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Estimation of overall properties of random polycrystals with the use of invariant decompositions of Hooke's tensor

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ABSTRACT

In the paper the theoretical analysis of bounds and self-consistent estimates of overall properties of linear random polycrystals composed of arbitrarily anisotropic grains is presented. In the study two invariant decompositions of Hooke's tensors are used. The applied method enables derivation of novel expressions for estimates of the bulk and shear moduli, which depend on invariants of local stiffness tensor. With use of these expressions the materials are considered for which at the local level constraints are imposed on deformation or some stresses are unsustained.

1. Introduction

Assessment of overall properties of heterogenous materials on the basis of a knowledge about their microstructure and local properties is the central problem of contemporary micromechanics which has its practical and theoretical aspects. This problem attracts researchers since the 50s of the previous century. Many important results and developments have been obtained and proposed since then (Christensen, 1979; Nemat-Nasser and Hori, 1999; Milton, 2002; Li and Wang, 2008). This work deals with the special class of heterogeneous materials which are the polycrystalline aggregates. Different estimates of overall properties of such materials are considered.

In the paper *linear crystals* are studied, i.e. it is assumed that mechanical behavior of constituent grains is governed by a *linear* constitutive law relating strain and stress measure, thus material properties are represented by fourth-order Hooke's tensor. The study encompasses for example linear elasticity but also linear viscous materials. Analytical expressions for uniform strain upper bound and uniform stress lower bound are provided. Moreover, more rigorous bounds, resulting from the theorems of minimum potential energy and of minimum complementary energy, proposed by Hashin and Shtrickman (Hashin and Shtrikman, 1962a,b) are analysed. The detailed theoretical treatment of these bounds as well as its generalizations are presented in Willis (1977, 1981), Walpole (1981), Talbot and Willis (1985), de Botton and Ponte Castañeda (1995), and Castañeda et al. (1998). In the present work *random* distribution of crystal orientations within the representative aggregate leading to the *isotropic overall behavior* is assumed. The developed procedure is also useful when analyzing polycrystal with other type of texture. Preliminary results concerning the polycrystals with fiber texture can be found in Kowalczyk-Gajewska (2011).

Next, the so-called self-consistent estimates of overall properties are considered. In the self-consistent scheme a single crystal is viewed as an ellipsoidal inclusion embedded in an infinite medium of unknown properties. For the theoretical formulations concerning a self-consistent method one is referred to the classical papers (Kröner, 1958; Hill, 1965; Willis, 1981; Walpole, 1981). Below they are specified 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. Existence and uniqueness of obtained solutions are discussed. Reductions of above estimates for incompressible materials, materials with *constrained* modes of *deformation* and materials with *unsustained stresses* are also derived. It seems that the most interesting results have been obtained within the context of materials with constraints. For example, the scaling law proposed in Nebozhyn et al. (2000, 2001) is here proven analytically. For viscous deformation by slip one has to do with the constrained deformation if crystal has an insufficient number of easy slip systems. It is the case for many metals and alloys of low symmetry e.g. Mg, Ti, Zr or γ-TiAl alloys. Many of them exhibit high specific strength and stiffness but suffer from low ductility.

Some of the derived results are already known in the literature. Uniform strain and uniform stress bounds in a concise form have been provided by Walpole (1981), and by Cowin et al. (1999) using the spectral theorem. A quartic equation for a self-consistent estimate of an overall shear modulus for cubic crystals has been found

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already by Hershey in Hershey (1954) (independently by Kröner (1958)) and then reduced to the cubic one e.g. in Kröner (1958), Hill (1965), and Willis (1981). Hexagonal crystals have been studied by Kneer (1963). Qui and Weng (1991) have discussed the influence of grain morphology on the self-consistent estimates for overall properties of such crystals. For hexagonal, trigonal and tetragonal crystals implicit equations for these estimates, depending on the components of a local stiffness tensor, were provided in different forms by Pham (1997), and Pham (2003) and by Berryman (2005). The Hashin–Shtrikman bounds have been provided for different crystal symmetries e.g. in Peselnick and Meister (1986), Watt (1965), Pham (2003), and Berryman (2005) (see also literature cited there). Optimal bounds on effective bulk and shear moduli of planar isotropic polycrystals composed of grains of orthotropic symmetry have been characterized by Avellaneda et al. (1996). The invariant decompositions of Hooke's tensor have been utilized to study the bounds and estimates of elastic properties for textured polycrystals of cubic symmetry in Böhlke and Bertram (2001), and Böhlke et al. (2010).

The originality of a presented analysis lies mainly in the method applied. In order to obtain the solutions, spectral and harmonic decompositions of fourth-order Hooke's tensor are used simultaneously. Thanks to that the important feature of the derived solutions is that they are expressed by means of invariants of local stiffness (compliance) tensors. The method has been proposed in Kowalczyk-Gajewska (2009) and applied to the analysis of the Voigt and Reuss bounds and self-consistent estimates. The most interesting result reported in Kowalczyk-Gajewska (2009) concerns the condition for an existence of the self-consistent estimate of the flow stress for the viscously linear random polycrystal with an insufficient number of independent slip systems. It has been proved that such estimate exists only if the constrained deviatoric space is one-dimensional. It means that crystal should have at least four independent slip systems in order to have a finite self-consistent estimate of an overall flow stress. It is a counterpart of the well-known Taylor condition of five independent slip systems, which guaranties acceptable solutions obtained by means of an uniform strain hypothesis. Here, the analysis is extended to the formulation of the Hashin–Shtrikman bounds. Additionally, new results, with respect to Kowalczyk-Gajewska (2009), concern the scaling laws for self-consistent estimates applicable to materials with constrained deformation. Moreover, crystals with unsustained stresses are discussed. For volumetrically isotropic crystals belonging to this class the condition of existence of a non-zero estimate of a shear modulus is formulated. As an example of material with unsustained stresses, again the creep of crystals of low symmetry can be indicated. When initiation of slip for some category of admissible slip systems is much smaller than for another ones, then the subspace of deviatoric stresses generated by geometry of independent easy slip systems can be identified as a subspace of unsustained stresses (see Section 4).

