Computers & Geosciences 80 (2015) 95–99

Contents lists available at ScienceDirect

Computers & Geosciences

journal homepage: www.elsevier.com/locate/cageo

Determination of Hashin–Shtrikman bounds on the isotropic effective elastic moduli of polycrystals of any symmetry

J. Michael Brown

Department of Earth and Space Sciences, University of Washington, Box 35-1310, Seattle, WA 98195, USA

ARTICLE INFO

Article history:
Received 20 August 2013
Received in revised form
10 March 2015
Accepted 11 March 2015
Available online 12 March 2015

Keywords:
Polycrystal
Aggregate
Elasticity
Hashin–Shtrikman
Voigt–Reuss–Hill
Isotropic-average

ABSTRACT

Although methods to determine optimal Hashin–Shtrikman bounds for polycrystals of cubic to monoclinic symmetry have been described, the calculation of bounds for triclinic crystals has not previously been possible. The recent determination of elastic moduli of common minerals with low symmetry provides motivation to extend the Hashin–Shtrikman formulation to lower symmetry. Here, Hashin–Shtrikman moduli, valid for crystals of any symmetry, are calculated as a function of the properties of a reference isotropic material. Defining the difference between moduli of the crystal and the moduli of the reference isotropic material as the residual tensor, the optimal lower (and upper) bounding moduli are found by a search along the boundary of positive (or negative) definite regimes of the residual elasticity tensor. The new numerical approach reproduces earlier results for higher symmetry crystals and successfully provides optimal bounds for triclinic crystals that have previously not been subject to analysis. The algorithm is sufficiently compact that implementation is relatively easy within any modern computational environment. Hashin–Shtrikman bounds for triclinic minerals in the plagioclase solid solution series are reported. These bounds are significantly narrower than extremal Voigt–Reuss bounds. The Hill averages moduli lie within the Hashin–Shtrikman bounds.

1. Introduction

Elastic properties of polycrystals (aggregates of many crystals) are relevant in engineering and technical applications (see the review by Adams and Olson, 1998) as well as in the geosciences. Since the elasticity of rocks (as polycrystalline aggregates) controls seismic wave speeds, efforts to understand Earth composition on the basis of its seismic structure require an ability to predict aggregate properties from single crystal properties (eg. Hacker et al., 2003).

The pioneering work of Hashin and Shtrikman (1962, 1963), who found limits of elastic energy deviations from a reference isotropic state, gave bounds for isotropic elastic properties of polycrystals where the shape and orientations of constituent crystals are uncorrelated. In contrast, the Voigt (uniform strain on all crystals), and Reuss (uniform stress on all crystals) bounds (Hill, 1952) are realized in multi-layered laminate structures (Avellaneda and Milton, 1989; Avellaneda et al. 1996). The Hashin–Shtrikman (H–S) optimal bounds must lie within the Voigt–Reuss (V–R) bounds.

Empirical evidence suggests that measurements of elastic properties of aggregates with random crystal orientations lie within H–S bounds (Watt et al., 1976; Brown et al., submitted for publication). Watt et al. (1976) argued that the Hashin–Shtrikman optimal bounds are the tightest constraints that can be determined without a detailed description of the microstructure of a material (the shape and size distributions of crystals within the aggregate). Thus, H–S optimal bounds provide a key constraint on the behavior of systems that are otherwise not well characterized. Investigations of the properties of polycrystals remain active. With an additional "symmetric cell" assumption tighter bounds have been reported (Pham, 2011a; 2011b; 2012).

