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Case study

Bounds and self-consistent estimates of the elastic constants of polycrystals

Christopher M. Kube [a,*], Andrea P. Arguelles [b]

[a] Vehicle Technology Directorate, Mechanics Division, Army Research Laboratory, 4603 Flare Loop, Aberdeen Proving Ground, MD 21005-5069, USA
[b] Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln, W342 Nebraska Hall, Lincoln, NE 68588-0526, USA

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ABSTRACT

The Hashin–Shtrikman bounds on the elastic constants have been previously calculated for polycrystalline materials with crystallites having general elastic symmetry (triclinic crystallite symmetry). However, the calculation of tighter bounds and the self-consistent estimates of these elastic constants has remained unsolved. In this paper, a general theoretical expression for the self-consistent elastic constants is formulated. An iterative method is used to solve the expression for the self-consistent estimates. Each iteration of the solution gives the next tighter set of bounds including the well-known Voigt–Reuss and Hashin–Shtrikman bounds. Thus, all of the bounds on the elastic constants and the self-consistent estimates for any crystallite symmetry are obtained in a single, computationally efficient procedure. The bounds and self-consistent elastic constants are reported for several geophysical materials having crystallites of monoclinic and triclinic symmetries.

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1. Introduction

Information related to the elastic properties of subsurface materials is obtained by relating seismic signatures to well-controlled laboratory experiments (Jones et al., 2009). Often, the laboratory measurements are conducted on single crystals of material, which have well known properties. Relating the single-crystal measurements to processes involving a larger system, e.g., a polycrystal, containing similar crystallites requires modeling the physical interaction of the crystallites and the resulting influence on the larger system. The most commonly employed models for polycrystals are based on statistically homogenizing the crystallites.

Homogenization of the elastic properties extends back to Voigt (1887) who considered the polycrystal's elastic constants to be equal to the average of the crystallite's elastic constants over all possible crystallite orientations. Inherent to Voigt's approach is the assumption of uniform strain throughout the polycrystal. The assumption of strain uniformity satisfies the kinematic compatibility at grain boundary interfaces, while losing continuity of surface traction or static compatibility. Reuss (1929) considered a uniform stress assumption, which satisfies static compatibility while sacrificing kinematic compatibility. Hill (1952) proved, based on the extreme assumptions of Voigt and Reuss, that the Voigt and Reuss estimates of the polycrystal's elastic constants bound the true elastic constants; i.e., the polycrystal's elastic constants that would result if both kinematic and static compatibility at the grain boundaries are satisfied. Hashin and Shtrikman (1962a, 1962b, 1963) developed new variational principles that allowed the next set of bounds to be determined by seeking values of the bulk and shear modulus that are near to regions of positive and negative definiteness of the first-order deviation between the crystallite's and polycrystal's elastic tensors. Watt et al. (1976) argued that the Hashin–Shtrikman bounds are the tightest bounds achievable without precise knowledge of the shapes, sizes, and correlations of the crystallites. Thus, the Hashin–Shtrikman bounds have been applied extensively in geophysical applications where it is difficult to ascertain such microstructural features (Jones et al., 2009; Xu and White, 1996; Berge et al., 1995; Vanorio et al., 2003). However, bounds tighter than those of Hashin–Shtrikman are possible if the microstructure is well characterized.

Watt and Peselnick (1980) and Watt (1986, 1979, 1980) considered the case of statistically isotropic and homogeneous polycrystals composed of uncorrelated, spherically shaped crystallites. Later, Watt (1987) published a computational procedure for the calculation of the Hashin–Shtrikman bounds for each of these cases. Berryman (2005, 2011) provided a convenient procedure to

* Corresponding author.
E-mail addresses: christopher.m.kube.ctr@mail.mil (C.M. Kube), arguelles1@gmail.com (A.P. Arguelles).

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calculate the Hashin–Shtrikman bounds for several cases of crystallite symmetry. More recently, Brown (2015) has provided a calculation scheme that includes the most general crystallite symmetry (triclinic).