For the derived results concerning crystals with constrained deformation and with unsustained stresses analogy can be drawn with the limitation of the self-consistent method indicated by Budiansky already in Budiansky (1965) when assessing the effective properties of two-phase isotropic material for which one phase is incompressible while the other corresponds to rigid inclusions (moduli $G = K \to \infty$) or holes (moduli $G = K = 0$). In the first case a finite overall shear modulus $\overline{G}$ is obtained when volume fraction of rigid inclusions is less than 2/5. In the second case, the non-zero overall bulk modulus $\overline{K}$ and shear modulus $\overline{G}$ are obtained when volume fraction of holes is less than 1/2. It can be also shown that if one phase is a non-viscous fluid ($K \neq 0$ and $G = 0$) and the second phase is isotropic (not necessarily incompressible) then the overall shear modulus is non-zero when the volume fraction of a fluid phase is less than 3/5 (Milton, 2002). One can wonder if the result proven in Kowalczyk-Gajewska (2009), for polycrystals with an insufficient number of easy slip systems, and the results obtained in Section 3, for materials with unsustained stresses, indicate similar limitation of the self-consistent method applied to polycrystalline one-phase materials or represent their real behavior. Although a definite answer to this question is not yet established, some support for the latter possibility can be found in Lebensohn et al. (2004); therefore a linear ice-type crystal and a Zr-type crystal studied in the latter paper are invoked as illustrative examples in the last section of this paper.

The paper consists of five sections. After this introductory part in which we state the problem, in Section 2 we shortly recall the results derived in Kowalczyk-Gajewska (2009) concerning uniform strain and uniform stress bounds and extend the analysis to the Hashin-Shtrickman bounds. In Section 3 we discuss the self-consistent estimates focusing on the crystals with constrained deformation and with unsustained stresses. In Section 4 the derived formulae are applied to estimate linear viscous properties of polycrystals of low symmetry. Section 5 contains a summary of results and concluding remarks. In Appendix A the spectral and harmonic decompositions of Hooke's tensor are recalled in a nutshell introducing the required notation. More details concerning the spectral theorem one may find e.g. in Rychlewski (1995), Cowin and Mehrabadi (1995), and Chadwick et al. (2001). The harmonic decomposition is presented e.g. in Forte and Vianello (1996), Rychlewski (2000), Rychlewski (2001b), and Rychlewski (2001a). The reader is referred to these publications for more details.

Throughout the paper the so-called "tensor" notation is used. Notation conventions are as follows: scalars are in mathematical italics, e.g. α, E, σ_Y; for vectors and second-order tensors boldface roman or greek symbols are used (meaning should be clear from the context), e.g. $\mathbf{n}$, $\boldsymbol{\sigma}$; the blackboard style is used for the fourth-order tensors, e.g. $\mathbb{L}, \mathbb{A}$. The second-order and the symmetrized fourth-order identity tensors are denoted as $\mathbf{I}$ and $\mathbb{I}^S$, respectively. Their components in any orthonormal basis are found to be δ_{ij} and $\frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{kj})$. Notation used for operations between tensors of different order is as follows (summation convention applies): $\mathbf{u} \otimes \mathbf{v}$ and $\mathbf{A} \otimes \mathbf{B}$ mean $u_i v_j$ and $A_{ij}B_{kl}$, respectively, $\mathbf{A} \cdot \mathbf{n}$ and $\mathbf{A} \cdot \mathbf{B}$ mean $A_{ij}n_j$ and $A_{ij}B_{ij}$, respectively, $\mathbf{AB}$ means $A_{ij}B_{jk}$, $\mathbf{B} \cdot \mathbb{A}$ and $\mathbb{A} \cdot \mathbf{B}$ mean $A_{ijkl}B_{ij}$ and $A_{ijkl}B_{kl}$, respectively, while $\mathbb{A} \circ \mathbb{B}$ means $A_{ijkl}B_{klmn}$, where $(\cdot)_{ijkl}, (\cdot)_{ij}, (\cdot)_i$ signify components of subsequent tensorial quantities in some orthonormal basis. The inverses of second- and fourth-order Hooke's tensors are denoted by $\mathbf{A}^{-1}$ and $\mathbb{A}^{-1}$, respectively and they are defined by relations $\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$, $\mathbb{A}^{-1} \circ \mathbb{A} = \mathbb{A} \circ \mathbb{A}^{-1} = \mathbb{I}^S$.

Let us now formulate the problem which is addressed within the paper. Assume a single-phase polycrystal with components (i.e. grains) of arbitrary anisotropy, with the same properties although axes of symmetry $\{\mathbf{a}_k\}$ rotated with respect to each other (see Fig. 1). 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 $\boldsymbol{\sigma}$ and strain tensor (or strain-rate tensor) $\boldsymbol{\varepsilon}$ is linear,

$$\boldsymbol{\varepsilon} = \mathbb{M} \cdot \boldsymbol{\sigma}, \quad \boldsymbol{\sigma} = \mathbb{L} \cdot \boldsymbol{\varepsilon}, \quad \mathbb{L} = \mathbb{M}^{-1}, \tag{1}$$

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

$$\mathbf{E} = \bar{\mathbb{M}} \cdot \boldsymbol{\Sigma}, \quad \boldsymbol{\Sigma} = \bar{\mathbb{L}} \cdot \mathbf{E}, \quad \bar{\mathbb{L}} = \bar{\mathbb{M}}^{-1}. \tag{2}$$

Moreover, all the introduced fourth-order tensors have the symmetries with respect to the permutation of indices of Hooke's tensor (see Appendix A). Note that major symmetry of the

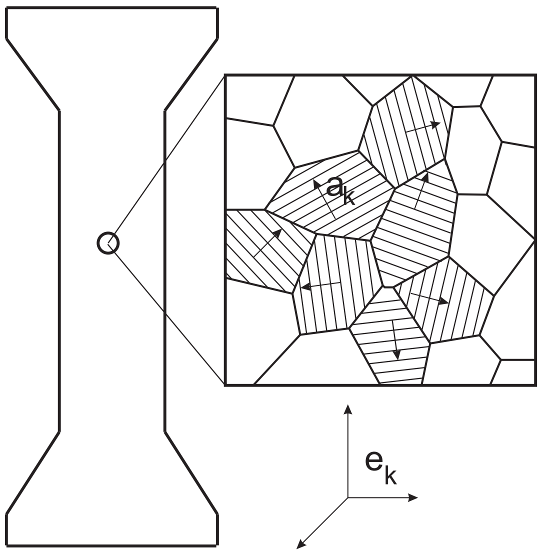

Fig. 1. Polycrystalline element.

constitutive tensor originates in the assumption of existence of a strain potential.

