T. BÖHLKE, A. BERTRAM

A Minimum Problem Defining Effective Isotropic Elastic Properties

Dedicated to Prof. D. Besdo on the event of his 60th birthday.

The paper discusses a special aspect of averages approximating the elastic properties of polycrystalline aggregates with a uniform orientation distribution. It is shown that the well known isotropic estimations by VOIGT *and* REUSS *and a recently suggested geometric mean of the local elasticity tensors minimize their distances to the single crystal elasticity tensors as well as to the corresponding volume averages. In this analysis, only the influence of the grain orientation distribution on the macroscopic response is considered.*

1. Single Crystal Elasticity

It is assumed that the symmetric stress tensor $\boldsymbol{T}$ is given as a linear invertible map of the symmetric strain tensor $\boldsymbol{E}$. The operators of this map - the fourth-order stiffness $\mathbf{C}$ and compliance tensor $\mathbf{S}$ - are specified by the symmetry group $\mathcal{S}$ of the material being a subgroup of the orthogonal group

$$\boldsymbol{T} = \mathbf{C}[\boldsymbol{E}], \qquad \boldsymbol{E} = \mathbf{S}[\boldsymbol{T}], \qquad \boldsymbol{H}^{\mathrm{T}}\mathbf{C}[\boldsymbol{E}]\boldsymbol{H} = \mathbf{C}[\boldsymbol{H}^{\mathrm{T}}\boldsymbol{E}\boldsymbol{H}], \qquad \forall\, \boldsymbol{H} \in \mathcal{S}. \tag{1}$$

The elasticity tensors are positive definite and possess the major symmetry in the case of hyperelastic materials. Without loss of generality, their right and left subsymmetry is assumed. Because of the aforementioned major symmetry, the following projector representations exist [2,8]

$$\mathbf{C} = \sum_{\alpha=1}^{\beta} \lambda_\alpha \mathbf{P}_\alpha, \qquad \mathbf{S} = \sum_{\alpha=1}^{\beta} \frac{1}{\lambda_\alpha} \mathbf{P}_\alpha, \qquad \beta \leq 6. \tag{2}$$

with λ_α and $\mathbf{P}_\alpha$ being the eigenvalues and eigenspace projectors of $\mathbf{C}$, respectively. Generally, the projectors $\mathbf{P}_\alpha$ are idempotent $\mathbf{P}_\alpha\mathbf{P}_\alpha = \mathbf{P}_\alpha$ (no summation) and biorthogonal $\mathbf{P}_\alpha\mathbf{P}_\gamma = \mathbf{0}$ $(\alpha \neq \gamma)$. Moreover, they are complete, i.e. $\sum_{\alpha=1}^{\beta} \mathbf{P}_\alpha$ is equal to the identity $\mathbf{I}^S$ on symmetric second-order tensors. In the case of isotropy, there are two distinct eigenvalues, and the corresponding projectors are given by $\mathbf{P}_1^I = \frac{1}{3}\boldsymbol{I} \otimes \boldsymbol{I}$ and $\mathbf{P}_2^I = \mathbf{I}^S - \mathbf{P}_1^I$ where $\boldsymbol{I}$ denotes the second-order identity tensor.

2. Polycrystal Elasticity

VOIGT's [9] and REUSS' [7] assumption of constant strain and stress fields, respectively, yield the most simple estimations of the elastic properties of the aggregate. The macroscopic elasticity tensors are then given by the volume averages of the corresponding local fields

$$\mathbf{C}^V = \frac{1}{V}\int_V \mathbf{C}\,\mathrm{d}V, \qquad \mathbf{S}^R = \frac{1}{V}\int_V \mathbf{S}\,\mathrm{d}V \neq \mathbf{C}^{V\,-1}. \tag{3}$$

The advantage of these approaches, which represent arithmetic means of the local properties, is that they give bounds for the strain energy density [4,6]. Their disadvantage is that these estimations differ the more the higher the degree of elastic anisotropy in the grains is. Therefore, alternative approaches have been developed in order to obtain more precise information from the texture data.

An approach that guarantees unique effective properties, such that the inverse of the mean compliance is equal to the mean stiffness, was given by ALEKSANDROV & AISENBERG [1] and further developed by MATTHIES & HUMBERT [5]. There the geometric mean of the local elastic moduli is used

$$\mathbf{C}^A = \exp\left(\frac{1}{V}\int \ln(\mathbf{C})\,\mathrm{d}V\right), \qquad \mathbf{S}^A = \exp\left(\frac{1}{V}\int \ln(\mathbf{S})\,\mathrm{d}V\right) \equiv \mathbf{C}^{A-1}. \tag{4}$$

In general, all these volume averages are anisotropic if applied to empirical texture data. An estimation of the elastic properties with the additional assumption of a uniform orientation distribution follows after transforming the integrals (3) and (4) into the orientation space with volume element $\mathrm{d}g$ using $\mathrm{d}V/V = f(g)\,\mathrm{d}g$ and setting the orientation distribution function $f(g)$ equal to one [3]

$$\mathbf{C}^{VI} = \int_g \mathbf{C}\,\mathrm{d}g, \qquad \mathbf{S}^{RI} = \int_g \mathbf{S}\,\mathrm{d}g, \qquad \mathbf{C}^{AI} = \exp\left(\int_g \ln(\mathbf{C})\,\mathrm{d}g\right). \tag{5}$$

If the orientation space is parameterized by EULER angles, the corresponding volume element is given by $\mathrm{d}g = \sin(\Phi)\,\mathrm{d}\Phi\,\mathrm{d}\varphi_1\,\mathrm{d}\varphi_2/8\pi^2$ [3]. HILL [4] proposed both an arithmetic and a geometric mean of the isotropic bounds $(5)_{1,2}$.

