Bounds and self-consistent estimates of overall properties for random polycrystals described by linear constitutive laws

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ANALYTICAL SOLUTIONS FOR BOUNDS of overall properties are derived for single-phase polycrystalline materials of random texture, composed of grains with arbitrary anisotropy and described by the linear constitutive law. Self-consistent estimates are found for these materials and they are studied in more details when anisotropic grains are volumetrically isotropic. Reduction of the above solutions for incompressible materials or materials with constraint modes of deformation is also derived. Existence and uniqueness of the obtained solutions are discussed. In order to obtain the solutions, simultaneously the spectral and harmonic decomposition of fourth order Hooke's tensor are used. Utility of the obtained results is demonstrated on the examples of metals and alloys of high specific strength and stiffness.

Key words: anisotropic materials, self-consistent estimates, polycrystals.

1. Introduction

ASSESSMENT OF OVERALL PROPERTIES of heterogenous materials on the basis of a knowledge of its microstructure and local properties is the central problem of contemporary micromechanics which has its practical and theoretical aspects. This problem attracts researchers since the fifties of the previous century. Many important results and developments have been obtained and proposed since then (see monographs [6, 15, 19, 22]).

This paper concerns the special class of heterogeneous materials which are the polycrystalline aggregates. Analytical solutions for upper and lower bounds, corresponding to the uniform strain and uniform stress assumptions, respectively, are derived for single-phase polycrystals. The aggregate of random texture is assumed leading to the isotropic overall behaviour. Mechanical behaviour of grains is arbitrarily anisotropic and described by linear constitutive law, relating strain and stress measure encompassing, for example, linear elastic but also linear viscous materials. More rigorous bounds, resulting from the theorems of minimum

potential energy and of minimum complementary energy, have been proposed by Hashin and Shtrickman [10, 11] and provided for different crystal symmetries, i.e. [3, 23, 25, 34] (see also literature cited there). They are not studied in this paper, however the developed procedure seems to be promising also for deriving these bounds. It could be also applied for the analysis of the bounds formulated and extensively discussed by Pham, in construction of which irregular and random nature of polycrystalline microgeometry is taken into account in asymptotic sense (see i.e. [26]).

In the self-consistent scheme, a single crystal is viewed as a spherical or ellipsoidal inclusion embedded in an infinite medium of unknown properties. For the theoretical formulations concerning self-consistent method one is referred to the classical papers [12] or [35]. In what follows, self-consistent estimates are found for a crystal of general anisotropy and of a spherical shape. Special attention is paid to these materials in which anisotropic grains are volumetrically isotropic. Reductions of the above estimates for incompressible materials or materials with constraint modes of deformation are also derived. The last case concerns i.e. metals or alloys of high specific strength and stiffness such as magnesium or titanium alloys and intermetallics. The utility of the obtained results is presented on the examples of these materials. Existence and uniqueness of the obtained solutions are discussed.

Some of the results obtained are already known in the literature. Upper and lower bounds in a concise form have been provided in [33]. Quartic equation for self-consistent estimate of an overall shear modulus for cubic crystals have been derived already by Hershey in 1954 (independently in [18]) and then reduced to the cubic one e.g. in [12, 18, 35]. Hexagonal crystals have been studied in [14]. In [27] the influence of grain morphology on the self-consistent estimates for overall properties of such crystals has been discussed. For hexagonal, trigonal and tetragonal crystals implicit equations for these estimates, depending on the local stiffness tensor components, were provided in different forms in [24, 25] and [3].

The originality of a paper lies mainly in the method applied. In order to obtain the solutions, simultaneously the spectral and harmonic decompositions of fourth-order Hooke's tensor are used. Thanks to that, the important feature of the derived solutions is that they are expressed by means of invariants of local stiffness (compliance) tensors. To the author's best knowledge, the presented analysis concerning incompressible crystals and crystals with constraint deformation modes is also new. Below, the spectral and harmonic decompositions of Hooke's tensor are recalled in a nutshell, mainly in order to introduce the required notation. More details concerning the spectral theorem one may find in [5, 8, 28]. The harmonic decomposition is presented in [9, 29–31]. The Reader is referred to these publications for more details.

1.1. Spectral decomposition

Hooke's tensor is the fourth-order tensor with the following symmetries with respect to the permutation of indices:

$$(1.1) \qquad T_{ijkl} = T_{jikl} = T_{ijlk} = T_{klij}.$$

Since in the same time Hooke's tensor is the symmetric second-order tensor in a 6-dimensional Euclidean space, the spectral theorem can be applied to such a tensor:

$$(1.2) \qquad \mathbb{T} = \sum_{K=1}^{M} T_K \mathbb{P}_K$$

where T_K are $M \leq 6$ mutually different eigenvalues and $\mathbb{P}_K$ are orthogonal projectors into the corresponding subspace of eigentensors. Orthogonal projectors fulfil the conditions

$$\mathbb{P}_K \mathbb{P}_L = \begin{cases} \mathbb{P}_K \text{ if } K = L \\ \mathbb{0} \ \text{ if } K \neq L \end{cases} \qquad \sum_{K=1}^{M} \mathbb{P}_K = \mathbb{I}$$

where $\mathbb{I}$ is the fourth-order symmetrized identity tensor. If T_K is an eigenvalue of multiplicity $m^{(K)}$ then the corresponding projector may be specified in the form

$$\mathbb{P}_K = \sum_{i=1}^{m^{(K)}} \boldsymbol{\omega}_i \otimes \boldsymbol{\omega}_i$$

where $\{\boldsymbol{\omega}_i\}$, $i = 1, \ldots, m^{(K)}$ constitute a basis in the corresponding m^K-dimensional eigen-subspace of second-order tensors. It should be stressed that decomposition (1.2) is unique.

The symmetry group of $\mathbb{T}$ is the product of symmetry groups of projectors $\mathbb{P}_K$. More on that issue one finds for example in [5, 16, 28].

1.2. Harmonic decomposition

Any Hooke's tensor can be also uniquely decomposed into five pairwise orthogonal parts (belonging to five pairwise orthogonal subspaces)

$$(1.3) \qquad \mathbb{T} = \underbrace{h_P \mathbb{I}_P + h_D \mathbb{I}_D}_{\text{the isotropic part}} + \underbrace{\mathbb{A}_{d1} + \mathbb{A}_{d2} + \mathbb{H}}_{\text{the anisotropic part}},$$

where the first two parts are isotropic and specified by second-order identity tensor $\mathbf{I}$ and fourth-order identity tensor $\mathbb{I}$:

$$\mathbb{I}_P = \frac{1}{3} \mathbf{I} \otimes \mathbf{I}, \qquad \mathbb{I}_D = \mathbb{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I},$$

and two scalars h_P and h_D. Second two parts are specified by two second-order deviators ϕ and ρ, namely

(1.4) $\qquad \mathbb{A}_{d1} = \mathbf{I} \otimes \phi + \phi \otimes \mathbf{I},$

(1.5) $\qquad \mathbb{A}_{d2} = \dfrac{1}{2} \left[\mathbf{I} \otimes \rho + \rho \otimes \mathbf{I} \right]^{T(23)+T(24)} - \dfrac{2}{3} \left[\mathbf{I} \otimes \rho + \rho \otimes \mathbf{I} \right],$

where

$$(\mathbb{A}^{T(23)+T(24)})_{ijkl} = (\mathbb{A})_{ikjl} + (\mathbb{A})_{ilkj}$$

and $\mathbb{H}$ is totally symmetric and traceless.

This decomposition allows for the following one-to-one correspondence:

$$\mathbb{T} \longleftrightarrow (h_P, \quad h_D, \quad \phi, \quad \rho, \quad \mathbb{H}).$$

Scalars are calculated as follows:

$$h_P = \frac{1}{3}\mathbf{I} \cdot \mathbb{T} \cdot \mathbf{I}, \qquad h_D = \frac{1}{5}(\mathrm{Tr}\mathbb{T} - h_P), \qquad h_P = \frac{1}{3}T_{iikk}, \qquad \mathrm{Tr}\mathbb{T} = T_{ikik},$$

while second-order deviators are calculated with use of the so-called Novozhilov's deviators μ_D and ν_D:

$$\phi = \frac{3}{7}\mu_D, \qquad \rho = \frac{2}{7}(\nu_D - 2\mu_D)$$

where μ_D and ν_D are deviators of the following tensors:

$$\mu = \mathbb{T} \cdot \mathbf{I}, \qquad \nu = \mathbb{T}^{T(23)} \cdot \mathbf{I}, \qquad \mu_{ij} = T_{ijkk}, \qquad \nu_{ij} = T_{ikjk}.$$

The symmetry group of the tensor $\mathbb{T}$ is the product of symmetry groups of the tensors ϕ, ρ and $\mathbb{H}$. The decomposition (1.3) is based on the presentations of [29, 31]. Different definitions of $\mathbb{A}_{d1}$ and $\mathbb{A}_{d2}$ have been utilized in [9].

2. Problem

Assume a single-phase polycrystal with components (i.e. grains) of arbitrary anisotropy with the same properties although of axes of symmetry rotated with respect to each other. Moreover, let the orientations ϕ^c of these components be randomly distributed within the considered representative volume element. It means that macroscopically polycrystalline material can be treated as an isotropic one.