In view of the above assumptions, the spectral decomposition (A.2) can be applied to the local stiffness and compliance tensors

$$\mathbb{L}(\phi^c)=\sum_{K=1}^{M}h_K\mathbb{P}_K(\phi^c),\quad \mathbb{M}(\phi^c)=\sum_{K=1}^{M}\frac{1}{h_K}\mathbb{P}_K(\phi^c),\tag{3}$$

where ϕ^c denotes orientation of local axes $\{\mathbf{a}_k\}$ with respect to some macroscopic frame $\{\mathbf{e}_k\}$ specified by e.g . three Euler angles. Moreover,

$$\mathbb{P}_K(\phi^c)=\mathbf{Q}(\phi^c)\star\mathbb{P}_K(0),\tag{4}$$

where $\mathbf{Q}(\phi^c)$ is the second-order orthogonal tensor and $\mathbb{P}_K(0)$ is the projector for some selected $\mathbf{Q}_0\in\mathcal{Q}_{tex}$, where $\mathcal{Q}_{tex}$ is the space of admissible orientations for the considered texture. In the case of un-textured polycrystal, one can select for example $\mathbf{Q}_0=\mathbf{I}$, so the crystals for which the local and macroscopic frames coincide. $\mathbf{Q}\star(\cdot)$ denotes the rotation operation for a n-th order tensor $\mathcal{A}$, namely

$$\begin{aligned}\mathbf{Q}\star\mathcal{A}&=\mathbf{Q}\star(A_{ij\ldots k}\mathbf{e}_i\otimes\mathbf{e}_j\otimes\ldots\otimes\mathbf{e}_k)\\&=A_{ij\ldots k}(\mathbf{Q}\mathbf{e}_i)\otimes(\mathbf{Q}\mathbf{e}_j)\otimes\ldots\otimes(\mathbf{Q}\mathbf{e}_k).\end{aligned}\tag{5}$$

Now, for each of projectors $\mathbb{P}_K$ the harmonic decomposition (A.5) of a fourth-order Hooke's tensor is applied

$$\mathbb{P}_K(\phi^c)=\eta_K^{\mathrm{P}}\mathbb{I}_{\mathrm{P}}+\eta_K^{\mathrm{D}}\mathbb{I}_{\mathrm{D}}+\mathbb{A}_K^{\mu}(\phi^c)+\mathbb{A}_K^{\nu}(\phi^c)+\mathbb{H}_K(\phi^c),\tag{6}$$

where $\mathbb{I}_{\mathrm{P}}$ and $\mathbb{I}_{\mathrm{D}}$ are specified by (A.6) while

$$\eta_K^{\mathrm{P}}=\frac{1}{3}\mathbf{I}\cdot\mathbb{P}_K(\phi^c)\cdot\mathbf{I}=\frac{1}{3}\mathbf{I}\cdot\mathbb{P}_K(0)\cdot\mathbf{I},\quad \eta_K^{\mathrm{D}}=\frac{1}{5}(m_K-\eta_K^{\mathrm{P}}),\tag{7}$$

$$\mathbb{A}_K^{\mu}(\phi^c)=\mathbb{A}^{\mu}(\boldsymbol{\mu}_{\mathrm{D}K}(\phi^c)),\quad \mathbb{A}_K^{\nu}(\phi^c)=\mathbb{A}^{\nu}(\boldsymbol{\nu}_{\mathrm{D}K}(\phi^c))\tag{8}$$

and m_K is the multiplicity of the corresponding modulus h_K.

The following identities are 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 corresponding rotated tensors as

$$\mathbf{h}(\phi^c)=\mathbf{Q}(\phi^c)\star\mathbf{h},\quad \mathbb{H}(\phi^c)=\mathbf{Q}(\phi^c)\star\mathbb{H},\tag{9}$$

one can prove that

$$\langle\mathbf{h}(\phi^c)\rangle_{\mathcal{Q}}=\mathbf{0},\quad \langle\mathbb{H}(\phi^c)\rangle_{\mathcal{Q}}=\mathbb{O},\tag{10}$$

where $\langle\cdot\rangle_{\mathcal{Q}}$ denotes averaging 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 (Bunge, 1982):

$$\langle\cdot\rangle_{\mathcal{Q}}=\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi}(\,\cdot\,)\sin\psi\,\mathrm{d}\varphi_1\mathrm{d}\psi\mathrm{d}\varphi_2.\tag{11}$$

It should be stressed that such formula for averaging is relevant for an isotropic orientation distribution (i.e. polycrystal with no texture). For other textures, e.g. fiber textures, the set of orientations over which the averaging is performed changes.

An interesting and important subgroup of the considered materials is the class of materials for which $\mathbf{I}$ is the eigenstate of $\mathbb{L}$ and $\mathbb{M}$. Materials with this property are called *volumetrically isotropic* (Burzyński, 1928), since its response to a hydrostatic stress state is the change of volume without the change of shape, similarly as in the case of isotropic materials. Let us denote the Kelvin bulk modulus of $\mathbb{L}$ by h^{P}, then the spectral decompositions (3) for the considered subclass of materials take the form

$$\mathbb{L}(\phi^c)=h^{\mathrm{P}}\mathbb{I}_{\mathrm{P}}+\sum_{K=2}^{M}h_K\mathbb{P}_K(\phi^c),\tag{12}$$

$$\mathbb{M}(\phi^c)=\frac{1}{h^{\mathrm{P}}}\mathbb{I}_{\mathrm{P}}+\sum_{K=2}^{M}\frac{1}{h_K}\mathbb{P}_K(\phi^c),\tag{13}$$

where

$$\mathbb{P}_K(\phi^c)=\eta_K^{\mathrm{D}}\mathbb{I}_{\mathrm{D}}+\mathbb{A}_K^{\nu}(\phi^c)+\mathbb{H}_K(\phi^c),\quad \sum_{K=2}^{M}\mathbb{P}_K(\phi^c)=\mathbb{I}_{\mathrm{D}}\tag{14}$$

and specifically

$$\eta_K^{\mathrm{D}}=\frac{1}{5}m_K,\quad \sum_{K=2}^{M}m_K=5,\quad \mathbb{A}_K^{\nu}(\phi^c)=\mathbb{A}_K^{\nu}(\boldsymbol{\nu}_{\mathrm{D}K}(\phi^c)).\tag{15}$$

Note that all crystals of cubic symmetry are volumetrically isotropic. In Kowalczyk-Gajewska and Ostrowska-Maciejewska (2004a) it has been shown that incompressible materials can be viewed as a special case of the volumetrically isotropic materials for which the bulk modulus is infinite

$$h^{\mathrm{P}}\to\infty.\tag{16}$$

Note that all linearly viscous materials, for which we assume that viscous deformation is incompressible, are volumetrically isotropic.