Inspection of the elasticity tensors resulting from integration (5) shows that these isotropic averages can be formulated in terms of the single crystal elasticity tensors and the projectors specifying a linear isotropic elastic law. By introducing the projector notation

$$\mathbf{C}^{VI} = \lambda_1^{VI}\mathbf{P}_1^I + \lambda_2^{VI}\mathbf{P}_2^I, \qquad \mathbf{C}^{RI} = \lambda_1^{RI}\mathbf{P}_1^I + \lambda_2^{RI}\mathbf{P}_2^I, \qquad \mathbf{C}^{AI} = \lambda_1^{AI}\mathbf{P}_1^I + \lambda_2^{AI}\mathbf{P}_2^I, \tag{6}$$

and defining the weights $W_{\gamma\alpha}$ by scalar products of the projectors

$$W_{1\alpha} = \mathbf{P}_\alpha \cdot \mathbf{P}_1^I, \qquad W_{2\alpha} = \mathbf{P}_\alpha \cdot \tfrac{1}{5}\mathbf{P}_2^I, \qquad (\alpha = 1,\ldots,\beta), \tag{7}$$

the eigenvalues of the fourth-order tensors (6) can be formulated as arithmetic, harmonic, and geometric means of the single crystal eigenvalues λ_α with respect to the weights $W_{\gamma\alpha}$

$$\lambda_\gamma^{VI} = \sum_{\alpha=1}^{\beta} W_{\gamma\alpha}\lambda_\alpha, \qquad \frac{1}{\lambda_\gamma^{RI}} = \sum_{\alpha=1}^{\beta} W_{\gamma\alpha}\frac{1}{\lambda_\alpha}, \qquad \lambda_\gamma^{AI} = \prod_{\alpha=1}^{\beta} \lambda_\alpha^{W_{\gamma\alpha}}. \tag{8}$$

The formulation of (5) in terms of projections onto the space of isotropic linear elastic laws implies that $\mathbf{C}^{VI}$, $\mathbf{C}^{RI}$, and $\mathbf{C}^{AI}$ solve the minimum problems

$$\begin{aligned}
&\min_{\lambda_1,\lambda_2\in\mathcal{R}^+} \|\,\mathbf{C} - \lambda_1\mathbf{P}_1^I - \lambda_2\mathbf{P}_2^I\,\| && \Rightarrow \quad \lambda_\gamma = \lambda_\gamma^{VI},\\
&\min_{\lambda_1,\lambda_2\in\mathcal{R}^+} \|\,\mathbf{S} - \frac{1}{\lambda_1}\mathbf{P}_1^I - \frac{1}{\lambda_2}\mathbf{P}_2^I\,\| && \Rightarrow \quad \lambda_\gamma = \lambda_\gamma^{RI},\\
&\min_{\lambda_1,\lambda_2\in\mathcal{R}^+} \|\,\ln(\mathbf{C}) - \ln(\lambda_1)\mathbf{P}_1^I - \ln(\lambda_2)\mathbf{P}_2^I\,\| && \Rightarrow \quad \lambda_\gamma = \lambda_\gamma^{AI},
\end{aligned} \tag{9}$$

with the FROBENIUS norm $\|\,\mathbf{C}\,\| := (C_{ijkl}C^{ijkl})^{1/2}$. Hence the isotropic estimations by VOIGT and REUSS represent the isotropic elastic laws nearest to both the single crystal law (2) and the volume averages (3). Furthermore, one can see that $\ln(\mathbf{C}^{AI})$ minimizes the distance to both $\ln(\mathbf{C})$ and $\int_V \ln(\mathbf{C})\,\mathrm{d}V/V$.

3. References

1 ALEKSANDROV, K.S.; AISENBERG, L.A.: Method of calculating the physical constants of polycrystalline metals. Soviet Physics-Doklady **11** (1966) 323–325

2 BERTRAM, A., OLSCHEWSKI, J.: Zur Formulierung anisotroper linear anelastischer Stoffgleichungen mit Hilfe einer Projektionsmethode. Z. angew. Math. Mech. **73** (1993) T401-T403

3 BUNGE, H.: Texture Analysis in Material Science. Cuviller Verlag Göttingen (1993)

4 HILL, R.: The elastic behaviour of a crystalline aggregate. Proc. Phys. Soc. Lond. **A 65** (1952) 349–354

5 MATTHIES, S.; HUMBERT, M. On the principle of a geometric mean of even-rank symmetric tensors for textured polycrystals. J. Appl. Cryst. **28** (1995) 254–266

6 NEMAT-NASSER, S.; HORI, M.: Micromechanics: Overall Properties of Heterogeneous Materials. Elsevier Science Publishers B.V., Amsterdam (1993)

7 REUSS, A.: Berechnung der Fließgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle. Z. Angew. Math. Mech. **9** (1929) 49–58

8 RYCHLEWSKY, J.: Unconventional approach to linear elasticity. Arch. Mech. **47**, 2 (1995) 149–171

9 VOIGT, W.: Lehrbuch der Kristallphysik. Leipzig Teubner (1910)

Addresses: A. BERTRAM, T. BÖHLKE, Otto-von-Guericke-Universität Magdeburg, Institut für Mechanik