Locally the constitutive relation between the stress tensor σ and strain tensor (or strain rate tensor) ε is linear, that is,

(2.1) $\qquad \varepsilon = \mathbb{M}^c \cdot \sigma, \qquad \sigma = \mathbb{L}^c \cdot \varepsilon, \qquad \mathbb{L}^c = (\mathbb{M}^c)^{-1}$

where $\mathbb{L}^c$ and $\mathbb{M}^c$ are stiffness and compliance tensors, respectively. Macroscopic relations for the averaged fields $\mathbf{E} = <\boldsymbol{\varepsilon}>$ and $\boldsymbol{\Sigma} = <\boldsymbol{\sigma}>$ are assumed to be linear as well, namely

$$\mathbf{E} = \overline{\mathbb{M}} \cdot \boldsymbol{\Sigma}, \qquad \boldsymbol{\Sigma} = \overline{\mathbb{L}} \cdot \mathbf{E}, \qquad \overline{\mathbb{L}} = \overline{\mathbb{M}}^{-1}.$$

Moreover, all the introduced fourth-order tensors have the symmetries with respect to the permutation of indices of Hooke's tensor. Note that major symmetry of the constitutive tensor originates in the assumption of existence of a strain potential.

In view of the above assumptions for the local stiffness and compliance tensors, the spectral decomposition (1.2) can be applied

$$(2.2) \qquad \mathbb{L}^c(\phi^c) = \sum_{K=1}^{M} h_K \mathbb{P}_K(\phi^c),$$

$$(2.3) \qquad \mathbb{M}^c(\phi^c) = \sum_{K=1}^{M} \frac{1}{h_K} \mathbb{P}_K(\phi^c),$$

where ϕ^c denotes orientation of local axes with respect to some macroscopic frame specified by three Euler angles. Moreover,

$$\mathbb{P}_K(\phi^c) = \mathbf{Q}(\phi^c) \star \mathbb{P}_K(0)$$

and $\mathbf{Q}(\phi^c) \star (\cdot)$ denotes the rotation operation for a n-th order tensor, $\mathbf{Q}(\phi^c)$ is the second-order orthogonal tensor and $\mathbb{P}_K(0)$ is the projector in the case when the local and macroscopic frames coincide.

Now, for each of projectors $\mathbb{P}_K$ the harmonic decomposition of a fourth-order tensor (1.3) can be applied

$$(2.4) \qquad \mathbb{P}_K(\phi^c) = \eta_P^{(K)} \mathbb{I}_P + \eta_D^{(K)} \mathbb{I}_D + \mathbb{A}_1^{(K)}(\phi^c) + \mathbb{A}_2^{(K)}(\phi^c) + \mathbb{H}^{(K)}(\phi^c)$$

where specifically

$$\eta_P^{(K)} = \frac{1}{3}\mathbf{I} \cdot \mathbb{P}_K(\phi^c) \cdot \mathbf{I} = \frac{1}{3}\mathbf{I} \cdot \mathbb{P}_K(0) \cdot \mathbf{I},$$

$$\eta_D^{(K)} = \frac{1}{5}(m^{(K)} - \eta_P^{(K)}),$$

$$\mathbb{A}_1^{(K)}(\phi^c) = \mathbb{A}_1^{(K)}(\boldsymbol{\mu}_D^{(K)}(\phi^c)),$$

$$\mathbb{A}_2^{(K)}(\phi^c) = \mathbb{A}_2^{(K)}(\boldsymbol{\nu}_D^{(K)}(\phi^c))$$

and $m^{(K)}$ is the multiplicity of the corresponding modulus h_K. One should note the following identities:

$$(2.5) \qquad \sum_{K=1}^{M} \mathbb{P}_K = \mathbb{I} \Rightarrow \sum_{K=1}^{M} \eta_P^{(K)} = 1, \qquad \sum_{K=1}^{M} \eta_D^{(K)} = 1, \qquad \sum_{K=1}^{M} m^{(K)} = 6,$$

where $0 \leq \eta_P^{(K)} \leq 1$, $0 \leq \eta_D^{(K)} \leq 1$ and

$$\sum_{K=1}^{M} \mathbb{A}_1^{(K)} = \mathbb{O} \quad \left(\sum_{K=1}^{M} \boldsymbol{\mu}_D^{(K)} = \mathbf{0} \right), \qquad \sum_{K=1}^{M} \mathbb{A}_2^{(K)} = \mathbb{O} \quad \left(\sum_{K=1}^{M} \boldsymbol{\nu}_D^{(K)} = \mathbf{0} \right),$$

$$\sum_{K=1}^{M} \mathbb{H}^{(K)} = \mathbb{O}.$$

The following identities are also important in the outlined analysis. Let $\mathbf{h}$ be any second-order deviator and $\mathbb{H}$ any fourth-order, fully symmetric and traceless tensor. Specifying the corresponding rotated tensors as

$$\mathbf{h}(\phi^c) = \mathbf{Q}(\phi^c) \star \mathbf{h}, \qquad \mathbb{H}(\phi^c) = \mathbf{Q}(\phi^c) \star \mathbb{H}$$

one can prove that

$$\langle \mathbf{h}(\phi^c) \rangle_{\mathcal{Q}} = \mathbf{0}, \qquad \langle \mathbb{H}(\phi^c) \rangle_{\mathcal{Q}} = \mathbb{O},$$

where $\langle \cdot \rangle_{\mathcal{Q}}$ denotes an average over the whole orientation space. If the orientation is specified by three Euler angles $\phi^c = \{\varphi_1, \psi, \varphi_2\}$ then this averaging is performed according to the following formula:

$$\langle \cdot \rangle_{\mathcal{Q}} = \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} (\cdot) \sin \psi \, d\varphi_1 \, d\psi \, d\varphi_2.$$

Interesting and important subgroup of the considered materials are the materials for which $\mathbf{I}$ is the eigenstate of $\mathbb{L}^c$ and $\mathbb{M}^c$. Materials with such a property are called volumetrically isotropic since its response to a hydrostatic stress state is the change of volume without the change of shape, similarly to the case of isotropic materials. Let us denote the Kelvin bulk modulus of $\mathbb{L}^c$ by h_P; then spectral decompositions (2.2)–(2.3) for the considered subclass of materials take the form

$$(2.6) \qquad\qquad \mathbb{L}^c(\phi^c) = h_P \mathbb{I}_P + \sum_{K=2}^{M} h_K \mathbb{P}_K(\phi^c),$$

$$(2.7) \qquad\qquad \mathbb{M}^c(\phi^c) = \frac{1}{h_P} \mathbb{I}_P + \sum_{K=2}^{M} \frac{1}{h_K} \mathbb{P}_K(\phi^c),$$

where

$$\mathbb{P}_K(\phi^c) = \eta_D^{(K)} \mathbb{I}_D + \mathbb{A}_2^{(K)}(\phi^c) + \mathbb{H}^{(K)}(\phi^c), \qquad \sum_{K=2}^{M} \mathbb{P}_K(\phi^c) = \mathbb{I}_D$$

and specifically

$$\eta_D^{(K)} = \frac{1}{5}m^{(K)}, \qquad \sum_{K=2}^{M} m^{(K)} = 5, \qquad \mathbb{A}_2^{(K)}(\phi^c) = \mathbb{A}_2^{(K)}(\boldsymbol{\nu}_D^{(K)}(\phi^c)).$$

Since macroscopically the material is isotropic, its stiffness and compliance tensors have the form

$$\overline{\mathbb{L}} = \bar{h}_P \mathbb{I}_P + \bar{h}_D \mathbb{I}_D, \qquad \overline{\mathbb{M}} = \frac{1}{\bar{h}_P}\mathbb{I}_P + \frac{1}{\bar{h}_D}\mathbb{I}_D$$

where $\bar{h}_P = 3\overline{K}$ is the overall Kelvin bulk modulus while $\bar{h}_D = 2\overline{\mu} = 2\overline{G}$ is the overall Kelvin shear modulus. In what follows we use notation *the bulk modulus* and *the shear modulus* for these quantities, but one should note the slight difference with respect to $\overline{K}$ and $\overline{G}$ which are usually called by these names[1]. Above formulae are in the same time spectral and harmonic decompositions of macroscopic constitutive tensors.

In the next sections we derive the upper and lower bounds for $\bar{h}_P$ and $\bar{h}_D$ as well as their self-consistent estimates.

3. Upper and lower bounds

The simplest upper bound for averaged properties of polycrystal is obtained by taking

$$(3.1) \qquad\qquad\qquad \boldsymbol{\varepsilon} = \mathbf{E}$$

everywhere in the polycrystal [35]. Such upper bound is called Voight bound for elastic materials or Taylor bound for rigid-plastic or viscoplastic materials. By averaging Eq. $(2.1)_2$ and applying hypothesis (3.1) one obtains

$$(3.2) \qquad\qquad \overline{\mathbb{L}} = \langle \mathbb{L}^c(\phi^c) \rangle, \qquad \overline{\mathbb{M}} = \overline{\mathbb{L}}^{-1} = \langle \mathbb{L}^c(\phi^c) \rangle^{-1}.$$

---

[1]Kelvin bulk and shear modulus are related with macroscopic Young modulus $\overline{E}$ and Poisson ratio $\bar{\nu}$ according to the known relations

$$\overline{E} = \frac{3\bar{h}_P \bar{h}_D}{\bar{h}_P + \bar{h}_D}, \qquad \bar{\nu} = \frac{\bar{h}_P - 2\bar{h}_D}{2(\bar{h}_P + \bar{h}_D)}.$$