Moreover, in Kowalczyk-Gajewska and Ostrowska-Maciejewska (2004a), considering linearly elastic materials with constraints imposed on deformation, it has been shown that the subspace of restricted deformation modes is the eigen-subspace of the corresponding constitutive fourth-order tensor (not necessarily volumetrically isotropic). Analogically, it can be proved that the subspace of unsustained stresses[1] is the eigen-subspace of the corresponding constitutive tensor. The dimension of this subspace is denoted as m^*, where m^* is also the multiplicity of the Kelvin modulus h^*. For material with constrained deformation $h^*\to\infty$, while for material with unsustained stresses $h^*\to 0$. Consequently, spectral decompositions (3) have the form

[1] If $\boldsymbol{\sigma}^*$ belongs to the subspace $\mathcal{P}^*$ of unsustained stresses for the material described by Hooke's tensors $\mathbb{L}$ then any stress state $\boldsymbol{\sigma}$ which can be achieved in the material fulfills

$$\boldsymbol{\sigma}^*\cdot\boldsymbol{\sigma}=0\Rightarrow\boldsymbol{\sigma}^*\cdot\mathbb{L}\cdot\boldsymbol{\varepsilon}=0\Rightarrow\mathbb{L}\cdot\boldsymbol{\sigma}^*=\mathbf{0}.\tag{17}$$

$$\mathbb{L}(\phi^c) = h^*\mathbb{P}^*(\phi^c) + \sum_{K=2}^{M} h_K \mathbb{P}_K(\phi^c), \tag{18}$$

$$\mathbb{M}(\phi^c) = \frac{1}{h^*}\mathbb{P}^*(\phi^c) + \sum_{K=2}^{M} \frac{1}{h_K}\mathbb{P}_K(\phi^c). \tag{19}$$

For material with constrained deformations the first component in (19) tends to zero, while for material with unsustained stresses the first component in (18) tends to zero. As it is seen an incompressible material is an example of a material with constrained deformation.

For macroscopically isotropic material its overall stiffness and compliance tensors have the form

$$\bar{\mathbb{L}} = \bar{h}^{\mathrm{P}}\mathbb{I}_{\mathrm{P}} + \bar{h}^{\mathrm{D}}\mathbb{I}_{\mathrm{D}}, \quad \bar{\mathbb{M}} = \frac{1}{\bar{h}^{\mathrm{P}}}\mathbb{I}_{\mathrm{P}} + \frac{1}{\bar{h}^{\mathrm{D}}}\mathbb{I}_{\mathrm{D}}, \tag{20}$$

where $\bar{h}^{\mathrm{P}} = 3\overline{K}$ is the overall Kelvin bulk modulus while $\bar{h}^{\mathrm{D}} = 2\bar{\mu} = 2\overline{G}$ is the overall Kelvin shear modulus. Below 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.[2] Formulae (20) are in the same time spectral and harmonic decompositions of macroscopic constitutive tensors. In the next subsections, when discussing untextured polycrystals (i.e. random polycrystals), we derive the upper and lower bounds for $\bar{h}^{\mathrm{P}}$ and $\bar{h}^{\mathrm{D}}$ as well as their self-consistent estimates.

2. Upper and lower bounds

2.1. Uniform stress and uniform strain (V–R) bounds

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

$$\boldsymbol{\varepsilon} = \mathbf{E}, \tag{22}$$

everywhere in the polycrystal (Hill, 1952). Such upper bound is called the Voigt (1889) bound for elastic materials or the Taylor (1938) bound for rigid-plastic or viscoplastic materials. By averaging Eq. $(1)_2$ and applying hypothesis (22) one obtains

$$\bar{\mathbb{L}} = \langle \mathbb{L}(\phi^c)\rangle, \quad \bar{\mathbb{M}} = \bar{\mathbb{L}}^{-1} = \langle \mathbb{L}(\phi^c)\rangle^{-1}. \tag{23}$$

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

$$\boldsymbol{\sigma} = \boldsymbol{\Sigma}, \tag{24}$$

everywhere in the polycrystal (Hill, 1952). Such lower bound is called the Reuss (1929) bound for elastic materials or the (Sachs, 1928) bound for rigid-plastic or viscoplastic materials. Averaging $(1)_1$ and applying hypothesis (24) one obtains

$$\bar{\mathbb{M}} = \langle \mathbb{M}(\phi^c)\rangle, \quad \bar{\mathbb{L}} = \bar{\mathbb{M}}^{-1} = \langle \mathbb{M}(\phi^c)\rangle^{-1}. \tag{25}$$

The bounds formulated above will be now specified for random polycrystals (untextured polycrystals). Introducing decompositions (3) and (6) into (23) and (25) it has been demonstrated in Kowalczyk-Gajewska (2009) that

$$\bar{h}^{\mathrm{P}}_{\mathrm{UP}} = \sum_{K=1}^{M} h_K \eta_K^{\mathrm{P}}, \quad \bar{h}^{\mathrm{D}}_{\mathrm{UP}} = \sum_{K=1}^{M} h_K \eta_K^{\mathrm{D}} \tag{26}$$

and

$$\bar{h}^{\mathrm{P}}_{\mathrm{LO}} = \left(\sum_{K=1}^{M}\frac{\eta_K^{\mathrm{P}}}{h_K}\right)^{-1}, \quad \bar{h}^{\mathrm{D}}_{\mathrm{LO}} = \left(\sum_{K=1}^{M}\frac{\eta_K^{\mathrm{D}}}{h_K}\right)^{-1}. \tag{27}$$

It can be shown that $1/3\bar{h}^{\mathrm{P}}_{\mathrm{UP}}$ is equal to the average bulk modulus of polycrystal while $3\bar{h}^{\mathrm{P}}_{\mathrm{LO}}$ is equal to the inverse of an average compressibility modulus (Kocks et al., 2000).

In the case of volumetrically isotropic materials the formulae above reduce to

$$\bar{h}^{\mathrm{P}}_{\mathrm{UP}*} = \bar{h}^{\mathrm{P}}_{\mathrm{LO}*} = h^{\mathrm{P}}, \quad \bar{h}^{\mathrm{D}}_{\mathrm{UP}*} = \frac{1}{5}\sum_{K=2}^{M} h_K m_K, \quad \bar{h}^{\mathrm{D}}_{\mathrm{LO}*} = 5\left(\sum_{K=2}^{M}\frac{m_K}{h_K}\right)^{-1}, \tag{28}$$

so the macroscopic bulk modulus is equal to the local one. Since upper and lower bounds for the bulk modulus coincide, $\bar{h}^{\mathrm{P}} = h^{\mathrm{P}}$ is the exact value.