Although the generalized theory for bounds as given by Hashin and Shtrikman is valid for any crystal symmetry, prior implementations (Peselnick and Meister, 1965; Watt, 1979, 1980, 1986; Watt and Peselnick, 1980) relied on (symmetry-dependent) analytical factoring of the residual elastic tensor. This tensor is defined as the difference between the actual anisotropic moduli and moduli of a reference isotropic material. As discussed in the next section, the optimal bounds are extremal values in regimes where the residual elastic tensor is either positive definite or negative definite. Low symmetry crystals have complicated expressions for the positive (negative) definite boundaries. In the case of monoclinic crystals, closed forms could not be determined for all conditions and iterative numerical solutions were required (eg. Watt, 1980). No attempt has been reported to factor the (more complicated) lower symmetry triclinic tensor. Efforts to realize

E-mail address: brown@ess.washington.edu

http://dx.doi.org/10.1016/j.cageo.2015.03.009
0098-3004/

practical calculations of optimal H–S bounds culminated with the publication by Watt (1987) of an algorithm, appropriate for cubic through monoclinic symmetries. That FORTRAN code required a complex mix of analytic and numerical calculations. Each symmetry class was handled differently as a result of the changing topology associated with the positive (negative) definite bounding conditions.

Despite the theoretical advantages of Hashin–Shtrikman bounds, the use of Voigt–Reuss–Hill bounds has remained ubiquitous in the geosciences. In part this may represent an implicit judgment that the Hill average of Voigt and Reuss bounds is adequate. However, Hashin–Shtrikman bounds may have also been avoided as a result of a perception that these bounds are too difficult to calculate. Maintaining an executable version of the older generation FORTRAN code was not an easy task. Furthermore, the complexity of the algorithm used in that code may have inhibited more widespread understanding and routine use of H–S bounds.

In this study, the fundamental equations for Hashin–Shtrikman moduli are implemented in a high-level language (MATLAB) and contemporary numerical methods are employed to search for the optimal bounds. The size of the code is dramatically smaller. The method is symmetry class independent. It exactly reproduces earlier (higher symmetry) results and is extended to applications in the case of triclinic crystals.

2. Theory

Key equations of the derivation given by Hashin and Shtrikman (1962, 1963) are reproduced here in order to identify necessary numerical steps. The elastic energy of a polycrystal is

$$U = \frac{1}{2}\int \sigma_{ij}\epsilon_{ij} dV \tag{1}$$

Given "effective" isotropic moduli $K*$ and $G*$ (the quantities to be bounded here), the elastic energy of the aggregate is approximated as

$$U_o \cong \frac{1}{2}\left[9K^*(\epsilon^o)^2 + 2G^*\epsilon^o_{ij}\epsilon^o_{ij}\right] \tag{2}$$

where σ_{ij} and ϵ_{ij} are the stress and strain tensors, $\epsilon^o = \frac{1}{3}\epsilon^o_{kk}$ is the isotropic non-deviatoric strain, and ϵ^o_{ij} is the isotropic deviatoric strain. Define the residual stress tensor as:

$$R_{ijkl} = C_{ijkl} - C^o_{ijkl} \tag{3}$$

where C_{ijkl} is the anisotropic elastic tensor for the crystal of interest and C^o_{ijkl} is the elastic tensor of a (variously described in the literature as the "fictive", "comparison" or) "reference" isotropic material:

$$C^o_{ijkl} = \left(K_o + \frac{2}{3}G_o\right)\delta_{ij}\delta_{kl} + 2G_o I_{ijkl} \tag{4}$$

where K_o and G_o are moduli for the "reference" material. Within the variational framework of the theory, these "reference" moduli are free parameters that can be adjusted to find the appropriate bounding "effective" elastic moduli.

With the 4th order tensor isotropic operator defined as

$$I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{5}$$

H_{ijkl} is determined by

$$H_{ijmn}R_{mnkl} = I_{ijkl} \tag{6}$$

If the differences between the actual stresses in a polycrystal and stresses in the "reference" material are defined by

$$p_{ij} = \sigma_{ij} - C^o_{ijkl}\epsilon_{kl} \tag{7}$$

Hashin and Shtrikman found that the extremes of elastic deviatoric energy with respect to p_{ij} required that

$$\left[H_{ijkl}(\Omega) - \beta I_{ijkl} - \gamma\delta_{ij}\delta_{kl}\right]p_{kl}(\Omega) = \epsilon^o_{ij} - \beta\left[I_{ijkl} - \gamma\delta_{ij}\delta_{kl}\right]\langle p_{kl}\rangle \tag{8}$$

