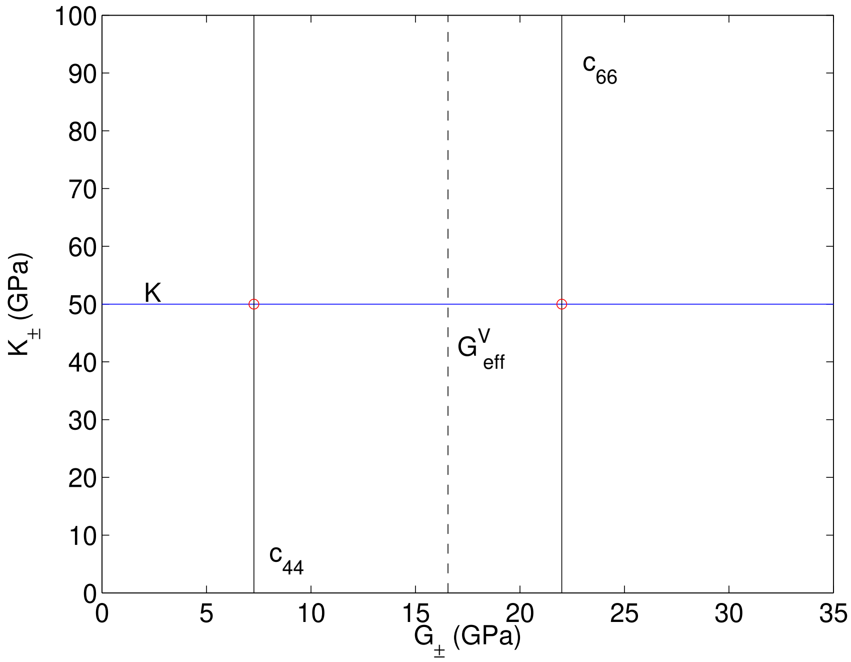


Figure 4: As in Figure 3 for the case of constant bulk modulus, in which case $K_V = K_R = K$, and $G^V_{\mathrm{eff}} = G^R_{\mathrm{eff}}$. Values of the constants entering the expressions (see Appendix A) are: $K = 50.0000$, $c_{44} = 7.2727$, $c_{66} = 22.0000$, $G^V_{\mathrm{eff}} = 16.5546$, in units of GPa. jim2-PMWconK [NR]

of a polycrystal of laminates when $K_n = K$ is:

$$\mu^{\pm}_{PM} = \left[\frac{1}{5}\left(\frac{1}{G^V_{\mathrm{eff}}+\zeta_\pm} + \frac{2}{c_{44}+\zeta_\pm} + \frac{2}{c_{66}+\zeta_\pm}\right)\right]^{-1} - \zeta_\pm, \tag{13}$$

where

$$\zeta_\pm = \frac{G_\pm}{6}\left(\frac{9K+8G_\pm}{K+2G_\pm}\right) \quad \text{with} \quad G_\pm = c_{44} \quad \text{or} \quad c_{66}. \tag{14}$$

Using standard methods, it is not hard to show that, if instead of optimum values of $\zeta_\pm$, we use $\zeta_\pm = 0$ or ∞, then (13) reduces to the formulas (8) and (5) for the correlated Reuss and Voigt bounds on the polycrystal's overall shear modulus.

We see that G^V_{eff} still plays a dominant role here — in the company of c_{44} and c_{66} — as one of the three values (after multiplication by 2) that are the shear eigenvalues of the elastic system. Furthermore, G^V_{eff} is determined for this case exactly by Eq. (6).

DISCUSSION

The results obtained so far show that, for the shear modulus G_{eff} of uniaxial shear for a transversely isotropic system, we have $2G^V_{\mathrm{eff}} = \omega_+$ when the bulk modulus of the system is uniform. In this case, the quasi-shear eigenvector is exactly in the same direction as the uniaxial shear component, so the quantity $2G^V_{\mathrm{eff}}$ — while more generally a strict upper bound on the eigenvalue ω_+ — is exactly equal to it in this special case. Thus, the uniaxial shear mode is in this instance an eigenvector of this system. This happens in particular when $K_n = K$ is a constant for random polycrystals of laminates. The simplified formula (13) for the bounds is therefore the main new result of this paper. When compared to (8), it is suggestive that some very simple forms for Hashin-Shtrikman bounds on shear can probably be found for many such polycrystalline systems, and especially so for granular laminates. The constant bulk modulus limit is a most convenient place to begin a search for such simplified expressions for the bounds.

