On the possibilities and limitations of modeling the elastic properties of textured multi-phase materials

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Abstract. The two ways of theoretical determination and modeling of the elastic properties of geological or modern technological materials are discussed. Such samples are characterized by a whole string of parameters or distributions (volume parts of the phases, sizes, shapes of the grains, or voids and their orientations etc.). The direct way uses first principles, averaging the strain field calculated by FEM techniques. The indirect way, without absolute spatial characteristics, uses distributions averaging the single-crystalline elastic properties, supposing infinite samples with ideal disorder and non-overlapping, space filling units. Overlapping can effectively been simulated by the DEM technique. The (GeoMixSelf) GMS-approximation able to consider ellipsoidal units, including voids, combines elements of the geometric mean and the self-consistent approximation. One example demonstrates the potentials, limitations and possible combinations of both ways.

1. Introduction
The description of the elastic properties of macroscopic samples (metals, alloys, compounds, minerals and rocks, cf. Fig. 1) is one of the first and typical application of quantitative texture analysis using

- the single-crystalline elastic parameters of their microscopic constituents (grains), and
- distribution characteristics, describing
- the texture of single-phase materials by the well-known ODF f(g),
- the volume fractions v, in case of multi-phase compounds (v = 1, 2, ...,N),
- grain shapes, grain sizes, shape orientations F(Ω),
- the orientation of the crystal lattice inside a given shape, or
- the elastic properties of an effective homogeneous matrix, in order to determine its response to inclusions that model single grains [1-3].
Starting with Hook's law that combines the stress $\sigma$ or strain $\varepsilon$ by the stiffness $C$ or compliance $S$ on the microscopic (single-crystalline ‘$0’’) level

$$\sigma = C^0 \cdot \varepsilon, \quad \varepsilon = S^0 \cdot \sigma, \quad C^0 = (S^0)^{-1},$$

the resulting effective elastic parameters $C$ or $S$ of a macroscopic sample follow as

$$\sigma = C \cdot \varepsilon, \quad \varepsilon = S \cdot \sigma, \quad C = (S)^{-1}.$$

The $\sigma$ and $\varepsilon$ are applied or describe the response of the macroscopic sample. It holds

$$\sigma = \langle \sigma \rangle, \quad \varepsilon = \langle \varepsilon \rangle,$$

where the brackets represent an average over all microscopic values in the whole sample. There are a ‘direct’ and an ‘indirect’ way to determine the asked $C$ or $S$.

2. The direct way

The direct way uses the first principle equations

$$u(r) \approx \sigma = C^0 \varepsilon = C^0 u(r)$$

(that combine the displacement $u(r)$ with the corresponding stresses and single-crystal data $C^0$ in the finite elements ‘FE’ of the regular representation of the sample, cf. Fig. 2) and the corresponding boundary conditions (continuity of stress and strain at the interfaces between the FE) in order to determine $\varepsilon(r)$. Then the asked $C$ follows from

$$\sigma \text{ (loaded, known)} = C \langle \varepsilon(r) \rangle$$

Obviously a concrete calculation can only consider a ‘mesoscopic’ unit of a sample to be described. The mesoscopic unit should statistically well represent the macroscopic homogenous sample in order to represent it by multiplying the mesoscopic units. The finer the FE mesh (in order to describe details of the grains) and the more phases with non-trivial lattice orientations or shape orientations have to be described, the number of the necessary FE (and correspondingly the number of equations to be resolved) will drastically rise. Moreover, the calculation of a unit represents only one ‘experiment’ and the repetition of the experiments (considering another equivalent units) gives an impression about the reached accuracy of the resulting $C$. However, this aspect of the problem (i.e. information on real numbers for the accuracy or the computing expenses) is quite scarcely reported in literature. A convincing example was already published in (1997) by Mullen et al. [5]. N centers of ‘grains’ have been statistically determined within a 2D box. Then the grains have been constructed by Voronoi tessellation. The orientation of the cubic crystal lattice in each grain was also statistically chosen in order to represent an isotropic texture $(f(g) = 1)$. The number of FE was determined by the criterion, that a narrowing of the mesh gives only a minor gain of accuracy. Each experiment with N grains have been repeated 100 times. The accuracy of the calculated Youngs modulus $E$ can be described by the spread around the corresponding mean value (for 100 experiments) coded as $(N, \Delta E [\%])$ : $(5, 26 \%), (10, 19 \%), (100, 6 \%), (1000, 2 \%)$ for Si with $A=1.65$ ; and $(5, 108 \%), (10, 83 \%), (100, 28 \%), (1000, 14 \%)$ for Cs with $A=6.98; \quad A = 2 C^0_{44} / (C^0_{11} - C^0_{12})$.