Introducing decompositions (2.2) and (2.4) into (3.2) one finds

$$
\begin{aligned}
\langle \mathbb{L}^c(\phi^c) \rangle &= \left\langle \sum_{K=1}^{M} h_K \mathbb{P}_K(\phi^c) \right\rangle \\
&= \left\langle \sum_{K=1}^{M} h_K \left(\eta_P^{(K)} \mathbb{I}_P + \eta_D^{(K)} \mathbb{I}_D + \mathbb{A}_1^{(K)}(\phi^c) + \mathbb{A}_2^{(K)}(\phi^c) + \mathbb{H}^{(K)}(\phi^c) \right) \right\rangle \\
&= \left(\sum_{K=1}^{M} h_K \eta_P^{(K)} \right) \mathbb{I}_P + \left(\sum_{K=1}^{M} h_K \eta_D^{(K)} \right) \mathbb{I}_D \\
&\quad + \sum_{K=1}^{M} h_K \left\langle \mathbb{A}_1^{(K)}(\phi^c) \right\rangle + \sum_{K=1}^{M} h_K \left\langle \mathbb{A}_2^{(K)}(\phi^c) \right\rangle + \sum_{K=1}^{M} h_K \underbrace{\left\langle \mathbb{H}^{(K)}(\phi^c) \right\rangle}_{=\mathbb{O}} \\
&= \left(\sum_{K=1}^{M} h_K \eta_P^{(K)} \right) \mathbb{I}_P + \left(\sum_{K=1}^{M} h_K \eta_D^{(K)} \right) \mathbb{I}_D \\
&\quad + \sum_{K=1}^{M} h_K \mathbb{A}_1^{(K)} \Big(\underbrace{\left\langle \boldsymbol{\mu}_D^{(K)}(\phi^c) \right\rangle}_{=\mathbf{0}} \Big) + \sum_{K=1}^{M} h_K \mathbb{A}_2^{(K)} \Big(\underbrace{\left\langle \boldsymbol{\nu}_D^{(K)}(\phi^c) \right\rangle}_{=\mathbf{0}} \Big),
\end{aligned}
$$

so finally

$$
\overline{\mathbb{L}}^{UP} = \langle \mathbb{L}^c(\phi^c) \rangle = \left(\sum_{K=1}^{M} h_K \eta_P^{(K)} \right) \mathbb{I}_P + \left(\sum_{K=1}^{M} h_K \eta_D^{(K)} \right) \mathbb{I}_D
$$

and

$$
(3.3) \qquad \bar{h}_P^{UP} = \sum_{K=1}^{M} h_K \eta_P^{(K)}, \qquad \bar{h}_D^{UP} = \sum_{K=1}^{M} h_K \eta_D^{(K)}.
$$

It can be shown that $1/3 \bar{h}_P^{UP}$ is equal to the average bulk modulus of polycrystal (see [15]). In the case of volumetrically isotropic materials, these formulae reduce to

$$
(3.4) \qquad \bar{h}_P^{UP*} = h_P, \qquad \bar{h}_D^{UP*} = \frac{1}{5} \sum_{K=2}^{M} h_K m^{(K)}
$$

so the macroscopic bulk modulus is equal to the local one.

The simplest lower bound for averaged properties of polycrystal is obtained by taking

$$
(3.5) \qquad \boldsymbol{\sigma} = \boldsymbol{\Sigma}
$$

everywhere in the polycrystal. Such lower bound is called Reuss bound for elastic materials or Sachs bound for rigid-plastic or viscoplastic materials. Averaging $(2.1)_1$ and applying hypothesis (3.5) one obtains

$$(3.6) \qquad \overline{\mathbb{M}} = \langle \mathbb{M}^c(\phi^c) \rangle , \qquad \overline{\mathbb{L}} = \overline{\mathbb{M}}^{-1} = \langle \mathbb{M}^c(\phi^c) \rangle^{-1} .$$

Performing similar calculations as for the upper bound solution one arrives at

$$\overline{\mathbb{M}}^{LO} = \langle \mathbb{M}^c(\phi^c) \rangle = \left(\sum_{K=1}^{M} \frac{\eta_P^{(K)}}{h_K} \right) \mathbb{I}_P + \left(\sum_{K=1}^{M} \frac{\eta_D^{(K)}}{h_K} \right) \mathbb{I}_D$$

and

$$(3.7) \qquad \bar{h}_P^{LO} = \left(\sum_{K=1}^{M} \frac{\eta_P^{(K)}}{h_K} \right)^{-1} , \qquad \bar{h}_D^{LO} = \left(\sum_{K=1}^{M} \frac{\eta_D^{(K)}}{h_K} \right)^{-1} .$$

It can be shown that $3\bar{h}_P^{LO}$ is equal to the inverse of an average compressibility modulus (see [15]). In the case of the volumetrically isotropic materials, the above formulae reduce to

$$(3.8) \qquad \bar{h}_P^{LO*} = h_P, \qquad \bar{h}_D^{LO*} = 5 \left(\sum_{K=2}^{M} \frac{m^{(K)}}{h_K} \right)^{-1} ,$$

so again the macroscopic bulk modulus is equal to the local one. Since upper and lower bounds for bulk modulus coincide, it is the exact value.

One should note that the upper bound and lower bound solutions depend only on local Kelvin moduli h_K, their multiplicity and $M-1$ independent values $\eta_P^{(K)}$, so maximum 11 independent function of 21 components of local stiffness tensor. All these functions are invariants of local elasticity tensor [4, 17]. Specific formula for $\{\bar{h}_P^{UP/LO}, \bar{h}_D^{UP/LO}\}$ for local symmetry groups covered by fourth-order tensor are collected in Table 1 (compare spectral decompositions of Hooke's tensor for different symmetry groups provided in [16]). It should be underlined that analytical formulas for lower and upper bounds specified by assumptions (3.1) and (3.5) for arbitrary anisotropic crystal are known in the literature [15, 33]. Their derivation is presented here in order to specify them in terms of invariants of $\mathbb{L}^c$ resultling from spectral and harmonic decompositions applied subsequently to the tensor $\mathbb{L}^c$ as well as in order to present the procedure, some part of which is common for the derivation of self-consistent estimates and can be applied also for the derivation of Hashin–Strikman bounds.

Table 1. Upper and lower bounds of overall bulk and shear modulae for different symmetry groups of single crystal.

Symmetry group	Bulk modulus $\bar{h}_P$	Shear modulus $\bar{h}_D$
monoclinic	$\bar{h}_P^{UP} = \sum_{K=1}^{4} h_K \eta_P^{(K)}$ $\bar{h}_P^{LO} = \left(\sum_{K=1}^{4} \frac{\eta_P^{(K)}}{h_K}\right)^{-1}$	$\bar{h}_D^{UP} = \frac{1}{5}\left[\sum_{k=1}^{4} h_K(1-\eta_P^{(K)}) + h_5 + h_6\right]$ $\bar{h}_D^{LO} = 5\left[\sum_{k=1}^{4} \frac{1-\eta_P^{(K)}}{h_K} + \frac{h_5+h_6}{h_5 h_6}\right]^{-1}$
orthotropy	$\bar{h}_P^{UP} = \sum_{K=1}^{3} h_K \eta_P^{(K)}$ $\bar{h}_P^{LO} = \left(\sum_{K=1}^{3} \frac{\eta_P^{(K)}}{h_K}\right)^{-1}$	$\bar{h}_D^{UP} = \frac{1}{5}\left[\sum_{k=1}^{3} h_K(1-\eta_P^{(K)}) + \sum_{K=4}^{6} h_K\right]$ $\bar{h}_D^{LO} = 5\left[\sum_{k=1}^{3} \frac{1-\eta_P^{(K)}}{h_K} + \frac{h_4+h_5+h_6}{h_4 h_5 h_6}\right]^{-1}$
trigonal and hexagonal	$\bar{h}_P^{UP} = (h_1-h_2)\eta_P^{(1)} + h_2$ $\bar{h}_P^{LO} = \frac{h_1 h_2}{h_1-(h_1-h_2)\eta_P^{(1)}}$	$\bar{h}_D^{UP} = \frac{1}{5}\left[h_1-(h_1-h_2)\eta_P^{(1)} + 2(h_3+h_4)\right]$ $\bar{h}_D^{LO} = 5\left[\frac{h_1 h_2 h_3 h_4}{h_3 h_4(h_2-(h_2-h_1)\eta_P^{(1)}) + 2h_1 h_2(h_3+h_4)}\right]$
tetragonal	$\bar{h}_P^{UP} = (h_1-h_2)\eta_P^{(1)} + h_2$ $\bar{h}_P^{LO} = \frac{h_1 h_2}{h_1-(h_1-h_2)\eta_P^{(1)}}$	$\bar{h}_D^{UP} = \frac{1}{5}\left[h_1-(h_1-h_2)\eta_P^{(1)} + h_3 + h_4 + 2h_5\right]$ $\bar{h}_D^{LO} = 5\left[\frac{h_1 h_2 h_3 h_4 h_5}{h_3 h_4 h_5(h_2-(h_2-h_1)\eta_P^{(1)}) + h_1 h_2(2h_3 h_4 + h_3 h_5 + h_4 h_5)}\right]$
cubic	$\bar{h}_P^{UP} = h_1$ $\bar{h}_P^{LO} = h_1$	$\bar{h}_D^{UP} = \frac{1}{5}(2h_2+3h_3)$ $\bar{h}_D^{LO} = \frac{5h_2 h_3}{2h_3 + 3h_2}$

4. Self-consistent estimates

Self-consistent estimate of an overall behaviour of polycrystal relays on Eshelby's solution for the ellipsoidal inclusion embedded in the infinite medium. Here a single grain is considered as an inclusion while the medium has averaged properties of a polycrystal. Following Hill's formulation of a self-consistent procedure [12], one finds the following localization equation for local strain

$$\boldsymbol{\varepsilon} = \mathbb{A}^c \cdot \mathbf{E}, \qquad \mathbb{A}^c = (\mathbb{L}^c + \mathbb{L}^*)^{-1}(\overline{\mathbb{L}} + \mathbb{L}^*), \qquad \langle \mathbb{A}^c \rangle = \mathbb{I}$$

where $\mathbb{A}^c$ is the localization tensor and $\mathbb{L}^*$ is the Hill tensor which depends on the shape of inclusion and the averaged properties $\overline{\mathbb{L}}$. Furthermore, it is shown that

$$(4.1) \qquad \overline{\mathbb{L}} = \langle \mathbb{L}^c \mathbb{A}^c \rangle,$$

which is an implicit equation since $\mathbb{A}^c$ depends on $\overline{\mathbb{L}}$. In the considered case we assume that grains have the same spherical shape and that macroscopic properties are isotropic, therefore the Hill tensor is specified as

$$(4.2) \qquad \mathbb{L}^* = h_P^* \mathbb{I}_P + h_D^* \mathbb{I}_D,$$

where

$$(4.3) \qquad h_P^* = 2\bar{h}_D, \qquad h_D^* = \bar{h}_D \frac{3\bar{h}_P + 4\bar{h}_D}{2(\bar{h}_P + 3\bar{h}_D)}.$$

Instead of (4.1), for derivation of $\overline{\mathbb{L}}$ an equivalent equation is used, namely

$$(4.4) \qquad \langle (\overline{\mathbb{L}} - \mathbb{L}^c)\mathbb{A}^c \rangle = \mathbb{O}.$$

Introducing (4.2) and (2.2) into $\mathbb{A}^c$ one notices that the inversion present in this formula is not straightforward unless all $\mathbb{P}_K(\phi^c)$ do not commute with $\mathbb{I}_P$. All $\mathbb{P}_K(\phi^c)$ commute with $\mathbb{I}_P$ if the material is volumetrically isotropic. Let us first consider this class of materials.