Following Brown (2015), a computational (MATLAB) procedure is offered that calculates the bounds on the elastic constants of statistically isotropic polycrystals composed of spherically-shaped crystallites belonging to any of the crystallographic symmetry classes. However, in this paper, all orders of bounds (including those of Voigt–Reuss and Hashin–Shtrikman) are considered. The calculation procedure stems from a theoretical expression of the effective elastic constants that one would find when the kinematic and static compatibility is satisfied throughout the polycrystal. An iterative solution is sought where each iteration gives the next tighter set of bounds. Convergence of the bounds produces estimates of the well-known self-consistent elastic constants. Crystals having additional symmetry can be treated as a limiting case of triclinic symmetry by employing the symmetry relations on the elastic constants (Brugger, 1965). The limiting case of cubic symmetry reproduces the formulas derived by Gairola and Kröner (1981).

2. Theory

This section describes the analytical steps to define and reduce the tensors needed in Eq. (7), which is the effective elastic moduli tensor that is used in the iterative computational procedure. Throughout the theory, the components of the fourth-rank tensors use the Voigt index convention where the pairs of indices obtain the following values: 11 → 1, 22 → 2, 33 → 3, 12 → 6, 13 → 5, and 23 → 4. For example, the (i=3, j=3, k=1, l=2) component of the elastic moduli tensor C_{ijkl} is c_{36}. Additionally, the standard summation convention over repeated indices from 1 to 3 is assumed.

Hooke's law for a linearly elastic polycrystalline medium is

$$\sigma_{ij}^{*} = C_{ijkl}^{*}\epsilon_{kl}^{*}, \tag{1}$$

where ϵ^{*} is the infinitesimal strain tensor and C_{ijkl}^{*} is the effective fourth-rank elastic modulus tensor for the medium. Similarly, Hooke's law for an individual spherical crystallite contained in the polycrystal is

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}, \tag{2}$$

where C_{ijkl} is the elastic modulus of the crystallite. In general, $\epsilon_{ij}^{*} \neq \epsilon_{ij}$ unless $C_{ijkl}^{*} = C_{ijkl}$. The connection between the strain field of the crystallite and polycrystal is

$$\epsilon_{ij} = H_{ijkl}\epsilon_{kl}^{*}. \tag{3}$$

H_{ijkl} is known as the concentration tensor given as (Lubarda, 2002; Qu and Cherkaoui, 2006)

$$H_{ijkl} = \left(C_{ijmn} + R_{ijmn}\right)^{-1}\left(C_{mnkl}^{*} + R_{mnkl}\right), \tag{4}$$

where

$$R_{ijkl} = C_{ijmn}^{*}\left[E_{mnkl}^{-1} - I_{mnkl}\right], \tag{5}$$

with E_{ijkl} being the Eshelby tensor (Eshelby, 1957) and I_{ijkl} being the identity tensor. The Eshelby tensor for a spherical crystallite embedded in the polycrystal is

$$E_{ijkl} = \frac{3c_{12}^{*} - 2c_{44}^{*}}{15\left(c_{12}^{*} + 2c_{44}^{*}\right)}\delta_{ij}\delta_{kl} + \frac{2\left(3c_{12}^{*} + 8c_{44}^{*}\right)}{15\left(c_{12}^{*} + 2c_{44}^{*}\right)}I_{ijkl}, \tag{6}$$

where c_{12}^{*} and c_{44}^{*} are the effective Lamé and shear constants of the polycrystal, respectively. The employment of this Eshelby tensor is not overly restrictive because only the average grain shape of the medium needs to be spherical. Alternate, more complicated forms of the Eshelby tensor may be consulted for the case of a polycrystal with (on the average) ellipsoidally shaped grains. ϵ_{ij} is dependent on the crystallographic orientation of the crystallite with respect to the principal directions of ϵ_{ij}^{*}. However, the volume average of ϵ_{ij} is equal to ϵ_{ij}^{*}. Substituting into Eq. (3), while letting $\langle\rangle$ denote the volume average ($\langle\epsilon_{ij}\rangle = \epsilon_{ij}^{*}$), yields $\langle H_{ijkl}\rangle = I_{ijkl}$. Applying the orientation average to Eq. (4) and rearranging then leads to expressions for the effective elastic moduli tensor,

$$C_{ijkl}^{*} = \langle\left(C_{ijkl} + R_{ijkl}\right)^{-1}\rangle^{-1} - R_{ijkl}, \tag{7}$$