where Ω is the orientation of a particular crystal relative to the co-ordinate system, angle brackets represent averages over all orientations, and

$$\beta = \frac{-3(K_o + 2G_o)}{5G_o(3K_o + 4G_o)} \tag{9}$$

$$\alpha = \frac{-3}{3K_o + 4G_o} \tag{10}$$

$$\gamma = \frac{1}{9}(\alpha - 3\beta) \tag{11}$$

Defining

$$A_{ijkl} = H_{ijkl} - \beta I_{ijkl} - \gamma\delta_{ij}\delta_{kl} \tag{12}$$

and determining B_{ijkl} such that:

$$B_{ijmn}A_{mnkl} = I_{ijkl} \tag{13}$$

Hashin and Shtrikman rewrote Eq. (8) in terms of B_{ijkl} and averaged over all orientations to give

$$\langle p_{ij}\rangle = \langle B_{ijkl}\rangle\left(\epsilon^o_{mn} - \beta I_{mnkl}\langle p_{kl}\rangle - \gamma\delta_{mn}\delta_{kl}\langle p_{kl}\rangle\right) \tag{14}$$

where the average of $\langle B_{ijkl}\rangle$ is

$$\langle B_{ijkl}\rangle = B_1\delta_{ij}\delta_{kl} + 2B_2 I_{ijkl} \tag{15}$$

This can be reduced to

$$B_{ijkl}\delta_{ij}\delta_{kl} = 9B_1 + 6B_2 \tag{16}$$

$$B_{ijkl}\delta_{ik}\delta_{jl} = 3B_1 + 12B_2 \tag{17}$$

Application of pure dilatational strain in Eq. (14) gives an "effective" bulk modulus

$$K^* = K_o + \frac{3B_1 + 2B_2}{3 + \alpha(3B_1 + 2B_2)} \tag{18}$$

Application of pure shear strain in Eq. (14) gives an "effective" shear modulus

$$G^* = G_o + \frac{B_2}{1 + 2\beta B_2} \tag{19}$$

Within the variational framework of the Hashin–Shtrikman derivation, the "effective" moduli are maximized or minimized through appropriate choices for K_o and G_o subject to whether the tensor of deviatoric stresses R_{ijkl} is either positive definite or negative definite. Such extremal values are the optimal bounding moduli.

The problem can be graphically understood with reference to Fig. 1. Here elastic moduli for the triclinic plagioclase feldspar, albite, as reported in (Brown et al., 2006) are used. However, the topology and trends are similar for all crystals of all symmetry classes. The horizontal axis is the parameter G_o and the vertical axis is the parameter K_o. Domains where R_{ijkl} is either positive or negative definite are given with dark shading. The tensor is always positive definite for small values of K_o and G_o. The tensor is always negative definite for large values. Boundary locations depend on the specific moduli of a particular crystal. As noted by Hill (1963), the lower positive definite boundary trends to the Reuss bulk