As already has been noted, incompressible materials, can be viewed as a special case of the volumetrically isotropic materials for which the bulk modulus is infinite

$$h^{\mathrm{P}} \to \infty. \tag{29}$$

As it has been shown above for such materials macroscopic bulk modulus is equal to the local one. Note that it is true independently of crystallographic texture. Therefore, we also have

$$\bar{h}^{\mathrm{P}} \to \infty. \tag{30}$$

The V–R bounds for an overall shear modulus $\bar{h}^{\mathrm{D}}$ are not changed and specified by Eq. (28).

In the case of materials with constrained deformation or unsustained stresses, formulae for upper and lower bounds for macroscopic bulk and shear moduli are rewritten as

$$\bar{h}^{\mathrm{P}}_{\mathrm{UP}} = h^*\eta^{\mathrm{P}*} + \sum_{K=2}^{M} h_K \eta_K^{\mathrm{P}}, \quad \bar{h}^{\mathrm{D}}_{\mathrm{UP}} = h^*\eta^{\mathrm{D}*} + \sum_{K=2}^{M} h_K \eta_K^{\mathrm{D}} \tag{31}$$

and

$$\bar{h}^{\mathrm{P}}_{\mathrm{LO}} = \left(\frac{\eta^{\mathrm{P}*}}{h^*} + \sum_{K=2}^{M}\frac{\eta_K^{\mathrm{P}}}{h_K}\right)^{-1}, \quad \bar{h}^{\mathrm{D}}_{\mathrm{LO}} = \left(\frac{\eta^{\mathrm{D}*}}{h^*} + \sum_{K=2}^{M}\frac{\eta_K^{\mathrm{D}}}{h_K}\right)^{-1}. \tag{32}$$

Consequently,

- For material with constrained deformation ($h^* \to \infty$) the bound $\bar{h}^{\mathrm{P}}_{\mathrm{UP}}$ is finite only when $\eta^{\mathrm{P}*} = 0$ (it means that the subspace $\mathcal{P}^*$ generated by $\mathbb{P}^*$ is the subspace of deviatoric tensors), while the modulus $\bar{h}^{\mathrm{D}}_{\mathrm{UP}}$ is finite when $\eta^{\mathrm{D}*} = 0$, which is equivalent to $\eta^{\mathrm{P}*} = m^*$. Apparently, both conditions cannot be fulfilled simultaneously and $\bar{h}^{\mathrm{D}}_{\mathrm{UP}}$ is finite only when $m^* = \eta_{\mathrm{P}*} = 1$. It is the case when material is incompressible. Lower bounds of $\bar{h}^{\mathrm{P}}$ and $\bar{h}^{\mathrm{D}}$ are finite until there exists at least one K for which h_K is finite and simultaneously

$$\eta_K^{\mathrm{P}} \neq 0 \quad \text{and} \quad \eta_K^{\mathrm{D}} \neq 0. \tag{33}$$

  If additional restrictions have been imposed on the incompressible materials, as far as an upper bound is concerned, both macroscopic moduli 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.
- For material with unsustained stresses ($h^* \to 0$) the bound $\bar{h}^{\mathrm{P}}_{\mathrm{LO}}$ is non-zero only when $\eta^{\mathrm{P}*} = 0$ (it means that the subspace $\mathcal{P}^*$ generated by $\mathbb{P}^*$ is the subspace of deviatoric tensors), while the modulus $\bar{h}^{\mathrm{D}}_{\mathrm{LO}}$ is non-zero when $\eta^{\mathrm{D}*} = 0$, which is equivalent to $\eta^{\mathrm{P}*} = m^*$. Again, both conditions cannot be fulfilled simultaneously and $\bar{h}^{\mathrm{D}}_{\mathrm{LO}}$ is non-zero only when $m^* = \eta_{\mathrm{P}*} = 1$. It is the case when hydrostatic stress states are not sustained. Upper bounds of $\bar{h}^{\mathrm{D}}$ and $\bar{h}^{\mathrm{P}}$ are both non-zero until there exist at least one K for which h_K is non-zero and (33) are simultaneously

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[2] Kelvin's bulk and shear moduli are related with the macroscopic Young modulus $\overline{E}$ and the Poisson ratio $\bar{\nu}$ according to the known relations, viz.:

$$\overline{E} = \frac{3\bar{h}^{\mathrm{P}}\bar{h}^{\mathrm{D}}}{2\bar{h}^{\mathrm{P}} + \bar{h}^{\mathrm{D}}}, \quad \bar{\nu} = \frac{\bar{h}^{\mathrm{P}} - \bar{h}^{\mathrm{D}}}{2\bar{h}^{\mathrm{P}} + \bar{h}^{\mathrm{D}}}, \quad (\bar{\nu} < 0 \Longleftrightarrow \bar{h}^{\mathrm{P}} < \bar{h}^{\mathrm{D}}). \tag{21}$$

valid. If for some incompressible material there are some unsustained deviatoric stresses, as far as a lower bound is concerned, the macroscopic shear modulus is zero so a non-zero lower bound does not exists, while there exists a non-zero upper bound for an overall shear modulus as long as some stress components are sustained.

One should note that the derived bounds depend only on local Kelvin moduli h_K, their multiplicity and $M-1$ independent values η_K^{P}, so maximum 11 independent function of 21 components of a local stiffness tensor. All these functions are invariants of the local elasticity tensor (Kowalczyk-Gajewska and Ostrowska-Maciejewska, 2004b). Specific formulae for $\left\{\bar{h}^{\mathrm{P}}_{\mathrm{UP/LO}}, \bar{h}^{\mathrm{D}}_{\mathrm{UP/LO}}\right\}$ for all local symmetry groups covered by the fourth-order tensor are collected in Kowalczyk-Gajewska (2009). It should be underlined that analytical formulae for bounds specified by assumptions (22) and (24) for an arbitrarily anisotropic crystal are known in the literature (Walpole, 1981; Kocks et al., 2000; Cowin et al., 1999). The originality of results derived in Kowalczyk-Gajewska, 2009 lie mainly in the method applied enabling the specification of them in terms of invariants of $\mathbb{L}$ coming from its spectral and harmonic decompositions applied subsequently. As it is shown further the proposed procedure can be also applied for the derivation of Hashin–Shtrikman bounds and self-consistent estimates.