4.1. Volumetrically isotropic crystals

Introducing formulae (2.6) into (4.4), the localization tensor is specified as

$$\mathbb{A}^c(\phi^c) = \frac{\bar{h}_P + h_P^*}{h_P^c + h_P^*} \mathbb{I}_P + \sum_{K=2}^{M} \frac{\bar{h}_D + h_D^*}{h_K + h_D^*} \mathbb{P}_K(\phi^c)$$

and

$$(\overline{\mathbb{L}} - \mathbb{L}^c(\phi^c))\mathbb{A}^c(\phi^c) = \underbrace{\frac{(\bar{h}_P - h_P^c)(\bar{h}_P + h_P^*)}{h_P^c + h_P^*}}_{\alpha_P}\mathbb{I}_P + \sum_{K=2}^{M}\underbrace{\frac{(\bar{h}_D - h_K)(\bar{h}_D + h_D^*)}{h_K + h_D^*}}_{\alpha_K}\mathbb{P}_K(\phi^c)$$

$$= \alpha_P\mathbb{I}_P + \sum_{K=2}^{M}\alpha_K\left(\frac{m^{(K)}}{5}\mathbb{I}_D + \mathbb{A}_2^{(K)}(\phi^c) + \mathbb{H}^{(K)}(\phi^c)\right).$$

Performing averaging over the whole orientation space we are left with

$$\left\langle(\overline{\mathbb{L}} - \mathbb{L}^c(\phi^c))\mathbb{A}^c(\phi^c)\right\rangle = \alpha_P\mathbb{I}_P + \frac{1}{5}\sum_{K=2}^{M}\alpha_K m^{(K)}\mathbb{I}_D,$$

hence the self-consistent estimates for $\bar{h}_P$ and $\bar{h}_D$ are obtained from the set of two equations

$$\alpha_P = \frac{(\bar{h}_P - h_P)(\bar{h}_P + h_P^*)}{h_P + h_P^*} = 0,$$

(4.5)
$$\sum_{K=2}^{M}\alpha_K m^{(K)} = (\bar{h}_D + h_D^*)\sum_{K=2}^{M}\frac{(\bar{h}_D - h_K)m^{(K)}}{h_K + h_D^*} = 0.$$

In view of positive definiteness of the local and macroscopic constitutive tensors, the first equation gives

(4.6)
$$\bar{h}_P = h_P$$

what confirms the result of previous subsection. Introducing (4.3) into the second equation one can reduce it to the polynomial equation of odd degree $2M - 3$ of the form

(4.7)
$$\sum_{K=2}^{M}(\bar{h}_D - h_K)m^{(K)}\prod_{L=2\,(L\neq K)}^{M}w^L(h_L, \bar{h}_P, \bar{h}_D) = 0,$$

where

(4.8)
$$w^L(h_L, \bar{h}_P, \bar{h}_D) = 4\bar{h}_D^2 + 3(\bar{h}_P + 2h_L)\bar{h}_D + 2h_L\bar{h}_P.$$

Equation (4.7) serves to obtain $\bar{h}_D$. We look for $\bar{h}_D$ among positive real roots of this polynomial. It is important to note that the solution depends only on the values of local Kelvin moduli and their multiplicity, so the invariants of local elasticity tensor. Moreover, it should be stressed that knowledge of the

multiplicity of Kelvin moduli is not necessary – formally one can solve this equation as a 9-degree one setting all $m^{(K)} = 1$ and assuming that all h_K are different:

$$(4.9) \qquad \sum_{k=0}^{9} \alpha_k \bar{h}_D^k = 0.$$

One can show that coefficients α_k depend then on invariant h_P and other invariants J_k of deviatoric part of elasticity tensor of the form, which are independent of ordering of the local Kelvin moduli (see Appendix). Analysis of coefficients α_k, presented in more detail in the Appendix, leads to the conclusion that polynomial (4.9) has always a single positive real root. Consequently, the admissible solution exists and is unique.

4.2. Anisotropic crystals

Now let us consider anisotropic crystals which are not volumetrically isotropic. To this end let us rewrite (2.2)–(2.3) as follows:

$$\mathbb{L}^c(\phi^c) = \underbrace{\sum_{K=1}^{N} h_K \mathbb{P}_K(\phi^c)}_{\widetilde{\mathbb{L}}^c(\phi^c)} + \sum_{K=N+1}^{M} h_K \mathbb{P}_K(\phi^c),$$

$$\mathbb{M}^c(\phi^c) = \underbrace{\sum_{K=1}^{N} \frac{1}{h_K} \mathbb{P}_K(\phi^c)}_{\widetilde{\mathbb{M}}^c(\phi^c)} + \sum_{K=N+1}^{M} \frac{1}{h_K} \mathbb{P}_K(\phi^c),$$

where projectors $\mathbb{P}_K(\phi^c)$ for $K = N+1, \ldots, M$ into deviatoric eigen-subspaces commute with $\mathbb{I}_P$ while $\mathbb{P}_K(\phi^c)$ for $K = 1, \ldots, N$ do not. Note that

$$\sum_{K=1}^{N} \mathbb{P}_K(\phi^c) = \widetilde{\mathbb{P}}(\phi_c) = \mathbb{I}_P + \widetilde{\mathbb{P}}_D(\phi_c),$$

where $\widetilde{\mathbb{P}}(\phi_c)$ and $\widetilde{\mathbb{P}}_D(\phi_c)$ fulfil $\mathbb{PP} = \mathbb{P}$, so these fourth-order tensors are projectors. Both commute with $\mathbb{I}_P$ and

$$\widetilde{\mathbb{L}}^c(\phi^c) = \widetilde{\mathbb{P}}(\phi^c) \mathbb{L}^c(\phi^c).$$

Consequently it is found

$$(\overline{\mathbb{L}} - \mathbb{L}^c)\mathbb{A}^c = \underbrace{(\widetilde{\overline{\mathbb{L}}} - \widetilde{\mathbb{L}}^c)\widetilde{\mathbb{A}}^c}_{\widetilde{\mathbb{R}}(\phi^c)} + \sum_{K=N+1}^{M} \underbrace{\frac{(\bar{h}_D - h_K)(\bar{h}_D + h_D^*)}{h_K + h_D^*}}_{\alpha_K} \mathbb{P}_K(\phi^c)$$

where

$$(4.10) \qquad \widetilde{\mathbb{A}}^c(\phi^c) = (\widetilde{\mathbb{L}}^c(\phi^c) + \widetilde{\mathbb{L}}^*(\phi^c))^{-1}(\widetilde{\overline{\mathbb{L}}}(\phi^c) + \widetilde{\mathbb{L}}^*(\phi^c)),$$

$$(4.11) \qquad \widetilde{\mathbb{L}}^*(\phi^c) = \widetilde{\mathbb{P}}(\phi^c)\mathbb{L}^* = h_P^*\mathbb{I}_P + h_D^*\widetilde{\mathbb{P}}_D(\phi^c),$$

$$(4.12) \qquad \widetilde{\overline{\mathbb{L}}}(\phi^c) = \widetilde{\mathbb{P}}(\phi^c)\overline{\mathbb{L}} = \bar{h}_P\mathbb{I}_P + \bar{h}_D\widetilde{\mathbb{P}}_D(\phi^c).$$

Harmonic decompositions of projectors $\mathbb{P}_K$, $(K = N+1, \ldots, M)$ and of $\widetilde{\mathbb{R}}(\phi^c)$,

$$\widetilde{\mathbb{R}}(\phi^c) = \widetilde{\alpha}_P\mathbb{I}_P + \widetilde{\alpha}_D\mathbb{I}_D + \widetilde{\mathbb{A}}_{d1}(\phi^c) + \widetilde{\mathbb{A}}_{d2}(\phi^c) + \widetilde{\mathbb{H}}(\phi^c),$$

are now performed. After averaging over the whole orientation space, two scalar equations which correspond to (4.5) are obtained:

$$(4.13) \qquad \widetilde{\alpha}_P = 0,$$

$$(4.14) \qquad \widetilde{\alpha}_D + \sum_{K=N+1}^{M} \alpha_K m^{(K)} = 0.$$

Let us specify the above equations for the materials in which $N = 2$ and corresponding h_1 and h_2 are of multiplicity one. In such a case there exists a uniquely defined (within the sign) deviatoric second-order tensor $\mathbf{d}(\phi^c)$ of a unit norm such that

$$\widetilde{\mathbb{P}}_D(\phi^c) = \mathbf{d}(\phi^c) \otimes \mathbf{d}(\phi^c), \qquad \mathbb{P}_K(\phi^c) \cdot \mathbf{d} = \mathbf{0}, \qquad K = N+1, \ldots, M$$

and

$$\widetilde{\mathbb{L}}^c(\phi^c) = L_{11}^c\mathbb{I}_P + L_{22}^c\widetilde{\mathbb{P}}_D(\phi^c) + \frac{1}{\sqrt{3}}L_{12}^c\left(\mathbf{I} \otimes \mathbf{d}(\phi^c) + \mathbf{d}(\phi^c) \otimes \mathbf{I}\right).$$