Once these HS bounds are known, it is an elementary operational exercise to determine self-consistent (SC) estimates based just on the analytical form of the bounds. Monotonicity of the functional

$$M(\zeta) = \left[\frac{1}{5}\left(\frac{1}{G^V_{\text{eff}}+\zeta} + \frac{2}{c_{44}+\zeta} + \frac{2}{c_{66}+\zeta}\right)\right]^{-1} - \zeta, \tag{15}$$

appearing in (13), is easy to prove [see Berryman (1982)] for examples of such proofs), and furthermore $\zeta(K,G) = (G/6)(9K+8G)/(K+2G)$ is a monotonic functional of both arguments. These facts guarantee that there is a unique solution to the self-consistency relation

$$\mu_{SC} \equiv M(\zeta(K,\mu_{SC})), \tag{16}$$

and, furthermore, this solution always lies between the bounds. To provide an example, consider the case of Figure 4 when the volume fractions are both 50%. Then, $\mu_{44} = 7.2727$, $\mu_{66} = 22.0000$, $G_{\text{eff}} = 16.5546$, $\mu_{PM^-} = 13.1164$, $\mu_{PM^+} = 13.8659$, and $\mu_{SC} = 13.5537$. So the self-consistent estimate is not closely correlated with the value of G_{eff}, which is itself usually found outside the correlated bounds on μ. Figure 5 illustrates these results for the full range of volume fractions with the same choice of constituents.

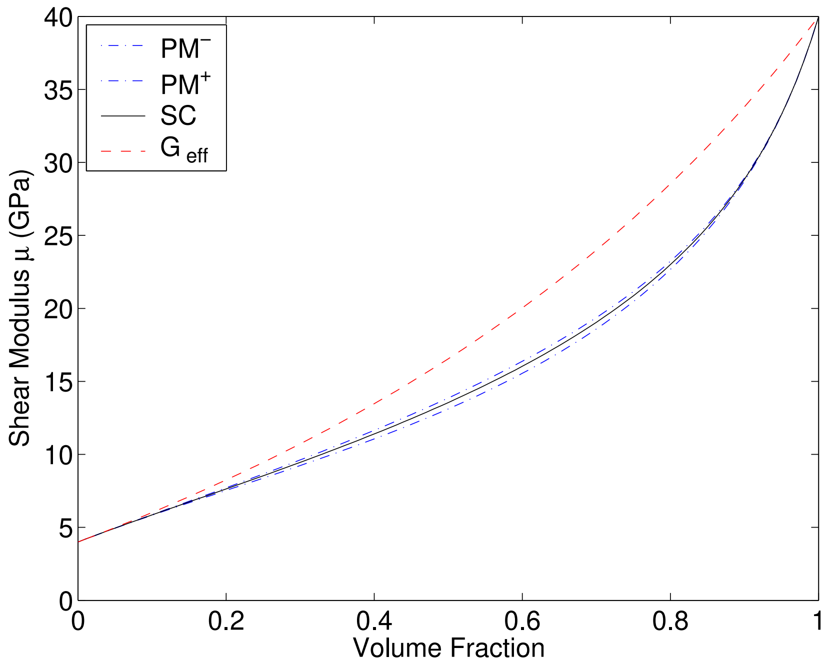


Figure 5: Comparison of the shear modulus estimates over all choices of volume fraction, for the same case considered in Figure 4. jim2-mucomparison [NR]

The results in Fig. 5 show very clearly that self-consistent values fall between the bounds as expected, and that the bounds themselves are in any case very close together for this high contrast example. Thus, an exact result for shear modulus has not been found [so the analogy to Hill's formula (1) is not perfect]. Nevertheless, for most practical purposes, the results show that the predictions of the theory using such correlated bounds — and related self-consistent estimates — will often be as good as, or perhaps better than, the precision of experimental measurements. (Maximum error incurred by using the self-consistent estimate in the example of Figure 5 is about 2%.) The value of G_{eff}, while playing an important role in the analysis, clearly should not be interpreted as the actual value of the effective overall shear modulus for the random polycrystal. G_{eff} does however contribute about 20% of the overall magnitude of the effective shear modulus.

