T. Böhlke, A. Bertram

Bounds for the Geometric Mean of 4th-Order Elasticity Tensors with Cubic Symmetry

Aggregates of cubic linear elastic crystals with arbitrary crystal orientation distribution are considered with respect to their effective elastic properties. It is shown that the effective elastic strain energy corresponding to a geometric averaging is bounded by the energies implied by the Voigt and Reuss estimates.

1. Simple Estimates of Effective Elastic Properties of Polycrystals

Based on the crystallite orientation distribution function $f(g)$ with $g \in SO(3)$, different orientational averages of elasticity tensors can be introduced. The function f specifies the volume of crystals having an orientation between g and $g + \mathrm{d}g$, i.e. $\mathrm{d}V/V = f(g)\,\mathrm{d}g$. As a result, volume averages can be transformed into averages over $SO(3)$. The most common mean values are the arithmetic and harmonic mean of the local stiffness tensors, which where first suggested by Voigt and Reuss

$$\mathbb{C}^V = \int_g f(g)\mathbb{C}(g)\,\mathrm{d}g, \qquad \mathbb{S}^R = \int_g f(g)\mathbb{S}(g)\,\mathrm{d}g \neq \mathbb{C}^{V\,-1}. \tag{1}$$

$\mathbb{C}$ and $\mathbb{S}$ denote the single crystal stiffness and compliance, respectively. These approaches give upper and lower bounds for the strain energy density. An approach that focuses on a homogenization resulting in unique effective properties was given in [1,5]. Here, the geometric mean of the local elastic moduli is used

$$\mathbb{C}^A = \exp\left(\int_g f(g)\ln(\mathbb{C}(g))\,\mathrm{d}g\right), \qquad \mathbb{S}^A = \exp\left(\int_g f(g)\ln(\mathbb{S}(g))\,\mathrm{d}g\right) \equiv \mathbb{C}^{A\,-1}. \tag{2}$$

For a uniform distribution of crystal orientations $f(g) = 1$ holds for all $g \in SO(3)$. In this case, the integrals (1) and (2) can be expressed solely in terms of the single crystal constants.

For aggregates of cubic crystals the following decomposition holds [3]

$$\mathbb{C}^V = \mathbb{C}^{VI} + \zeta^V \mathbb{A}', \qquad \ln(\mathbb{C}^A) = \ln(\mathbb{C}^{AI}) + \zeta^A \mathbb{A}', \qquad \mathbb{S}^R = \mathbb{S}^{RI} + \zeta^R \mathbb{A}', \tag{3}$$

where $\mathbb{C}^{VI}$, $\mathbb{C}^{AI}$, and $\mathbb{S}^{RI}$ represent the elasticity tensors which are obtained for a uniform orientation distribution. These isotropic parts allow for the classical projector decomposition into a dilatational and a distorsional deformation mode, e.g., $\mathbb{C}^{VI} = \lambda_1^{VI}\mathbb{P}_1^I + \lambda_2^{VI}\mathbb{P}_2^I$ with $\mathbb{P}_1^I = \mathbf{I}\otimes\mathbf{I}/3$ and $\mathbb{P}_2^I = \mathbb{I} - \mathbb{P}_1^I$. $\mathbf{I}$ denotes the 2nd-order identity tensor and $\mathbb{I}$ the identity on symmetric 2nd-order tensors. The scalar factors in equations (3) are given by

$$\zeta^V = \sqrt{\tfrac{6}{5}}\,(\lambda_3 - \lambda_2), \qquad \zeta^A = \sqrt{\tfrac{6}{5}}\,(\ln(\lambda_3) - \ln(\lambda_2)), \qquad \zeta^R = \sqrt{\tfrac{6}{5}}\left(\frac{1}{\lambda_3} - \frac{1}{\lambda_2}\right). \tag{4}$$