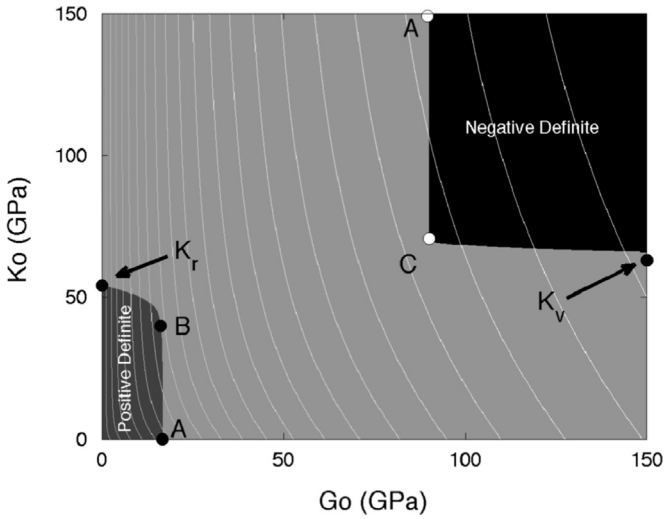

Fig. 1. Isotropic averaging of elastic moduli for albite (An_0) as a function of the reference isotropic moduli. In the lower left corner (dark shade) the residual elastic tensor R_{ijkl} is positive definite. In the upper corner (shaded black) R_{ijkl} is negative definite. The Reuss average bulk modulus is plotted at $G_o=0$ and the Voigt average bulk modulus is plotted on the right side. The contours (intervals of about 0.4 GPa) are values of the Hashin–Shtrikman shear modulus (function of K_o and G_o) that increase from left to right. Two points labeled A define the limits of the positive (negative) boundaries with respect to G_o. Point B marks the location on the boundary where the optimal maximum lower limit Hashin–Shtrikman moduli are found. Point C is the location on the boundary where the optimal minimum upper limit Hashin Shtrikman moduli are found.

modulus as G_o goes to zero. As G_o goes to infinity, the negative definite boundary trends to the Voigt average bulk modulus. Both K^* and G^* are monotonic functions of K_o and G_o. Contours of constant G^* (Eq. (19)) are plotted as the light lines in the figure. As shown, a maximal (optimal) value of G^* occurs in the positive definite region and a minimal (optimal) value for G^* occurs in the negative definite region. These points are marks as B and C and represent the optimal Hashin–Shtrikman bounds on the shear modulus. Similar contours in K^* provide the graphical solution for optimal bulk moduli. As graphically demonstrated, the optimal bounds always lie on the boundary of the positive (negative) definite regions.

3. Implementation

The following MATLAB code fragments illustrate numerical implementation of the theory described above. All 4th order elastic tensor quantities are mapped, using the Voigt notation (Nye, 1957), into 6×6 elasticity matrixes. There is no loss in generality.

Determination of the Hashin–Shtrikman moduli (Eqs. (18) and (19)) can be accomplished as follows. Given scalar values for the reference material moduli, the compliance factors (Eqs. (9)–(11)) are calculated:

```
alpha=-3/(3*ko+4*go);
beta=-3*(ko+2*go)/(5*go*(3*ko+4*go));
gamma=(alpha-3*beta)/9;
```

The form of the isotropic operator for elastic tensors is defined in Eq. (5). In the 6×6 matrix representation, the first three diagonal terms are always one while the last three elements can be either 1/2 or 2, depending on how the operator is invoked. These two forms are labeled `I` and `Iinv`.

```
I=eye(6,6);
Iinv=I;
Iinv(4:6,4:6)=2*I(4:6,4:6);
I(4:6,4:6)=.5*I(4:6,4:6);
```

The 6×6 isotropic modulus matrix (Eq. (4)) is given by

```
co=2*go*I;
co(1:3,1:3)=co(1:3,1:3)+(ko-2/3*go)*ones(3,3);
```

The residual matrix (Eq. (3)) and its inverse (Eq. (6)) are

```
R=cij-co;
H=inv(R);
```

Eqs. (12) and (13) are implemented as follows (note the use of the inverse isotropic operator when working with compliances):

```
A=H-beta*Iinv;
A(1:3,1:3)=A(1:3,1:3)-gamma*ones(3,3);
B=inv(A);
```

Orientationally averaged values for the B matrix (Eqs. (16) and (17)) are given by

```
sumB1=sum(sum(B(1:3,1:3)));
dB=diag(B);
sumB2=sum(dB(1:3))+2*sum(dB(4:6));
B1=(2*sumB1-sumB2)/15;
B2=(3*sumB2-sumB1)/30;
```

The Hashin–Shrtikman effective moduli ("`khs`" and "`ghs`") are then determined (Eqs. (18) and (19)):

```
khs=ko+(3*B1+2*B2)/(3+alpha*(3*B1+2*B2));
ghs=go+B2/(1+2*beta*B2);
```

As shown in the previous section, the optimal bounds on the Hashin–Shtrikman moduli lie on the boundaries of the positive (negative) definite regions of matrix `R`. `R` is positive (negative) definite if and only if all eigenvalues of `R` are either all positive or all negative. The following code sets the variable `value` to 1 if positive definite and to -1 if negative definite.

```
[~,D]=eig(R);
s=sum(sign(diag(D)));
value=0;
if s==6,
   value=1;
elseif s==-6,
   value=-1;
 end
```

The fragments given above are assembled into the MATLAB function `hscalc` with inputs being the reference material moduli (`ko` and `go`) and (as a 6×6 matrix) the crystal (anisotropic) elastic moduli `cij`. Output by this function are the H–S effective moduli and the variable `value` (1 for positive definite, -1 for negative definite and 0 otherwise).