In conclusion, we note that, applications of the analytical results presented here include benchmarking of numerical procedures used for studying elastic behavior of complex composites, as well as estimating coefficients needed in up-scaled equations for elasticity and/or poroelasticity of heterogeneous systems. In particular, up-scaling methods typically determine the form of the effective equations of motion, but most often do not provide any means (or at least any very useful means) of estimating/computing the elastic/poroelastic coefficients. The methods described here are therefore expected to be especially useful for earth sciences and oil reservoir engineering applications, as well as for obvious uses in the practice and theory of elastic composites and heterogeneous media.

APPENDIX A: PESELNICK-MEISTER-WATT BOUNDS FOR HEXAGONAL SYMMETRY

Hashin-Shtrikman-style bounds (Hashin and Shtrikman, 1962; 1963) on the bulk and shear moduli of isotropic random polycrystals composed of hexagonal grains have been derived by Peselnick and Meister (1965), with later corrections by Watt and Peselnick (1980) The main results are presented here using notation consistent with that of our text, in order to emphasize the connections to the analysis presented. To keep this summary brief, we will merely quote the results and refer the reader to the original papers for the derivations.

Parameters used to optimize the Hashin-Shtrikman bounds are $K_\pm$ and $G_\pm$, which have the significance of being the bulk and shear moduli of two isotropic comparison materials. G_+, K_+ are the values used in the formulas for the upper bounds, and G_-, K_- for the lower bounds. Formulas for the bounds are:

$$K_{PM}^{\pm} = K_\pm + \frac{K_V - K_\pm}{1 - 2\beta_\pm (G_{\text{eff}}^V - G_\pm)}, \tag{17}$$

and

$$\mu_{PM}^{\pm} = G_\pm + \frac{B_2^\pm}{1 + 2\beta_\pm B_2^\pm}, \tag{18}$$

where

$$\alpha_\pm = \frac{-1}{K_\pm + 4G_\pm/3}, \qquad \beta_\pm = \frac{2\alpha_\pm}{15} - \frac{1}{5G_\pm}, \qquad \gamma_\pm = \frac{1}{9}(\alpha_\pm - 3\beta_\pm), \tag{19}$$

and

$$B_2^{\pm} = \frac{1}{5}\Big[\frac{G_{\rm eff}^V - G_{\pm}}{\mathcal{D}_{\pm}} + \frac{2(c_{44} - G_{\pm})}{1 - 2\beta_{\pm}(c_{44} - G_{\pm})} + \frac{2(c_{66} - G_{\pm})}{1 - 2\beta_{\pm}(c_{66} - G_{\pm})}\Big], \tag{20}$$

with

$$\mathcal{D}_{\pm} = 1 - \beta_{\pm}(c_{11} + c_{12} + c_{33} - 3K_{\pm} - 2G_{\pm}) - 9\gamma_{\pm}(K_V - K_{\pm}). \tag{21}$$

Optimum values of the moduli for the comparison materials have been shown to be (in our notation)

$$K_- = \frac{K_V(G_{\rm eff}^R - G_-)}{(G_{\rm eff}^V - G_-)} \tag{22}$$

with

$$0 \le G_- \le \min(c_{44}, G_{\rm eff}^R, c_{66}), \tag{23}$$

and

$$K_+ = \frac{K_V(G_+ - G_{\rm eff}^R)}{(G_+ - G_{\rm eff}^V)} \tag{24}$$

with

$$\max(c_{44}, G_{\rm eff}^V, c_{66}) \le G_+ \le \infty. \tag{25}$$

Note that, when $G_- = 0$, $K_- = K_R$, because $K_R = K_V G_{\rm eff}^R / G_{\rm eff}^V$ from the product formulas (Berryman, 2004). Also, note that, if $K_n = K$ is constant, then $K_{\pm} = K_V = K_R = K$ for any choice of $G_{\pm}$, since then we also have that $G_{\rm eff}^V = G_{\rm eff}^R$.