2.2. Hashin–Shtrikman (H–S) bounds

More rigorous bounds, resulting from the theorems of minimum potential energy and of minimum complementary energy have been derived by Hashin and Shtrikman (Hashin and Shtrikman, 1962a; Hashin and Shtrikman, 1962b), cf. (Willis, 1977; Willis, 1981; Walpole, 1981). In view of these derivations some $\widetilde{\mathbb{L}}$ provides an upper (correspondingly: lower) bound on the tensor of effective properties $\bar{\mathbb{L}}$ according to the following implications

$$\gamma \cdot (\widetilde{\mathbb{L}}(\mathbb{L}_0) - \bar{\mathbb{L}}) \cdot \gamma \geqslant (\leqslant) 0 \text{ if } \bigwedge_{\phi^c \in \mathcal{Q}_{tex}} \gamma \cdot (\mathbb{L}_0 - \mathbb{L}(\phi^c)) \cdot \gamma \geqslant (\leqslant) 0, \tag{34}$$

where γ is any strain state. The $\mathbb{L}_0$ is a stiffness tensor for some comparison material of the same symmetry as $\bar{\mathbb{L}}$. For the analysed polycrystalline materials of grains with the same shape and orientation of ellipsoid axes the estimate $\widetilde{\mathbb{L}}$ is specified as

$$\widetilde{\mathbb{L}} = \langle (\mathbb{L}(\phi^c) + \mathbb{L}_*(\mathbb{L}_0))^{-1} \rangle^{-1} - \mathbb{L}_*(\mathbb{L}_0), \tag{35}$$

where $\mathbb{L}_*(\mathbb{L}_0)$ is the Hill tensor depending on the assumed shape of inclusions and properties of comparison material $\mathbb{L}_0$. If overall properties are isotropic it can be shown that bounding estimates (35) are valid for an arbitrary shape of inclusions (Christensen, 1979) with the isotropic $\mathbb{L}_*$ specified by (see e.g. (Li and Wang, 2008))

$$\mathbb{L}_* = h_*^{\mathrm{P}} \mathbb{I}_{\mathrm{P}} + h_*^{\mathrm{D}} \mathbb{I}_{\mathrm{D}}, \tag{36}$$

where

$$h_*^{\mathrm{P}} = 2h_0^{\mathrm{D}}, \quad h_*^{\mathrm{D}} = h_0^{\mathrm{D}} \frac{3h_0^{\mathrm{P}} + 4h_0^{\mathrm{D}}}{2\left(h_0^{\mathrm{P}} + 3h_0^{\mathrm{D}}\right)}. \tag{37}$$

Positive quantities h_0^{P} and h_0^{D} are bulk and shear moduli of isotropic comparison material. Note that right-hand side of an inequality in implication (34) is equivalent to semi-positive (semi-negative) definiteness of the tensor $\mathbb{L}_0 - \mathbb{L}(\phi^c)$ for any ϕ^c. One can show that $\widetilde{\mathbb{L}}$ specified by (35) is a monotonically increasing function of $h_0^{\mathrm{P}}, h_0^{\mathrm{D}}$ (Walpole, 1981; Berryman, 2005), thus the upper (lower) bound is the tightest when the bulk and shear moduli of a comparison material are as small (correspondingly: large) as possible. It leads to the conclusion of Nadeau and Ferrari (2001) that for an optimal $\mathbb{L}_0$ the smallest (largest) eigenvalue of the difference $\mathbb{L}_0 - \mathbb{L}(\phi^c)$ should be equal to zero.

Procedure of deriving the H–S bounds involves two important steps, namely:

1. An appropriate selection of a comparison material $\mathbb{L}_0$ which does not violate the condition of semi-positive (semi-negative) definiteness of $\Delta\mathbb{L}(\phi^c) = \mathbb{L}_0 - \mathbb{L}(\phi^c)$ and in the same time provides the tightest possible upper (lower) bound[3]
2. Specification of $\widetilde{\mathbb{L}}$ according to the formula (35) with use of the selected $\mathbb{L}_0$

Procedure is not as straightforward as derivation of the V–R bounds because in general the local tensor $\mathbb{L}(\phi^c)$ and the isotropic Hill tensor $\mathbb{L}_*(\mathbb{L}_0)$ as well as the estimate $\widetilde{\mathbb{L}}$ do not commute. Two steps simplify this considerably if locally material is volumetrically isotropic and the latter property holds.

2.2.1. Volumetrically isotropic crystals

Analysis of the V–R bounds indicated that $\bar{h}^{\mathrm{P}} = h^{\mathrm{P}}$. Therefore also $\tilde{h}^{\mathrm{P}}_{\mathrm{UP}} = \tilde{h}^{\mathrm{P}}_{\mathrm{LO}} = h^{\mathrm{P}}$, and $h_0^{\mathrm{P}} = h^{\mathrm{P}}$. Consider that for volumetrically isotropic crystal, under $h_0^{\mathrm{P}} = h^{\mathrm{P}}$ we have

$$\Delta\mathbb{L}(\phi^c) = \sum_{K=2}^{M} \left(h_0^{\mathrm{D}} - h_K\right) \mathbb{P}^{(K)}(\phi^c), \tag{38}$$

therefore it is easy to see that

$$\bigwedge_{\phi^c \in \mathcal{Q}} \gamma \cdot \Delta\mathbb{L}(\phi^c) \cdot \gamma \geqslant (\leqslant) 0 \Longleftrightarrow h_0^{\mathrm{D}} \geqslant \max_{K>1}\{h_K\} \quad \left(h_0^{\mathrm{D}} \leqslant \min_{K>1}\{h_K\}\right). \tag{39}$$

Consequently the tightest upper and lower bounds $\widetilde{\mathbb{L}}_{\mathrm{HS}}$ are obtained by setting, correspondingly, $h_0^{\mathrm{D}} = \max_{K>1}\{h_K\}$ and $h_0^{\mathrm{D}} = \min_{K>1}\{h_K\}$ in the following formula derived from (35) with use of (10),

$$\tilde{h}^{\mathrm{D}}_{\mathrm{HS}} = 5\left(\sum_{K=2}^{M} \frac{m_K}{h_K + h_*^{\mathrm{D}}(h^{\mathrm{P}}, h_0^{\mathrm{D}})}\right)^{-1} - h_*^{\mathrm{D}}\left(h^{\mathrm{P}}, h_0^{\mathrm{D}}\right). \tag{40}$$

The above specification of optimal bounds is equivalent to the one obtained by Nadeau and Ferrari (2001) for this class of polycrystals.