One can show that quantities L_{11}^c, L_{22}^c and $(L_{12}^c)^2$ are invariants of the local elasticity tensor since they are specified as follows:

$$(4.15) \qquad L_{11}^c = \frac{1}{3}\mathbf{I} \cdot \mathbb{L}^c(\phi^c) \cdot \mathbf{I} = h_1\eta_P^{(1)} + h_2\eta_P^{(2)} > 0,$$

$$(4.16) \qquad L_{22}^c = \mathbf{d} \cdot \mathbb{L}^c(\phi^c) \cdot \mathbf{d} = h_1 + h_2 - L_{11}^c > 0,$$

$$(4.17) \qquad (L_{12}^c)^2 = L_{11}^c L_{22}^c - h_1 h_2 > 0.$$

It can be easily checked that L_{11}^c provides the Voight-type upper bound (3.3) for an overall bulk modulus. Introducing the above formulae into (4.10)–(4.12),

after some algebra it is found that

$$\widetilde{\alpha}_P = \frac{(\bar{h}_P + h_P^*)((L_{12}^c)^2 + (\bar{h}_P - L_{11}^c)(h_D^* + L_{22}^c))}{(h_P^* + L_{11}^c)(h_D^* + L_{22}^c) - (L_{12}^c)^2},$$

$$\widetilde{\alpha}_D = \frac{(\bar{h}_D + h_D^*)((L_{12}^c)^2 + (h_P^* + L_{11}^c)(\bar{h}_D - L_{22}^c))}{(h_P^* + L_{11}^c)(h_D^* + L_{22}^c) - (L_{12}^c)^2}$$

and Eqs. (4.13)–(4.14) are equivalent to

$$(4.18) \qquad\qquad (L_{12}^c)^2 + (\bar{h}_P - L_{11}^c)(h_D^* + L_{22}^c) = 0,$$

$$(4.19) \qquad \frac{(L_{12}^c)^2 + (h_P^* + L_{11}^c)(\bar{h}_D - L_{22}^c)}{(h_P^* + L_{11}^c)(h_D^* + L_{22}^c) - (L_{12}^c)^2} + \sum_{K=3}^{M} \frac{(\bar{h}_D - h_K)m^{(K)}}{h_K + h_D^*} = 0.$$

Due to relations (4.3), contrary to volumetrically isotropic materials, $\bar{h}_P$ cannot be calculated independently of $\bar{h}_D$.

The class of materials considered above is not artificial. All materials of transversal (hexagonal), trigonal and tetragonal symmetry belong to the considered group. For these materials deviatoric tensor $\mathbf{d}$ is specified as

$$\mathbf{d} = \pm\frac{1}{\sqrt{6}}(\mathbf{I} - 3\mathbf{m} \otimes \mathbf{m}),$$

where $\mathbf{m}$ is the unit vector coaxial with the main axis of symmetry. Formulas for self-consistent estimates for these classes of single crystal anisotropy have been provided in [3] in the form of implicit equations which are equivalent to (4.18) and (4.19). In [3], the quantity denoted as G_{eff}^V is introduced which is called "uniaxial shear energy" per unit volume for an applied unit shear strain. It is easily verified that $2G_{\text{eff}}^V = L_{22}^c$.

5. Materials with constraints

5.1. Incompressible materials

In [16] it was shown that incompressible materials can be viewed as a special case of the volumetrically isotropic materials for which the bulk modulus is infinite

$$h_P \to \infty.$$

Solutions for upper and lower bounds as well as the self-consistent estimate presented in previous sections indicate that macroscopic bulk modulus is equal to the local one; therefore we also have

$$\bar{h}_P \to \infty.$$

Upper and lower bounds for an overall shear modulus $\bar{h}_D$ have not changed and are specified by Eqs. $(3.4)_2$ and $(3.8)_2$.

As far as a self-consistent estimate for the macroscopic shear modulus is concerned, calculating the limit values for h_P^* and h_D^* one obtains

$$\lim_{\bar{h}_P \to \infty} h_{P*} = 2\bar{h}_D, \qquad \lim_{\bar{h}_P \to \infty} h_{D*} = \frac{3}{2}\bar{h}_D,$$

so Eq. (4.5) reduces to

$$(5.1) \qquad 5\bar{h}_D \sum_{K=2}^{M} \frac{(\bar{h}_D - h_K)m^{(K)}}{2h_K + 3\bar{h}_D} = 0, \qquad \sum_{K=2}^{M} m^{(K)} \leq 5$$

which, due to the assumptions $h_K > 0$ and $\bar{h}_D > 0$, is equivalent to the following polynomial equation of $M - 1$ degree:

$$(5.2) \qquad \sum_{K=2}^{M} (\bar{h}_D - h_K)m^{(K)} \prod_{L=2\,(L \neq K)}^{M} (2h_K + 3\bar{h}_D) = 0.$$

One can prove that this polynomial has always exactly one real root which is positive. Consequently, the solution exists and is unique. Eq. (5.2), similarly like for volumetrically isotropic materials, can be formulated with use of J_k invariants (see Appendix, Eq. (A.7)).

5.2. Materials with restricted deformation modes

It was shown in [16] that the subspace of restricted deformation modes is the eigenspace of the corresponding constitutive fourth-order tensor. The dimension of this subspace is m^* where m^* is also the multiplicity of the infinite Kelvin modulus $h^* \to \infty$. Spectral decompositions (2.2)–(2.3) have the form

$$(5.3) \qquad \mathbb{L}^c(\phi^c) = h^* \mathbb{P}^*(\phi^c) + \sum_{K=2}^{M} h_K \mathbb{P}_K(\phi^c),$$

$$(5.4) \qquad \mathbb{M}^c(\phi^c) = \underbrace{\frac{1}{h^*}}_{\to 0} \mathbb{P}^*(\phi^c) + \sum_{K=2}^{M} \frac{1}{h_K}\mathbb{P}_K(\phi^c) = \sum_{K=2}^{M} \frac{1}{h_K}\mathbb{P}_K(\phi^c).$$

Formulae for an upper bound for macroscopic bulk and shear moduli are rewritten as

$$(5.5) \qquad \bar{h}_P^{UP} = h^*\eta_P^* + \sum_{K=2}^{M} h_K \eta_P^{(K)}, \qquad \bar{h}_D^{UP} = h^*\eta_D^* + \sum_{K=2}^{M} h_K \eta_D^{(K)}.$$

It is seen that $\bar{h}_P^{UP}$ is finite only when $\eta_P^* = 0$ (it means that the space $\mathcal{P}^*$ is the subspace of deviatoric tensors), while the modulus $\bar{h}_D^{UP}$ is finite when $\eta_D^* = 0$ which is equivalent to $\eta_P^* = m^*$. Apparently, both situations cannot take place simultaneously and $\bar{h}_D^{UP}$ is finite only when $m^* = \eta_P^* = 1$. It is the case when the material is incompressible.

Formulae for lower bounds are rewritten as

$$(5.6) \qquad \bar{h}_P^{LO} = \left(\underbrace{\frac{\eta_P^*}{h^*}}_{\to 0} + \sum_{K=2}^{M} \frac{\eta_P^{(K)}}{h_K} \right)^{-1} = \left(\sum_{K=2}^{M} \frac{\eta_P^{(K)}}{h_K} \right)^{-1},$$

$$(5.7) \qquad \bar{h}_D^{LO} = \left(\underbrace{\frac{\eta_D^*}{h^*}}_{\to 0} + \sum_{K=2}^{M} \frac{\eta_D^{(K)}}{h_K} \right)^{-1} = \left(\sum_{K=2}^{M} \frac{\eta_D^{(K)}}{h_K} \right)^{-1}$$

and both are finite until there exists at least one K for which h_K is finite and simultaneously

$$\eta_D^{(K)} \neq 0 \qquad \text{and} \qquad \eta_D^{(K)} \neq 0.$$

If additional restrictions have been imposed on the incompressible materials, as far as an upper bound is concerned both macroscopic modulae are infinite so there is no upper bound, while there exists a lower bound for an overall shear modulus as long as some modes of deformation are not restricted.

Let us pass to self-consistent estimates for volumetrically isotropic materials with constraint deformation modes. We begin with the situation when the space of constraint deformation is the subspace of the deviatoric second-order tensors. As previously, m^* denotes the dimension of this subspace and at the same time, the multiplicity of the corresponding Kelvin modulus h^*. Consequently, the estimate (4.6) for the overall bulk modulus is still valid. Introducing (5.3), Eq. (4.7) can be rewritten as follows:

$$\frac{(\bar{h}_D - h^*)m^*}{2h^*(h_P + 3\bar{h}_D) + \bar{h}_D(3h_P + 4\bar{h}_D)} + \sum_{K=3}^{M} \frac{(\bar{h}_D - h_K)m^{(K)}}{w^K(h_K, h_P, \bar{h}_D)} = 0.$$

Taking the limit for $h^* \to \infty$ we are left with

$$\frac{-m^*}{2(h_P + 3\bar{h}_D)} + \sum_{K=3}^{M} \frac{(\bar{h}_D - h_K)m^{(K)}}{w^K(h_K, h_P, \bar{h}_D)} = 0$$

which, under assumptions of $\bar{h}_D > 0$ and $h_K > 0$, is equivalent to the polynomial equation of degree $2(M - 2)$:

$$(5.8) \quad \sum_{K=3}^{M} 2(\bar{h}_D - h_K)(h_P + 3\bar{h}_D)m^{(K)} \prod_{L=3\,(L \neq K)}^{M} w^L(h_L, \bar{h}_P, \bar{h}_D)$$
$$- m^* \prod_{K=3}^{M} w^K(h_K, \bar{h}_P, \bar{h}_D) = 0.$$

Analysis of this polynomial leads to the conclusion that it has at least one positive root as long as $m^* \leq 2$. In other words, a finite self-consistent estimate for the overall shear modulus exists as long as the dimension of a space of constraint deviatoric deformation modes is less than three.