For the laminated materials considered here, the minimum condition in (23) will never be satisfied by c_{66} except in the trivial case of constant shear modulus. Each of the other two arguments can possibly become the minimum under certain nontrivial circumstances. For the materials considered here, it follows from (7) that the maximum condition in (25) will always be uniquely satisfied by c_{66}, except again for the trivial case of constant shear modulus.

Peselnick and Meister (1965) had originally obtained all the results here except for the additional condition in (23) that permits c_{44} to be replaced in certain circumstancs by $G_{\rm eff}^R$. This new condition was added later by Watt and Peselnick (1980).

APPENDIX B: BOUNDS OF DEDERICHS AND ZELLER FOR MULTIPHASE MEDIA

One of the bounds of Dederichs and Zeller (1973) is based on the assumption that, inside each grain of a multiphase material, the distribution of different phases is independent of the shape of the grain, and also independent of the phases of contiguous grains. Grains are therefore assumed to be completely uncorrelated, both internally and externally. The results obtained for bulk modulus are:

$$K_{DZ}^{\pm} = \left[\sum_{n=1}^{N} \frac{f_n}{K_n + 4g_\pm/3} \right]^{-1} - 4g_\pm/3, \tag{26}$$

where

$$g_- = c_{44} \qquad \text{and} \qquad g_+ = c_{66} \tag{27}$$

in our present notation [see eq. (7)]. Similarly, for shear modulus, we have

$$\mu_{DZ}^{\pm} = \left[\sum_{n=1}^{N} \frac{f_n}{\mu_n + \zeta_\pm} \right]^{-1} - \zeta_\pm, \tag{28}$$

where

$$\zeta_- = \frac{c_{44}}{6} \frac{\langle 9/\mu + 8/K \rangle}{\langle 1/\mu + 2/K \rangle} = \frac{g_-}{6} \left(\frac{9\langle 1/K \rangle^{-1} + 8g_-}{\langle 1/K \rangle^{-1} + 2g_-} \right) \tag{29}$$

and

$$\zeta_+ = \frac{c_{66}}{6} \frac{\langle 9K + 8\mu \rangle}{\langle K + 2\mu \rangle} = \frac{g_+}{6} \left(\frac{9\langle K \rangle + 8g_+}{\langle K \rangle + 2g_+} \right). \tag{30}$$

These bounds on bulk modulus are the same as those of Beran and Molyneux (1966) and Miller (1969). The upper bound on shear modulus is the same as that of McCoy (1970) and Silnutzer (1972). Because of the simple functional form of both sets of bounds, it is easy to show (Berryman, 1982) that they are always at least as restrictive as — and, for non-negligible volume fractions of inclusions, normally a significant improvement upon — the Hashin-Shtrikman bounds (Hashin and Shtrikman, 1962; 1963).

We chose to consider these bounds here because they depend only on simple volume averages of the constituent elastic constants, and also because they show — by way of contrast to the other bounds (see Figures 1 and 2) — that it does indeed matter what assumptions are made about the microstructure of the composite.

REFERENCES

Avellaneda, M., 1987, Iterated homogenization, differential effective medium theory and applications: *Commun. Pure Appl. Math.*, **40**, 527–554.

Backus, G. E., 1962, Long-wave elastic anisotropy produced by horizontal layering: *J. Geophys. Res.*, **67**, 4427–4440.

Berryman, J. G., 1980, Long-wavelength propagation in composite elastic media II. Sphericaal inclusions: *J. Acoust. Soc. Am.*, **68**, 1809–1819.

Berryman, J. G., 1980, Long-wavelength propagation in composite elastic media II. Ellipsoidal inclusions: *J. Acoust. Soc. Am.*, **68**, 1820–1831.

Berryman, J. G., 1982, Effective medium theory for elastic composites: in *Elastic Wave Scattering and Propagation*, edited by V. K. Varadan and V. V. Varadan, (Ann Arbor Science, Ann Arbor, Michigan), pp. 111–129.

Berryman, J. G., 1994, Role of porosity in estimates of composite elastic constants: *Trans. ASME J. Energy Resources Tech.*, **116**, 87–96.

Berryman, J. G., 2004a, Poroelastic shear modulus dependence on pore-fluid properties arising in a model of thin isotropic layers: *Geophys. J. Int.*, **157**, pp. 415–425.