Evaluation of Eq. (7) is completed using the following steps. Find R_{ijkl} by observing that the tensor E_{ijkl} has isotropic symmetry, which permits a straightforward evaluation of E_{ijkl}^{-1}. E_{ijkl}^{-1} also has isotropic symmetry and can be written in terms of the isotropic basis functions $\delta_{ij}\delta_{kl}$ and I_{ijkl}. Thus, the inner products over the repeated indices m and n reduce to simple inner products between the isotropic basis functions. Then, R_{ijkl} can be written in the isotropic form, $R_{ijkl} = r_{12}\delta_{ij}\delta_{kl} + 2r_{44}I_{ijkl}$, where r_{12} and r_{44} are the only independent components of R_{ijkl}. C_{ijkl} and R_{ijkl} can be written with respect to an alternative coordinate system through the use of orthogonal transformation operators, $C'_{ijkl} = a_{i\alpha}a_{j\beta}a_{k\gamma}a_{l\delta}C_{\alpha\beta\gamma\delta}$ and $R'_{ijkl} = a_{i\alpha}a_{j\beta}a_{k\gamma}a_{l\delta}R_{\alpha\beta\gamma\delta}$. Expanding over the repeated indices, and applying the isotropic symmetry relations to R_{ijkl} allows the sum $C_{ijkl} + R_{ijkl}$ to be constructed in the following manner:

$$\begin{aligned} C_{ijkl} + R_{ijkl} = a_{i\alpha}a_{j\beta}a_{k\gamma}a_{l\delta}\left(C_{\alpha\beta\gamma\delta} + R_{\alpha\beta\gamma\delta}\right) = a_{i1}a_{j1}a_{k1} \\ a_{l1}\left(c_{11} + r_{12} + 2r_{44}\right) \\ + a_{i1}a_{j1}a_{k1}a_{l2}c_{16} + a_{i1}a_{j1}a_{k1}a_{l3}c_{15} + a_{i1}a_{j1}a_{k2}a_{l1}c_{16} \\ + a_{i1}a_{j1}a_{k2}a_{l2}\left(c_{12} + r_{12}\right) + \cdots \end{aligned} \tag{8}$$

$C_{ijkl} + R_{ijkl}$ in Eq. (8) has triclinic symmetry like C_{ijkl}. Hence, the inverse of $C_{ijkl} + R_{ijkl}$ follows the same procedure as constructing the inverse of C_{ijkl}. The inverse $L_{ijkl} = \left(C_{ijkl} + R_{ijkl}\right)^{-1}$ is determined by solving the overdetermined system of 81 equations for the 21 unknown components of L_{ijkl} generated by

$$\left(C_{ijmn} + R_{ijmn}\right)L_{mnkl} = I_{ijkl}. \tag{9}$$

For example, the first equation follows from considering $i = j = k = l = 1$ and summing over the repeated indices m and n. Repeating this process for all combinations of i, j, k, l leads to the 81 equations. The average $\langle L_{ijkl}\rangle = \langle\left(C_{ijmn} + R_{ijmn}\right)^{-1}\rangle$ is obtained by equating the invariants of L_{ijkl} and $\langle L_{ijkl}\rangle$ and solving for the two independent components of $\langle L_{ijkl}\rangle$, which are

$$15\ell_{12}^{*} = \ell_{11} + \ell_{22} + \ell_{33} + 4\left(\ell_{12} + \ell_{13} + \ell_{23}\right) - 2\left(\ell_{44} + \ell_{55} + \ell_{66}\right), \tag{10a}$$

$$15\ell_{44}^{*} = \ell_{11} + \ell_{22} + \ell_{33} - \left(\ell_{12} + \ell_{13} + \ell_{23}\right) + 3\left(\ell_{44} + \ell_{55} + \ell_{66}\right). \tag{10b}$$

The evaluation of $\langle L_{ijkl}\rangle^{-1} = \langle\left(C_{ijmn} + R_{ijmn}\right)^{-1}\rangle^{-1}$ is straightforward because $\langle L_{ijkl}\rangle$ has isotropic symmetry. At this point, all of the necessary tensors and operations contained in Eq. (7) are defined. Solving Eq. (7) for C_{ijkl}^{*} in closed form is not possible, except for the special case of cubic crystallographic symmetry, because it is transcendental with C_{ijkl}^{*} appearing in the definitions of R_{ijkl} and E_{ijkl} on the righthand side of Eq. (7). For polycrystals having crystallites of cubic symmetry, the bulk modulus of the polycrystal is equal to the bulk modulus of the crystallites, which leads to the expression $c_{12}^{*} = \left(c_{11} + 2c_{12} - 2c_{44}^{*}\right)/3$ and allows c_{12}^{*} and c_{44}^{*} to be

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