3. The indirect way

The indirect way considers infinite samples with space filling, non-overlapping units, without any explicit correlations, i.e. realizing an ‘ideal disorder’. All absolute spatial characteristics
(of meaning in the direct way) are lost, becoming relative quantities. Describing e.g. the half-axes \(a, b, c\) of a ellipsoidal grain, effectively all grains of the kind \(a/c, b/c, 1\) will be meant. Distributions are used, characterizing the sample, like those mentioned in the introduction. Instead of the averaging relations (3) and the resulting connection (5), the asked \(\mathbf{C}\) or \(\mathbf{S}\) are determined using averages \(\mathbf{C}^<\) or \(\mathbf{S}^<\) by variants of ‘micromechanical models’. There are three levels of approximations.

The first level considers non-interacting point-like grains (voids cannot be considered because of \(\mathbf{S}^>\) inclusion. The key element is the dimension-less Eshelby-tensor. Therefore the ‘inversion relation’ \(\mathbf{C} = \mathbf{S}^\perp\), that works on the microscopic (1) and macroscopic (2) levels, is not obeyed by \(>\) (6). So long the bounds differ by percents only, there are no problems. But the more anisotropic the \(\mathbf{C}^>\), are, the more \(\mathbf{C}^<\) and \(\mathbf{C}^R\) differ. E.g. for biotite with isotropic oriented grains the VOIGT and REUSS values of the Young’s modulus \(1/\mathbf{S}^\perp\) differ by about 300% [6]. There are several attempts to ‘narrow’ the bounds (Hashin & Shtrikman bounds, really applicable to cases with \(f(g)\) only [2]) or using ‘means’ of them, like HILL’s approximations \(\mathbf{HILL}^<\mathbf{C}^< = (\mathbf{C}^< + \mathbf{C}^R)/2\) \(\mathbf{HILL}^<\mathbf{C}^R = ((\mathbf{S}^< + \mathbf{S}^>)^2)/2\). The ‘SuperHILL’ approximation \([6,7]\) \(\mathbf{SUPER} = \mathbf{S}^{\text{QUOT}}\mathbf{C}^<\mathbf{C}^R = [\mathbf{S}^{\text{QUOT}}\mathbf{C}^<\mathbf{C}^R]^{-1} = (\mathbf{SUPER}^<\mathbf{S})^{-1}\). The ‘group’ principle \([7]\) should be obeyed by the ‘inversion relation. The geometric mean ‘GEO’ \(\mathbf{C}^{\text{GEO}} = \exp(<\mathbf{LN}\mathbf{C}^<>)\) obeys the inversion relation as well the ‘group’ principle \([7]\), that should be obeyed by systems with non-interacting units. Consequently the geometric mean leads to results quite narrow to experimental ones (even for multi-phase cases) if the sample corresponds to the conditions: macroscopic homogeneous, almost spherical grain shapes, minimum correlations between the sort and orientations of the grains. The first level approximations explicitly neglect any interactions between the in reality ‘hard-wired’ to each other grains?! Already about 100 years there are manifold (‘second level’) attempts to include elements of interaction into the consideration, finally using in any way the Green-function of a real or working matrix of the sample [2]. A very constructive step was done by Eshelby (1957) who succeeded to describe in a closed form the strain field \(\mathbf{e}(\mathbf{r})\) for a system of a loaded anisotropic homogeneous matrix that contains an anisotropic ellipsoidal \((a, b, c)\) (not point-like!) inclusion. The key element is the dimension-less Eshelby-tensor \(\mathbf{S}^{\text{Esh}}\) that depends on \(\mathbf{C}\) of the matrix and \(a, b, c\). Basing on that result several kinds of self-consistent ‘SC’ schemes have been developed. The SC-idea is: the \(\mathbf{C}\) or \(\mathbf{S}\) of a ‘system’ consisting of a ‘matrix’ and inclusions are iteratively determined. The next iteration step \((i+1)\) uses the \(\mathbf{C}\) or \(\mathbf{S}\) of the system as the elastic properties of the matrix up to the moment when the properties of the system and the matrix coincide. In the variant of Williams (1970) it reads:

\[
\begin{align*}
\mathbf{C}^{i+1} &= \mathbf{C} + \mathbf{p}, \quad \mathbf{S}^{i+1} = \mathbf{S} + \mathbf{q}, \\
\mathbf{u} &= ([\mathbf{C}^< - (\mathbf{C} - \mathbf{E}^\perp)]^{-1} \cdot \mathbf{E}^\perp - \mathbf{I}) \cdot \mathbf{S} = \mathbf{S}^{\text{Esh}}(\mathbf{C}_i(a_1, a_2, a_3)) \cdot \mathbf{S}; \quad \mathbf{C}^{\text{GMS}} \equiv \mathbf{C}, \quad \mathbf{S}^{\text{GMS}} \equiv \mathbf{S} \text{ for } (i \to \infty).
\end{align*}
\]

Commonly the results of the two branches \(\mathbf{C}^{\text{SC}}\) and \(\mathbf{S}^{\text{SC}} = (\mathbf{S}^{\text{SC}})^{-1}\) do not coincide. In order to obey the inversion relation the GeoMixSelf (‘GMS’) approximation was introduced \([7]\), that applies the SUPER-relation (with the character of a geometric mean) at each iteration step \(i\):

\[
\begin{align*}
\mathbf{C}^i &= \mathbf{C} + \mathbf{p}, \quad \mathbf{S}^i = \mathbf{S} + \mathbf{q}, \\
\mathbf{C}_i &= (\mathbf{C}^<)^{-1}, \quad \mathbf{C}^{\text{GMS}} = \mathbf{C} \text{ } (i \to \infty) \equiv (\mathbf{S}^{\text{GMS}})^{-1}.
\end{align*}
\]
The averaging procedure $<>$ in (7) can be generalized without difficulties to the case of mixed phases, with their own $v_\nu$, $f_\nu(g)$, $F_\nu(\Omega)$, and $\{a_1, a_2, a_3\}$-sets. The GMS approximation is also able to consider pores, because the critical $S_0$ are never asked in (8). The second level can describe non-overlapping ellipsoidal grains or voids only. In porous geologic samples or ceramics ‘nets’ of voids that can be imagined as overlapped ellipsoids. In third level approximations such overlaps can effectively be considered by the differential element method (‘DEM’). A small amount of ellipsoidal pores (with may be other orientation) is added to a working matrix (may be calculated by GMS) with a starting porosity of non-overlapping ellipsoidal pores. The resulting system (used as the matrix for the next iteration step, up to the final porosity) effectively contains overlapping effects. E.g. considering porous materials (cf. Fig. 3) by non-overlapping pores only, the critical porosity (decay of the sample) will earlier be reached than for overlapped pores with a more stable skeleton of the embedding matrix. Sample specific correlations between constituents of the sample (like in graphite or shale’s) can also effectively be modeled ([8], [9]) combining e.g. the $F_\nu(\Omega)$ of flat ellipsoidal grains with those of flat pores or cracks.

4. Example, comparisons
Because of the limited space, only one example can be given. Fig. 3 demonstrates in a sufficient manner the discussed points of interest.

Fig. 3 Dependence of Young’s modulus on porosity for $\text{Al}_2\text{O}_3$ modeled and calculated by FEM [10] and the corresponding results applying SC-, GMS- and DEM- techniques.

5. Conclusion
The direct way is of universal character limited by computing expenses only. The ‘simpler’ indirect way can successfully be applied, especially investigating the dependence of properties on sample parameters in cases, if the to be modeled samples belong to the class of the simplifying assumptions. A general problem is to get the necessary amount of reliable microscopic (experi- mental or in any way estimated) ‘INPUT’-data.

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