The eigenvalues λ_2 and λ_3 refer to the anisotropic projectors of a elasticity tensor of a cubic single crystal with the lattice vectors $\{\mathbf{g}_i\}$: $\mathbb{P}_2^C = \sum_{k=1}^3 \mathbf{g}_k\otimes\mathbf{g}_k\otimes\mathbf{g}_k\otimes\mathbf{g}_k - \mathbb{P}_1^I$, $\mathbb{P}_3^C = \mathbb{I} - \mathbb{P}_2^C - \mathbb{P}_1^I$. The tensor $\mathbb{A}'$ depends only on the distribution of crystal lattice vectors $\{\mathbf{g}_i\}$ and is given by [3]

$$\mathbb{A}' = \frac{\sqrt{30}}{30}\left(\mathbf{I}\otimes\mathbf{I} + 2\mathbb{I} - 5\int_g \sum_{k=1}^{3} f(g)\;\mathbf{g}_k(g)\otimes\mathbf{g}_k(g)\otimes\mathbf{g}_k(g)\otimes\mathbf{g}_k(g)\,\mathrm{d}g\right). \tag{5}$$

2. Bounds for the Eigenvalues of the Geometric Mean

The question arises whether the elastic energy of the geometric mean is bounded by those of the arithmetic and the harmonic mean for arbitrary crystal orientation distributions. Here, the question is answered for aggregates of cubic

crystals. The starting point is a projector decomposition (e.g., [2]) of the three different averages

$$\mathbb{C}^V = \sum_{\gamma=1}^{\beta^V} \lambda_\gamma^V \mathbb{P}_\gamma^V = \sum_{\alpha=1}^{\beta} \lambda_\alpha \bar{\mathbb{P}}_\alpha, \quad \ln(\mathbb{C}^A) = \sum_{\gamma=1}^{\beta^A} \ln(\lambda_\gamma^A)\mathbb{P}_\gamma^A = \sum_{\alpha=1}^{\beta} \ln(\lambda_\alpha)\bar{\mathbb{P}}_\alpha, \quad \mathbb{S}^R = \sum_{\gamma=1}^{\beta^R} \frac{1}{\lambda_\gamma^R}\mathbb{P}_\gamma^R = \sum_{\alpha=1}^{\beta} \frac{1}{\lambda_\alpha}\bar{\mathbb{P}}_\alpha, \tag{6}$$

where β^V, β^A, and β^R denote the number of distinct eigenvalues of the different averages. β is the number of distinct eigenvalues of the cubic single crystal, i.e., $\beta = 3$. $\bar{\mathbb{P}}_\alpha$ represents the mean value of the projector $\mathbb{P}_\alpha$, i.e. $\bar{\mathbb{P}}_\alpha = \int_g f(g)\mathbb{P}_\alpha(g)\,\mathrm{d}g$. From the decomposition (6) and the orthogonality of the corresponding projectors, one concludes that the eigenvalues of the three averages can be written in terms of weights

$$\lambda_\gamma^V = \sum_{\alpha=1}^{\beta} W_{\gamma\alpha}^V \lambda_\alpha, \qquad \lambda_\gamma^A = \prod_{\alpha=1}^{\beta} \lambda_\alpha^{W_{\gamma\alpha}^A}, \qquad \frac{1}{\lambda_\gamma^R} = \sum_{\alpha=1}^{\beta} W_{\gamma\alpha}^R \frac{1}{\lambda_\alpha}, \qquad (\gamma = 1 \ldots \beta^{V,A,R}) \tag{7}$$

with

$$W_{\gamma\alpha}^V = \frac{\mathbb{P}_\gamma^V}{\|\mathbb{P}_\gamma^V\|^2} \cdot \bar{\mathbb{P}}_\alpha, \qquad W_{\gamma\alpha}^A = \frac{\mathbb{P}_\gamma^A}{\|\mathbb{P}_\gamma^A\|^2} \cdot \bar{\mathbb{P}}_\alpha, \qquad W_{\gamma\alpha}^R = \frac{\mathbb{P}_\gamma^R}{\|\mathbb{P}_\gamma^R\|^2} \cdot \bar{\mathbb{P}}_\alpha. \tag{8}$$