Finding optimal bounds for the effective moduli requires a search along the positive (negative) definite boundaries. As illustrated in Fig. 1, the positive definite boundary at $K_o=0$ (lower point A) is found with a search along the lower (G_o) axis as shown below. The smallest possible reference shear modulus (essentially zero) is given by `gmin` and `gmax` is an upper bound that is pragmatically set large (1000 GPa).

```
  dg=(gmax-gmin)/2;
  go=gmin+dg;
  dg=dg/2;
  [~,vo]=hscalc(kmin,go,cij); % vo is 1, 0, or -1
while du>.01
  if vo==0
    gn=go-dg; % point is on right side of boundary -
move left
  else
    gn=go+dg; % point is on left side of boundary -
move right
  end
  [hs,vn]=hscalc(kmin,gn,cij);
  dg=abs(gn-go)/2; % now search in smaller region
  go=gn;
  vo=vn;
end
```

With the "reference" shear modulus set to range from zero to point A of Fig. 1, the positive definite boundary is searched to find the point with maximal values of the H–S moduli (point B). Either the bulk or shear modulus can be tested for the maximal value with little change in results. The boundary is found for each specified value of `go` by searching along `ko` (using similar coding as given above). The search is controlled by the standard MATLAB function `fminbnd`, a bounded search algorithm for the maximum (minimum) of a function of a single variable. `fminbnd` uses the "golden section" method (Brent, 1973) with parabolic interpolation. Since both H–S moduli are monotonically increasing functions of `ko` and `go`, a single extremal value exists along the boundary as shown in Fig. 1.

Since one or more eigenvalues of the residual elasticity matrix R_{ijkl} goes to zero on the positive (negative) definite boundary, it is necessary to move slightly off the boundary in order to insure that necessary matrix inversions are adequately scaled. However, since Hashin–Shtrikman moduli vary relatively slowly (as shown in Fig. 1) negligible changes to the calculated bounds result from avoiding the exact boundary. The search along the negative definite boundary (minimum `go` found at upper point A of Fig. 1), to find the smallest upper values of the H–S moduli (point C of Fig. 1) proceeds in a similar way.

The MATLAB function included with this paper, `HSBounds`, returns the optimal H–S bounds. This function makes use of "nested" sub-functions within the main function. In MATLAB, variables defined within `HSBounds` are locally available to any nested function. In particular, the elastic moduli matrix `cij_local` can be used by `lowerbound`, `upperbound`, and the functions called by these functions. This avoids the need to define global variables in order to use the built-in MATLAB function `fminbnd`.

Minimal error checking is provided. `HSBounds` checks that the input matrix is appropriately 6×6, symmetric, and positive definite. Thus, the user is expected to construct the correct 6×6 matrix of elastic moduli. Moduli could be passed to `HSBounds` as a (more compact) vector. However, problems arise in deciding on the order of moduli and in tracking the symmetry-differing number of moduli. The current implementation avoids difficulties (in the sense that conventions to construct the matrix from a vector can differ) between the user and the function.

Four matrix arrays are returned by `HSBounds`. The first is a 2×2 array that contains upper and lower optimal H–S bounds for the bulk modulus and shear modulus. The second array (3×2) contains the V–R–H bounds. The third array (2×2) is a listing of the "reference" moduli at the optimal points. The fourth array (1×2) gives values of the reference shear modulus at the points labeled A in Fig. 1. The third and fourth output arrays are provided in order to confirm that reasonable results have been obtained. All returned results should be interrelated as shown by the topology plotted in Fig. 1. In all currently tested cases, results have been sensible.