Now, let us consider incompressible materials in which additionally some subspace of deviatoric deformation modes is constraint. As it was already shown, the overall bulk modulus is infinite in this case. Let us rewrite Eq. (5.1) as follows:

$$5\bar{h}_D \frac{(\bar{h}_D - h^*)m^*}{2h^* + 3\bar{h}_D} + 5\bar{h}_D \sum_{K=3}^{M} \frac{(\bar{h}_D - h_K)m^{(K)}}{2h_K + 3\bar{h}_D} = 0, \qquad \sum_{K=3}^{M} m^{(K)} \leq 4$$

where as previously m^* denotes the dimension of the constraint subspace of deviatoric deformation modes (due to incompressibility, total dimension of the space of constraint deformation modes is $m^* + 1$). Now we take a limit of this equation for $h^* \to \infty$ and find the counterpart of polynomial equation (5.2)

$$(5.9) \quad \sum_{K=3}^{M} 2(\bar{h}_D - h_K)m^{(K)} \prod_{L=3\,(L \neq K)}^{M} (2h_L + 3\bar{h}_D) - m^* \prod_{K=3}^{M} (2h_K + 3\bar{h}_D) = 0$$

which is of degree $M - 2$. Positive solution for the above polynomial equation exists and is unique only if $m^* = 1$. In other words, in the case of incompressible materials the self-consistent estimate for the overall shear modulus is finite only when the subspace of restricted deviatoric modes is one-dimensional.

5.3. Examples

In order to illustrate the utility of the obtained general results of this section we specify the solution for the selected incompressible linear viscous materials. For metals, usually the viscoplastic regularization is used for the description of their inelastic deformation taking place by crystallographic slip on N slip systems. The number and geometry of slip systems depend on the geometry of crystallographic lattice of a single crystal. The local constitutive relation is formulated as a power law in the form

$$(5.10) \quad \dot{\varepsilon}^{vp} = v_0 \sum_{r=1}^{N} \left(\frac{\tau^r}{\tau_c^r}\right)^n \mathbf{P}^r,$$

where v_0 is a reference slip rate, τ^r, τ_c^r are the resolved shear on the slip system r and the corresponding critical shear stress, where

$$\tau^r = \boldsymbol{\sigma} \cdot \mathbf{P}^r, \qquad \mathbf{P}^r = \frac{1}{2}(\mathbf{m}^r \otimes \mathbf{n}^r + \mathbf{n}^r \otimes \mathbf{m}^r).$$

Two unit vectors $\mathbf{m}^r$ and $\mathbf{n}^r$ define the slip system denoting the slip direction and plane normal to the slip, respectively. Clearly, material described by (5.10) is incompressible. When $n = 1$, the linear relation is obtained

$$(5.11) \qquad \dot{\boldsymbol{\varepsilon}}^{vp} = \mathbb{M}^v \cdot \boldsymbol{\sigma}, \qquad \mathbb{M}^{vp} = v_0 \sum_{r=1}^{N} \frac{1}{\tau_c^r} \mathbf{P}^r \otimes \mathbf{P}^r.$$

Below, the solutions are derived for bounds and self-consistent estimate of overall viscous shear modulus $\bar{h}_D$ for fcc polycrystals, γ-TiAl polycrystal of near-gamma microstructure and hcp Mg polycrystals of random texture, assuming $n = 1$. Note that usually $n > 1$ is identified for these materials. Then a single crystal is described by a non-linear constitutive law. Consequently, solutions for bounds and self-consistent estimates require an appropriate linearization of a problem and depend on the loading scheme. Estimates are found numerically by discretization of the orientation space, see e.g. [13, 21] or [20]. In these calculations, knowledge of the analytical solutions for the limit case $n = 1$ is beneficial from the point of view of verification of the applied numerical procedures as well as it provides good initial approximation of a solution.

5.3.1. Fcc polycrystals. Single crystal of a fcc unit cell has 12 slip systems $\{111\} < 110 >$ of the same type ($\tau_c^r = \tau_c$). One finds

$$\mathbb{M}^{vp} = \frac{v_0}{\tau_c} \left(\frac{1}{h_2} \mathbb{P}_2 + \frac{1}{h_3} \mathbb{P}_3 \right), \qquad h_2 = \frac{1}{2}, \qquad h_3 = \frac{3}{2},$$

where h_2 is of multiplicity 2 and h_3 of multiplicity 3, and $\mathbb{P}_2$ and $\mathbb{P}_3$ are specified as for cubic symmetry [16]. Using formulas (3.4), (3.8) and (A.8) one finds immediately

$$\bar{h}_D^{LO} = \frac{5}{6} \left[\frac{\tau_c}{v_0} \right], \qquad \bar{h}_D^{SC} = 1 \left[\frac{\tau_c}{v_0} \right], \qquad \bar{h}_D^{UP} = \frac{11}{10} \left[\frac{\tau_c}{v_0} \right].$$

Equivalent solution was obtained in [13].

5.3.2. γ-TiAl intermetallic. Titanium aluminide of near-gamma microstructure can be modelled as a polycrystal composed of spherical grains. Single crystal has a fcc-like unit cell with 12 possible slip systems but they are subdivided

into two groups: 4 ordinary dislocations $\{111\} < 1\bar{1}0]$ and 8 super-dislocations $\{111\} < 10\bar{1}]$ [2]. Denoting $\rho = \frac{\tau_c^{\text{sup}}}{\tau_c^{\text{ord}}}$ one finds

$$\mathbb{M}^{vp} = \frac{v_0}{\tau_c^{\text{ord}}} \left(\frac{1}{h_2}\mathbb{P}_2 + \frac{1}{h_3}\mathbb{P}_3 + \frac{1}{h_4}\mathbb{P}_4 + \frac{1}{h_5}\mathbb{P}_5 \right),$$

Projectors $\mathbb{P}_K$ are specified as for volumetrically isotropic material of tetragonal symmetry (see [16]) and

$$h_2 = \frac{\rho}{2}, \qquad h_3 = \frac{3\rho}{2+4\rho}, \qquad h_4 = \frac{3\rho}{2}, \qquad h_5 = \frac{3\rho}{1+\rho}.$$

where h_5 is of multiplicity 2. Using formulae (3.4) and (3.8) one finds upper and lower bounds

$$(5.12) \quad \bar{h}_D^{LO} = \frac{5\rho}{4+2\rho} \left[\frac{\tau_c^{\text{ord}}}{v_0} \right], \qquad \bar{h}_D^{UP} = \frac{1}{5}\rho \left(2 + \frac{6}{1+\rho} + \frac{3}{2+4\rho} \right) \left[\frac{\tau_c^{\text{ord}}}{v_0} \right]$$

while the self-consistent estimate is the single positive real root of the following polynomial equation of degree 4:

$$3\bar{h}_D^4 + \frac{\rho(7+8\rho)}{2(1+2\rho)}\bar{h}_D^3 - \frac{\rho^2(7+8\rho)}{(1+\rho)(1+2\rho)}\bar{h}_D^2 - \frac{3\rho^3(7+3\rho)}{2(1+\rho)(1+2\rho)}\bar{h}_D$$
$$- \frac{3\rho^4}{(1+\rho)(1+2\rho)} = 0.$$

Figure 1 presents the solution of the above equation for different values of ρ together with the corresponding upper and lower bounds specified by (5.12). It is observed in experiments [2] that super-dislocations are more difficult to initiate than ordinary dislocations, therefore $\rho > 1$ is physically meaningful.
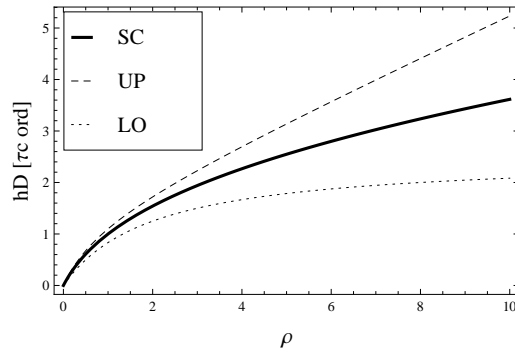

Fig. 1. Dependence of bounds and self-consistent estimate of an overall viscous stiffness of TiAl random polycrystal on $\rho = \tau_c^{\text{sup}}/\tau_c^{\text{ord}}$.

Now, let us look at the limit situation when $\rho \longrightarrow \infty$ which means that the inelastic deformation is possible only by ordinary dislocations. In this case, the

subspace of deviatoric strain-rate tensors which are possible to realize by this reduced set of slip systems is three-dimensional. Taking the limit values of h_k one obtains

$$h_2 = h_4 \longrightarrow \infty, \qquad h_3 = \frac{3}{4}, \qquad h_5 = 3,$$

therefore the multiplicity of the infinite deviatoric Kelvin moduli is two. According to the analysis performed in the preceding subsection, a finite self-consistent estimate does not exist in such a case. The limited number of easy slip systems is the main source of poor ductility of titanium aluminides which inhibits its industrial use in spite of its high specific strength and stiffness. It should be noted that the lack of easy slip systems is partially balanced by the activation of a twinning mechanism which can be described as pseudo-slip (see [7]). However, twin systems cannot be directly included in the presented analysis as far as, due to their uni-directionality, they introduce non-linearity into the constitutive relation even for $n = 1$.