Berryman, J. G., 2004b, Bounds on elastic constants of random polycrystals of laminates: in press, to appear in *J. Appl. Phys.*

Bruggeman, D. A. G., 1935, Berechnung verschiedener physikalischer Konstanten von heterogenen Substanzen: I. Dielectrizitätskonstanen und Leitfahigkeiten der Mischkörper aus Isotropen Substanzen: *Ann. Phys. (Leipzig)*, **24**, 636–679.

Drugan, W. J., and Willis, J. R., 1996, A micromechanics-based nonlocal constitutive equation and estimates of representative volume element size for elastic composites: *J. Mech. Phys. Solids*, **44**, 497–524.

Einstein, A., 1905, Eine neue Bestimmung der Moleküldimensionen: *Ann. Phys.*, **19**, 289–306.

Gibiansky, L. V., and Milton, G. W., 1993, On the effective viscoelastic moduli of two-phase media. I. Rigorous bounds on the complex bulk modulus: *Proc. Roy. Soc. London A*, **440**, 163–188.

Gibiansky, L. V., Milton, G. W., and Berryman, J. G., 1999, On the effective viscoelastic moduli of two-phase media. III. Rigorous bounds on the complex shear modulus in two dimensions: *Proc. Roy. Soc. London A*, **455**, 2117–2149.

Hashin, Z., and Shtrikman, S., 1961, Note on a variational approach to the theory of composite elastic materials: *J. Franklin Inst.*, **271**, 336–341.

Hashin, Z., and Shtrikman, S., 1962, On some variational principles in anisotropic and nonhomogeneous elasticity: *J. Mech. Phys. Solids*, **10**, 335–342.

Hashin, Z., and Shtrikman, S., 1963, A variational approach to the theory of the elastic behavior of multiphase materials: *J. Mech. Phys. Solids*, **11**, 127–140.

Hill, R., 1952, Elastic properties of reinforced solids: Some theoretical principles: *Proc. Phys. Soc. London A*, **65**, 349–354.

Maxwell, J. C., 1873, *Treatise on Electricity and Magnetism*: Clarendon Press, Oxford, England.

Milton, G. W., 1981, Bounds on the electromagnetic, elastic, and other properties of two-component composites: *Phys. Rev. Lett.*, **46**, 542–545.

Milton, G. W., 1985, The coherent potential approximation is a realizable effective medium scheme: *Comm. Math. Phys.*, **99**, 463–500.

Milton, G. W., and Berryman, J. G., 1997, On the effective viscoelastic moduli of two-phase media. II. Rigorous bounds on the complex shear modulus in three dimensions: *Proc. Roy. Soc. London A*, **453**, 1849–1880.

Milton, G. W., 2002, *The Theory of Composites*: Cambridge, University Press, Cambridge, UK, pp. 77-78, 163, 457–498.

Norris, A. N., 1985, A differential scheme for the effective moduli of composites: *Mech. Mater.*, **4**, 1–16.

Peselnick, L., and Meister, R., 1965, Variational method of determining effective moduli of polycrystals: (A) Hexagonal symmetry, (B) trigonal symmetry: *J. Appl. Phys.*, **36**, 2879–2884.

Postma, G. W., 1955, Wave propagation in a stratified medium: *Geophysics*, **20**, 780–806.

Rayleigh, L., 1892, On the influence of obstacles arranged in a rectangular order upon the properties of medium: *Phil. Mag.*, **34**, 481–502.

Reuss, A., 1929, Berechung der Fliessgrenze von Mischkristallenx auf Grund der Plastizitätsbedingung für Einkristalle: *Z. Angew. Math. Mech.*, **9**, 49–58.

Voigt, W., 1928, *Lehrbuch der Kristallphysik*: Teubner, Leipzig, 964 pp.

Walpole, L. J., 1966, On bounds for the overall elastic moduli of inhomogeneous systems I.: *J. Mech. Phys. Solids*, **14**, 151–162.

Watt, J. P., and Peselnick, L., 1980, Clarification of the Hashin-Shtrikman bounds on the effective elastic moduli of polycrystals with hexagonal, trigonal, and tetragonal symmetries: *J. Appl. Phys.*, **51**, 1525–1531.