If the m-files HSBounds.m and test_HSBounds.m are in the MATLAB path, invoking the script test_HSBounds will calculate bounds for the examples used in Watt (1987). The current code should reproduce his results to 0.01 GPa. Newly reported (Brown et al., submitted for publication) elastic moduli for triclinic plagioclase feldspars are also included in the script. H–S bounds based on these data are further discussed below.

4. Discussion

The current implementation has been tested against the examples provided by Watt (1987). Results for reported moduli agree to 0.01 GPa, the least significant figure given in the earlier work. Since the current implementation and the former implementation used ~0.01 GPa internally as a convergence criteria, this agreement is acceptable and exceeds typical experimental uncertainty by about an order of magnitude.

Hashin–Shrtikman bounds for recently reported triclinic plagioclase feldspars elastic moduli (Brown et al. submitted for publication) are given in Table 1. The underlying data are listed in `test_HSBounds`. The seven crystals range in composition in the solid solution series from albite ($NaSi_3AlO_8$) to anorthite ($CaSi_2Al_2O_8$). Compositions are reported in terms of anorthite content (An_x where $x=0$ for albite and $x=100$ for anorthite). In all cases, the H–S bounds are significantly tighter that the V–R bounds and the (Hill) average of the V–R bounds lies between the H–S bounds. There is a decrease in the width of all bounds between An_0 and An_{96} as the overall anisotropy of plagioclase feldspars decrease with increasing anorthite composition.

5. Conclusions

A new implementation, based on a straightforward and transparent algorithm, for calculation of isotropic polycrystal aggregate elastic behavior is reported. The method allows calculation of bounds derived by Hashin and Shtrikman (1962, 1963) for crystals having any symmetry. The method is given here as a MATLAB function. However, it is easily transferable to any modern computational environment that has access to standard numerical algorithms. For the first time Hashin–Shtrikman bounds have been calculated and reported for crystals of triclinic symmetry. In all cases examined, the Hill average of Voigt and Reuss bounds lies

Table 1
Isotropic average moduli for plagioclase feldspars based on the triclinic elastic moduli reported by Brown et al. (submitted for publication).

Composition	Modulus (GPa)	Voigt	+HS	Hill	–HS	Reuss
An_0	K	63.1	60.3	58.6	57.1	54.1
	G	41.4	36.7	35.6	32.9	29.8
An_{25}	K	69.2	67.5	66.7	66.0	64.3
	G	39.5	36.2	35.3	33.7	31.1
An_{37}	K	73.0	71.6	70.9	70.3	68.8
	G	42.3	38.8	37.9	36.2	33.6
An_{48}	K	77.6	76.4	75.8	75.3	74.1
	G	42.9	39.3	38.4	36.6	33.9
An_{60}	K	77.0	76.1	75.4	75.2	73.9
	G	41.2	38.4	37.6	36.3	33.9
An_{78}	K	82.3	81.1	80.3	80.0	78.3
	G	41.1	38.4	37.7	36.5	34.3
An_{96}	K	88.7	87.3	86.4	86.1	84.1
	G	42.5	39.9	39.1	38.0	35.7

between the upper and lower Hashin–Shtrikman bounds.

Although Watt et al. (1976) argued compellingly that Hashin–Shtrikman bounds are preferable in situations where the shape and size distributions of grains are not constrained, the use of Voigt–Reuss–Hill bounds has remained ubiquitous in the geosciences. In part this represents an implicit judgment that, within uncertainties, the Hill average of Voigt–Reuss bounds may be adequate. However, Hashin–Shtrikman bounds may have also been avoided as a result of prior calculational difficulties. Maintaining an executable version of the older generation FORTRAN code was not an easy task. Furthermore, the complexity of the previous algorithm may have inhibited more widespread understanding and use of Hashin–Shtrikman bounds. The current implementation is accomplished with a compact code that will hopefully be more routinely used by the community.

Acknowledgements

The National Science Foundation through Grant EAR-0711591 provided partial support. Discussions with K.C. Creager and E. Abramson and comments by an anonymous reviewer improved this manuscript.

Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.cageo.2015.03.009.

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