5.3.3. hcp Mg polycrystals. Other materials of high specific strength and stiffness but of limited ductility are the Mg alloys. The Mg single crystal of a hcp lattice structure has hexagonal symmetry. Usually four groups of slip systems are reported for magnesium [1, 32]: 3 basal $(0001)<11\bar{2}0>$, 3 prismatic $\{1100\}<11\bar{2}0>$, 6 pyramidal $<a>$ $\{1\bar{1}01\}<11\bar{2}0>$ and 6 pyramidal $<c+a>$ $\{1122\}<11\bar{2}3>$. Only basal slip systems are considered to be the easy ones, however, the subspace of deviatoric strain-rate states which are possible to take place by this reduced set of slip systems is two-dimensional. Addition of prismatic or pyramidal $<a>$ slip systems (or both of them) makes this subspace four-dimensional. Only the set of pyramidal $<c+a>$ slip systems covers the whole deviatoric space. Again, due to the reasons explained above, twinning mechanism is not considered.

Let us denote

$$\rho_1 = \frac{\tau_c^{\mathrm{prism}}}{\tau_c^{\mathrm{basal}}}, \qquad \rho_2 = \frac{\tau_c^{\mathrm{pyram}<a>}}{\tau_c^{\mathrm{basal}}}, \qquad \rho_3 = \frac{\tau_c^{\mathrm{pyram}<c+a>}}{\tau_c^{\mathrm{basal}}}.$$

If all 18 slip systems can be initiated, using (5.11) one obtains local viscous compliance tensor in the form

$$(5.13) \qquad \mathbb{M}^{vp} = \underbrace{\frac{9d^2}{(1+d^2)^2\rho_3}}_{1/h_2} \mathbb{P}_2 + \underbrace{\frac{3}{4}\left(\frac{1}{\rho_1} + \frac{8d^2}{(3+4d^2)\rho_2} + \frac{2d^2}{(1+d^2)^2\rho_3}\right)}_{1/h_3} \mathbb{P}_3$$

$$+ \underbrace{\left(\frac{3}{4} + \frac{9}{(6+8d^2)\rho_2} + \frac{3(1-d^2)^2}{2(1+d^2)^2\rho_3}\right)}_{1/h_4} \mathbb{P}_4,$$

where d is the c/a ratio describing lattice geometry (see [15] for its definition) while projectors $\mathbb{P}_K$ are specified as for a volumetrically isotropic material of transversal isotropy (see [16]). In the case of Mg crystal, lattice geometry parameter d is equal to 1.624 [15]. Identifying h_K, $K = 2, 3, 4$ as indicated by (5.13), where h_2 is of multiplicity one and h_3, h_4 of multiplicity 2, one easily obtains lower and upper bounds using Eq. $(3.4)_2$ and Eq. $(3.8)_2$ as well as the self-consistent estimate from cubic equation (A.9).
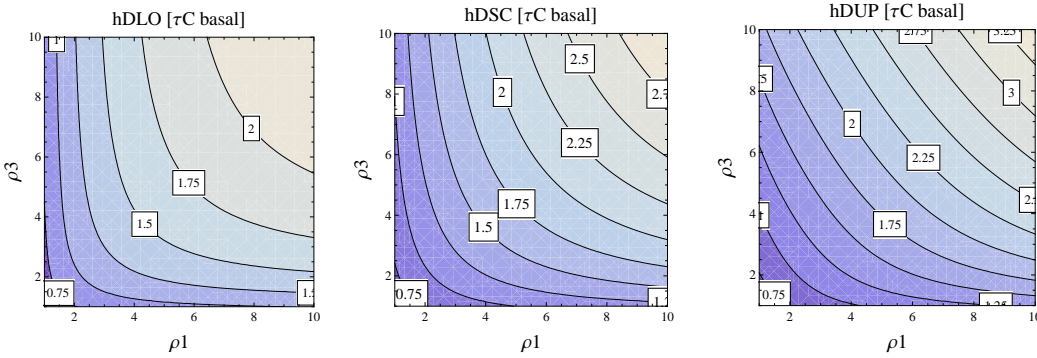
Fig. 2. Bounds and self-consistent estimate of an overall viscous shear modulus of a hcp Mg random polycrystal for $\rho_1 = \rho_2$.

It is interesting to analyse some special cases of the above solutions. First, let us assume that $\rho_1 = \rho_2$, then the solutions concerning bounds and self-consistent estimate depend on two parameters ρ_1 and ρ_3. They are presented in Fig. 2. Two limit situations can be considered: $\rho_3 \to \infty$ and $\rho_1 = \rho_2 \to \infty$ corresponding to blocking pyramidal $<c+a>$ or prismatic+pyramidal $<a>$ sets of slip systems, respectively. For the first case, local Kelvin moduli are

$$\rho_3 \to \infty \Rightarrow h_2 \to \infty, \qquad h_3 = \frac{4(3+4d^2)}{9(1+4d^2)}\rho_1, \qquad h_4 = \frac{4(3+4d^2)\rho_1}{3(6+(3+4d^2)\rho_1)}$$

and since the infinite local modulus h_2 is of multiplicity one, a finite self-consistent estimate can be found from the quadratic equation with one positive root

$$15\bar{h}_D^2 - 3f(\rho_1)(3+\rho_1)\bar{h}_D - 8\rho_1 f(\rho_1) = 0,$$

where

$$f(\rho_1) = \frac{40(3+4d^2)^2 \rho_1}{27(1+4d^2)(6+(3+4d^2)\rho_1)}.$$

The corresponding upper bound is infinite while the lower bound is:

$$\bar{h}_D^{LO} = \frac{10\rho_1}{3(3+\rho_1)}.$$

Resulting values are presented in Fig. 3a. In the second case the local Kelvin moduli are

$$\rho_1 = \rho_2 \to \infty \Rightarrow h_2 = \frac{(1+d^2)^2}{9d^2}\rho_3, \qquad h_3 = \frac{2(1+d^2)^2}{3d^2}\rho_3,$$

$$h_4 = \frac{4(1+d^2)^2\rho_3}{3(2(1-d^2)^2 + (1+d^2)^2\rho_3)},$$

so all of them are finite and bounds and a self-consistent estimate can be found using formulae (3.4), (3.8) and the cubic Eq. (A.9). Results are presented in Fig. 3b.
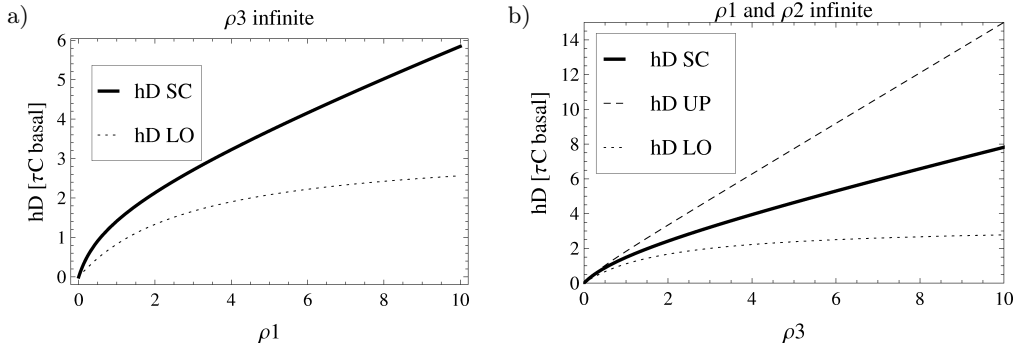

Fig. 3. Bounds and self-consistent estimate of an overall viscous shear modulus of a hcp Mg random polycrystal for a) $\rho_3 \to \infty$ (pyramidal $<c+a>$ slip systems are blocked) b) $\rho_1 = \rho_2 \to \infty$ (prismatic and pyramidal $<a>$ slip systems are blocked).

Finally, it is easy to see that if all slip systems except the easy ones are blocked (that is $\rho_1 \to \infty$, $\rho_2 \to \infty$ and $\rho_3 \to \infty$), then only the local Kelvin modulus h_4 is finite, therefore a finite self-consistent estimate of $\bar{h}_D$ does not exist.

Let us add that finite self-consistent estimates can be also found for the cases when both the prismatic and pyramidal $<c+a>$ slip systems are blocked ($\rho_1 \to \infty$ and $\rho_3 \to \infty$) or when both the pyramidal $<a>$ and pyramidal $<c+a>$ slip systems are blocked ($\rho_2 \to \infty$ and $\rho_3 \to \infty$).