In the case of incompressible crystals the estimate of bulk modulus is infinite, while formula (40) for the H–S bounds of $\bar{h}^{\mathrm{D}}$ remains unaffected, with an exception that

$$h_*^{\mathrm{P}} = \lim_{h_0^{\mathrm{P}} \to \infty} h_*^{\mathrm{P}} = 2h_0^{\mathrm{D}}, \quad h_*^{\mathrm{D}} = \lim_{h_0^{\mathrm{P}} \to \infty} h_*^{\mathrm{D}} = \frac{3}{2} h_0^{\mathrm{D}}. \tag{41}$$

2.2.2. Anisotropic crystals

Now, let us consider anisotropic crystals which are not volumetrically isotropic. To this end let us rewrite (3) as follows

$$\mathbb{L}(\phi^c) = \underbrace{\sum\nolimits_{K=1}^{N} h_K \mathbb{P}_{(\phi^c)}}_{\widehat{\mathbb{L}}(\phi^c)} + \sum_{K=N+1}^{M} h_K \mathbb{P}_K(\phi^c), \tag{42}$$

$$\mathbb{M}(\phi^c) = \underbrace{\sum\nolimits_{K=1}^{N} \frac{1}{h_K} \mathbb{P}_K(\phi^c)}_{\widehat{\mathbb{M}}(\phi^c)} + \sum_{K=N+1}^{M} \frac{1}{h_K} \mathbb{P}_K(\phi^c), \tag{43}$$

[3] The quality of bounds will be assessed in view of the norm $\|\widetilde{\mathbb{L}}\|$.

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

$$\sum_{K=1}^{N}\mathbb{P}_K(\phi^c) = \widehat{\mathbb{P}}(\phi_c) = \mathbb{I}_P + \widehat{\mathbb{P}}_D(\phi_c), \tag{44}$$

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

$$\widehat{\mathbb{L}}(\phi^c) = \widehat{\mathbb{P}}(\phi^c)\circ\mathbb{L}(\phi^c) = \mathbb{L}(\phi^c)\circ\widehat{\mathbb{P}}(\phi^c), \tag{45}$$

while $\hat{\mathbb{M}}(\phi^c)$ is a partial inverse of $\widehat{\mathbb{L}}(\phi^c)$.

With use of the above notation $\Delta\mathbb{L}(\phi^c)$ is specified as

$$\Delta\mathbb{L}(\phi^c) = \Delta\widehat{\mathbb{L}}(\phi^c) + \sum_{K=N+1}^{M}\left(h_0^D - h_K\right)\mathbb{P}_K(\phi^c) \tag{46}$$

and $\Delta\widehat{\mathbb{L}}(\phi^c) = \widehat{\mathbb{L}}_0 - \widehat{\mathbb{L}}(\phi^c)$. Requirement of semi-positive (semi-negative) definiteness of the tensor $\Delta\mathbb{L}(\phi^c)$ is fulfilled when

$$\bigwedge_{\phi^c\in\mathcal{Q}_{tex}}\boldsymbol{\gamma}\cdot\Delta\widehat{\mathbb{L}}(\phi^c)\cdot\boldsymbol{\gamma}\geqslant(\leqslant)0 \;\text{ and }\; h_0^D\geqslant\max_{K>N}\{h_K\}\;\left(h_0^D\leqslant\min_{K>N}\{h_K\}\right). \tag{47}$$

Above inequalities specify an admissible set $A_0\in R^2$ of pairs $\{h_0^P, h_0^D\}$ for the comparison isotropic tensor $\mathbb{L}_0$. Now, we derive estimator $\widetilde{\mathbb{L}}$ for the selected pair of these scalars. Let us denote (inverse means the partial inverse)

$$\widehat{\mathbb{R}}(\phi^c) = \left(\widehat{\mathbb{L}}(\phi^c) + \widehat{\mathbb{L}}_*(\mathbb{L}_0)\right)^{-1} \tag{48}$$

and perform its harmonic decomposition

$$\widehat{\mathbb{R}}(\phi^c) = \hat{\mu}^P\mathbb{I}_P + \hat{\mu}^D\mathbb{I}_D + \widehat{\mathbb{R}}(\phi^c)_{ani} \tag{49}$$

as well as harmonic decompositions (14) of deviatoric projectors $\mathbb{P}_K$ for $K > N$. After introducing above decompositions into (35) and using the property (10) one finds

$$\tilde{h}^P = \frac{1}{\hat{\mu}^P} - h_*^P, \quad \tilde{h}^D = \left(\hat{\mu}^D + \sum_{K=N+1}^{M}\frac{m^K}{5\left(h_K + h_*^D\right)}\right)^{-1} - h_*^D. \tag{50}$$

As already discussed moduli $\tilde{h}^P$ and $\tilde{h}^D$ are monotonically increasing functions of h_0^P, h_0^D, therefore the optimal upper (lower) bounds are obtained for $\{h_0^P, h_0^D\}$ lying on the boundary of the admissible set $\mathcal{A}_0$ specified by relations (47). As it will be demonstrated, contrary to volumetrically isotropic polycrystals such restrictions do not specify the optimum $\mathbb{L}_0$ uniquely. An additional requirement is needed. The choice of such requirement is not unique. For example in Nadeau and Ferrari (2001) it has been suggested that optimal bounds are specified by $\mathbb{L}_0$ with minimum (maximum) trace, where $\mathrm{Tr}\mathbb{L}_0 = h_0^P + 5h_0^D$. In this paper it is proposed to calculate the upper (lower) bound on the isotropic $\widetilde{\mathbb{L}}$ for a pair $\{h_0^P, h_0^D\}\in A_0$ for which the function $F_0 = \|\widetilde{\mathbb{L}}\|^2$, specified as

$$F_0\left(h_0^P, h_0^D\right) = \tilde{h}^P\left(h_0^P, h_0^D\right)^2 + 5\tilde{h}^D\left(h_0^P, h_0^D\right)^2 \tag{51}$$

reaches minimum (maximum). Note that $F_0(h_0^P, h_0^D)$ is a monotonically increasing function of its arguments.