For all of the three averages the dilatational and distorsional deformation modes are decoupled as it is the case for singlecrystalline elasticity tensors with a cubic symmetry. The eigentensors corresponding to the dilatational deformation mode are the same for all three averages and are given by $\mathbf{I}/\sqrt{3}$. In what follows we assume $\lambda_2 \neq \lambda_3$, i.e. $\zeta^V \neq 0$. Since $\mathbb{P}_2^I$ represents the identity on 2nd-order traceless tensors, the eigenvalue problem corresponding to distorsional deformation modes reads

$$0 = (\mathbb{C}^V - \lambda^V \mathbb{P}_2^I)[\hat{\mathbf{E}}'] = (\lambda_2^{VI}\mathbb{P}_2^I + \zeta^V \mathbb{A}' - \lambda^V \mathbb{P}_2^I)[\hat{\mathbf{E}}'] = \zeta^V (\mathbb{A}' - \frac{\lambda^V - \lambda_2^{VI}}{\zeta^V}\mathbb{P}_2^I)[\hat{\mathbf{E}}']. \tag{9}$$

One concludes that a deviatoric eigentensor $\hat{\mathbf{E}}'$ of $\mathbb{C}^V$ is also an eigentensor of $\mathbb{A}'$, and vice versa. The same statement is true for the two other averages. If the eigentensors of $\mathbb{C}^V$, $\mathbb{C}^A$, and $\mathbb{S}^R$ coincide with those of $\mathbb{A}'$, then the eigentensors of the arithmetic, geometric, and harmonic mean are identical in the case of aggregates of cubic crystals. This statement holds independently of the crystal orientation distribution in the aggregate. From the identity of the eigentensors one concludes those of the projectors and of the weights in (8)

$$\mathbb{P}_\gamma^V = \mathbb{P}_\gamma^A = \mathbb{P}_\gamma^R, \qquad W_{\gamma\alpha}^V = W_{\gamma\alpha}^A = W_{\gamma\alpha}^R, \qquad (\gamma = 1, \ldots, \bar{\beta} = \beta^V = \beta^A = \beta^R;\ \alpha = 1, \ldots, \beta). \tag{10}$$

Now, the eigenvalues (7) can be written as

$$\lambda_\gamma^V = \sum_{\alpha=1}^{\beta} W_{\gamma\alpha}\lambda_\alpha, \qquad \lambda_\gamma^A = \prod_{\alpha=1}^{\beta} \lambda_\alpha^{W_{\gamma\alpha}}, \qquad \frac{1}{\lambda_\gamma^R} = \sum_{\alpha=1}^{\beta} W_{\gamma\alpha}\frac{1}{\lambda_\alpha}, \qquad W_{\gamma\alpha} = W_{\gamma\alpha}^V = W_{\gamma\alpha}^A = W_{\gamma\alpha}^R \tag{11}$$

$(\gamma = 1 \ldots \bar{\beta})$. Based on Jensen's inequality [4, p.50], one concludes from (11) that the eigenvalues λ_γ^A of $\mathbb{C}^A$ are bounded by the eigenvalues of the Voigt and Reuss estimates

$$\lambda_\gamma^V \geq \lambda_\gamma^A \geq \lambda_\gamma^R, \qquad (\gamma = 1 \ldots \bar{\beta}). \tag{12}$$

From eqns (10) and (12) it follows that the elastic energy predicted the geometric mean is bounded by the energies implied by the arithmetic and the harmonic mean. This statement holds for arbitrary crystal orientation distributions in the polycrystal.

3. References

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Addresses: T. Böhlke, A. Bertram, Otto-v.-Guericke-Universität Magdeburg, Institut für Mechanik, Postfach 4120, D-39016 Magdeburg