Self-consistent estimates for the single crystal with different groups of slip systems blocked are compared in Fig. 4. Surprisingly, although pyramidal $<c+a>$ slip systems are sufficient to realize any deviatoric strain-rate state, the self-consistent estimate for $\bar{h}_D$ in the case when only basal and pyramidal $<c+a>$ slip systems can operate is higher than for the case, when pyramidal $<c+a>$ slip systems are blocked while other groups of slip system can be activated with the same level of the corresponding critical shear stresses. It means that in the first case, the polycrystal is more stiff than in the latter one. Variation of a self-consistent estimate and a lower bound for this case when $\rho_1 \neq \rho_2$ is presented
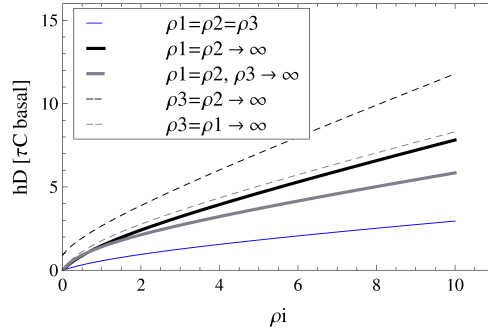
Fig. 4. Comparison of self-consistent estimates of an overall viscous shear modulus of a Mg random polycrystal for different active sets of slip systems.

in Fig. 5. Moreover, one can also observe that activation of the pyramidal $<a>$ slip systems is more beneficial, from the point of view of polycrystal ductility, than activation of the prismatic slip systems.
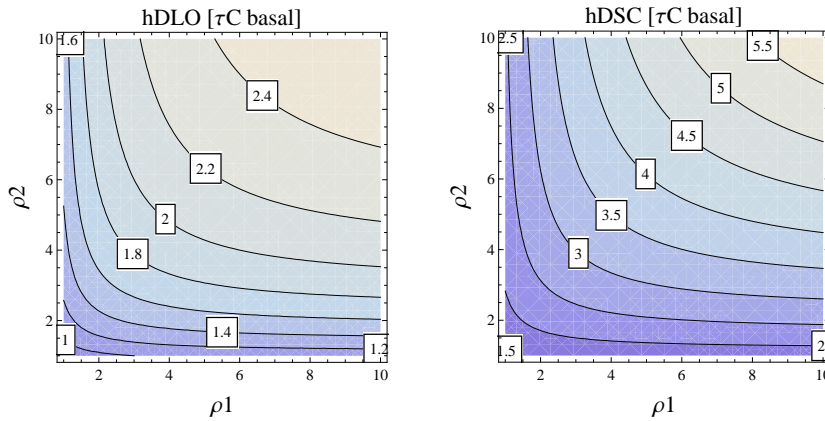

Fig. 5. Lower bounds and a self-consistent estimate of an overall viscous stiffness of a hcp Mg random polycrystal for $\rho_1 \neq \rho_2$ and pyramidal $<c + a>$ slip systems blocked.

6. Summary

Using the spectral and harmonic decompositions of Hooke's tensors, the bounds and self-consistent estimates have been derived for random polycrystals composed of elements of arbitrary anisotropy. For the wide class of anisotropic crystals, solutions have been provided in the form of polynomial equations with coefficients depending on the invariants of a local stiffness tensor. Incompressible materials as well as materials with constraint deformation modes have been considered. It was demonstrated that the existence of a finite self-consistent es-

timate for an overall shear modulus depends on the dimension of a subspace of constrained deviatoric deformation. Utility of the analysis has been demonstrated on the examples of metals and alloys of high specific strength and stiffness.

Acknowledgment

Appendix

The crystal bulk modulus h_P and the following functions of deviatoric Kelvin moduli

$$J_1 = h_2 + h_3 + h_4 + h_5 + h_6 > 0,$$
$$J_2 = h_2 h_3 + h_2 h_4 + \ldots + h_5 h_6 > 0,$$
$$J_3 = h_2 h_3 h_4 + h_2 h_3 h_5 + \ldots + h_4 h_5 h_6 > 0,$$
$$J_4 = h_2 h_3 h_4 h_5 + h_2 h_3 h_4 h_6 + \ldots + h_3 h_4 h_5 h_6 > 0,$$
$$J_5 = h_2 h_3 h_4 h_5 h_6 > 0$$

are invariants of a local $\mathbb{L}$ for the volumetrically isotropic material, which are independent of ordering of h_K and can be calculated without performing the spectral decomposition. The coefficients α_k of the polynomial equation (4.9) for a self-consistent estimate of an overall shear modulus $\bar{h}_D$ are specified with use of the above invariants as follows:

$$\alpha_0 = -16 J_5 h_P^4 < 0,$$
$$\alpha_1 = -h_P^3 \left(192 J_5 + 16 J_4 h_P\right) < 0,$$
$$\alpha_2 = -h_P^2 \left(864 J_5 + 160 J_4 h_P + 12 J_3 h_P^2\right) < 0,$$
$$\alpha_3 = -h_P \left(1728 J_5 + 576 J_4 h_P + 88 J_3 h_P^2\right) < 0,$$
$$\alpha_4 = -\left(1296 J_5 + 864 J_4 h_P + 204 J_3 h_P^2 - 36 J_2 h_P^3 - 27 J_1 h_P^4\right),$$
$$\alpha_5 = -\left(432 J_4 + 144 J_3 h_P - 204 J_2 h_P^2 - 216 J_1 h_P^3 - 81 h_P^4\right),$$
$$\alpha_6 = 352 J_2 h_P + 576 J_1 h_P^2 + 432 h_P^3 > 0,$$
$$\alpha_7 = 192 J_2 + 640 J_1 h_P + 864 h_P^2 > 0,$$
$$\alpha_8 = 256 J_1 + 768 h_P > 0,$$
$$\alpha_9 = 256.$$

Analysis of α_k indicates that the polynomial (4.9) has at least one and no more than three positive real roots. Three positive roots are obtained if simultaneously

(A.1) $$\alpha_4 > 0 \quad \text{and} \quad \alpha_5 < 0.$$

Now, we prove that both inequalities cannot be true at the same time which ensures that Eq. (4.9) has a unique positive solution.

To this end, note that α_4 and α_5 are linear functions of J_K and 4th-order polynomial functions of h_P. Domains of admissible arguments of these functions are defined as $J_K > 0$ and $h_P > 0$. Let us consider α_4 and α_5 as linear functions of J_1. Condition $(A.1)_2$ can be then rewritten as

(A.2) $$27h_P^4 J_1 < 54J_4 h_P + 18J_3 h_P^2 - 51/2 J_2 h_P^3 - 81/8 h_P^5.$$

There exists such $J_1 \in (0, J_1^{(0)})$ for which the above inequality is true only if

(A.3) $$51/2 J_2 h_P^3 < 54 J_4 h_P + 18 J_3 h_P^2 - 81/8 h_P^5.$$

Otherwise the condition (A.1) cannot be fulfilled. Inequality $(A.1)_1$ is specified as

(A.4) $$27h_P^4 J_1 > 1296 J_5 + 864 J_4 h_P + 204 J_3 h_P^2 - 36 J_2 h_P^3.$$

Combining (A.2) and (A.4) it is obtained that

$$51/2 J_2 h_P^3 > 17/7(1296 J_5 + 810 J_4 h_P + 186 J_3 h_P^2 + 81/8 h_P^5).$$

Now, combining the above inequality with (A.3) we arrive at an inequality

$$22032 J_5 + 13392 J_4 h_P + 3036 J_3 h_P^2 + 243 h_P^5 < 0$$

which apparently cannot be true for any positive J_K and h_P, therefore we have proved that condition (A.1) cannot be fulfilled for any combination of J_K and h_P. Consequently, the polynomial equation (4.9) has always a unique positive solution.

The form (4.7) of the polynomial equation is simplified as compared to (4.9), as far as it takes into account information about the multiplicity of Kelvin moduli what enables one to lower the degree of a polynomial. Now, we specify the polynomial equation for $M = 3$ with $m^K = \{2, 3\}$ and $M = 4$ with $m^K = \{1, 2, 2\}$, which cases correspond, for example, to cubic symmetry and hexagonal symmetry (transversal isotropy) of single crystal, respectively. In the first case, polynomial equation (4.7) takes the form of the third-order equation

(A.5) $$4\bar{h}_D^3 + \bar{h}_D^2 (3h_P + 2h_2) - \bar{h}_D (6h_2 + h_P) h_3 - 2h_2 h_3 h_P = 0.$$

It corresponds to the equation for an overall shear modulus of cubic crystals found by Kröner [18] (see also [12, 35]), specified in terms of components of local stiffness tensor. In the second case (4.7) is the 5-th order equation of the form

$$(A.6) \qquad -4h_2h_3h_4h_P^2 - 2(12h_2h_3h_4 + (h_2h_3 + h_2h_4 + 2h_3h_4)h_P)h_P\bar{h}_D$$
$$- (36h_2h_3h_4 + (6h_2h_3 + 6h_2h_4 + 16h_3h_4)h_P - 3h_2h_P^2)\bar{h}_D^2$$
$$- (12h_3h_4 - (16h_2 + 6h_3 + 6h_4)h_P - 9h_P^2)\bar{h}_D^3$$
$$+ (16h_2 + 8h_3 + 8h_4 + 24h_P)\bar{h}_D^4 + 16\bar{h}_D^5 = 0.$$

Equation for a self-consistent estimate of an overall shear modulus for incompressible material can also be expressed in terms of invariants J_k, assuming $m^{(K)} = 1$ for all deviatoric Kelvin moduli h_K, $K = 2, \ldots, 6$. It has the following form:

$$(A.7) \qquad 81\bar{h}_D^5 + 27J_1\bar{h}_D^4 - 12J_3\bar{h}_D^2 - 16J_4\bar{h}_D - 16J_5 = 0.$$

This equations has a single positive real root.

Let us specify Eq. (5.2) for incompressible crystals of cubic symmetry and of hexagonal symmetry. In the first case we have to do with two deviatoric Kelvin moduli h_2 and h_3 of multiplicity 2 and 3, respectively. Polynomial equation (5.2) reduces to the quadratic one with one positive root

$$(A.8) \qquad 3\bar{h}_D^2 - h_3\bar{h}_D - 2h_2h_3 = 0 \Rightarrow \bar{h}_D = \frac{h_3}{6}\left(1 + \sqrt{1 + 24\frac{h_2}{h_3}}\right).$$

In the second case there are three deviatoric moduli: h_2 of multiplicity 1, h_3 and h_4 of multiplicity 2 (hexagonal symmetry from the point of view of the form of $\mathbb{L}$ is equivalent to the transversal isotropy). Polynomial equation is now cubic

$$(A.9) \qquad 9\bar{h}_D^3 + 3h_2\bar{h}_D^2 - 2(h_2h_3 + h_2h_4 + 2h_3h_4)\bar{h}_D - 4h_2h_3h_4 = 0$$

and the exact, though complicated, formula can be provided for the single positive root using the known procedure for solving cubic equations.

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