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

$$\widehat{\mathbb{P}}_D(\phi^c) = \mathbf{d}(\phi^c)\otimes\mathbf{d}(\phi^c), \quad \mathbb{P}_K(\phi^c)\cdot\mathbf{d}(\phi^c) = \mathbf{0} \quad \text{for} \quad K = 3,\ldots,M \tag{52}$$

and

$$\widehat{\mathbb{L}}(\phi^c) = L_{11}\mathbb{I}_P + L_{22}\widehat{\mathbb{P}}_D(\phi^c) + \frac{1}{\sqrt{3}}L_{12}(\mathbf{I}\otimes\mathbf{d}(\phi^c) + \mathbf{d}(\phi^c)\otimes\mathbf{I}). \tag{53}$$

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

$$L_{11} = \frac{1}{3}\mathbf{I}\cdot\mathbb{L}(0)\cdot\mathbf{I} = h_1\eta_1^P + h_2\eta_2^P > 0, \tag{54}$$

$$L_{22} = \mathbf{d}(0)\cdot\mathbb{L}(0)\cdot\mathbf{d}(0) = h_1 + h_2 - L_{11} > 0, \tag{55}$$

$$(L_{12})^2 = L_{11}L_{22} - h_1h_2 > 0. \tag{56}$$

It can be easily checked that L_{11} provides the Voigt-type upper bound (26) for an overall bulk modulus. With use of above definitions one can show that the condition of semi-positive (semi-negative) definiteness of the tensor $\Delta\widehat{\mathbb{L}}(\phi^c)$ is equivalent to the condition of semi-positive (semi-negative) definiteness of the 2×2 matrix of the form

$$\begin{bmatrix} h_0^P - L_{11} & -L_{12} \\ -L_{12} & h_0^D - L_{22}\end{bmatrix}, \tag{57}$$

which, using the fact that $\mathbb{L}(\phi_c)$ is positive definite, implies the following inequalities

$$h_0^P\geqslant(\leqslant)L_{11}, \quad h_0^D\geqslant(\leqslant)L_{22}, \quad h_0^P\geqslant(\leqslant)L_{11} + \frac{(L_{12})^2}{h_0^D - L_{22}}. \tag{58}$$

The admissible subspaces of h_0^P and h_0^D specified by above inequalities and (47) are presented in Fig. 2.

For the specified h_0^P and h_0^D estimators (35) become

$$\tilde{h}^P = L_{11} - \frac{(L_{12})^2}{L_{22} + h_*^D}, \quad \tilde{h}^D = 5\left(\frac{h_*^P + L_{11}}{J_*} + \sum_{K=3}^{M}\frac{m^K}{\left(h_K + h_*^D\right)}\right)^{-1} - h_*^D, \tag{59}$$

where

$$J_* = \left(L_{11} + h_*^P\right)\left(L_{22} + h_*^D\right) - (L_{12})^2. \tag{60}$$

As already stressed the tightest upper (lower) bound is obtained for values lying on the boundary of the admissible set $\mathcal{A}_0$ of solutions marked in Fig. 2a–b(c–d) by a thick black line. Points on this line fulfill equation

$$h_0^P = h_0^P(h_0^D) = L_{11} + \frac{(L_{12})^2}{h_0^D - L_{22}}, \quad \text{and} \quad h_0^D\geqslant h_{max}(\leqslant h_{min}) \tag{61}$$

and $h_{max} = \max\{h_{max}^D, L_{22}\}$ ($h_{min} = \min\{h_{min}^D, L_{22}\}$). The above conditions are equivalent to the requirements formulated by Berryman (2005) for polycrystals of hexagonal, trigonal, and tetragonal symmetries. Relation $(61)_1$ is also equivalent to the corresponding formula derived by Nadeau and Ferrari (2001) when constructing the procedure of finding the optimal bounds. According to the relation $(61)_1$ the modulus h_0^P is a decreasing function of h_0^D; therefore the requirement that the optimum bounds are obtained for h_0^P and h_0^D as small (large) as possible is inconclusive for points lying on the boundary of $\mathcal{A}_0$. The additional requirement imposed on $F_0 = ||\mathbb{L}_0||^2$ is used to specify $\{h_0^P(h_0^D), h_0^D\}$ uniquely. Denote by $\hat{h}_0^D$ the solution of the following extremum condition

$$\frac{dF_0}{dh_0^D} = \frac{\partial F_0}{\partial h_0^D} + \frac{\partial F_0}{\partial h_0^P}\frac{dh_0^P}{dh_0^D} = \frac{\partial F_0}{\partial h_0^D} - \frac{(L_{12})^2}{(h_0^D - L_{22})^2}\frac{\partial F_0}{\partial h_0^P} = 0. \tag{62}$$

If $\hat{h}_0^D\geqslant h_{max}$ (correspondingly: $0\leqslant\hat{h}_0^D\leqslant h_{min}$) then the tightest upper (correspondingly lower) bound on $\mathbb{L}$ will be obtained for the isotropic comparison material with moduli $\{h_0^P(\hat{h}_0^D), \hat{h}_0^D\}$. If it is not the case, one should take isotropic material with moduli

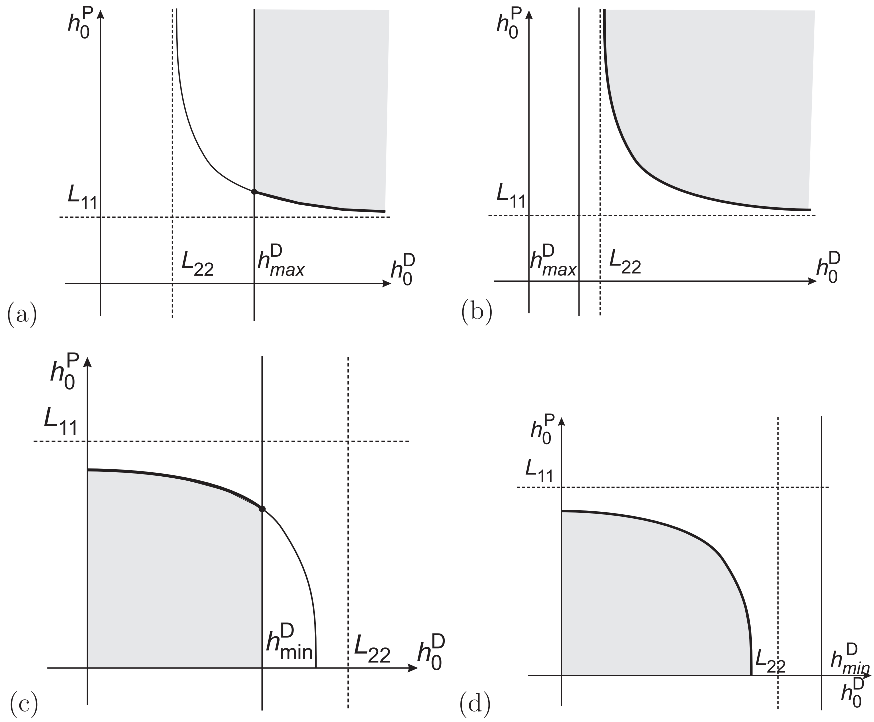

Fig. 2. The admissible subspaces of h_0^P and h_0^D specified by (58) when calculating the H–S bounds for random polycrystal of local properties defined by (42) and (53): (a) $h_{max}^D > L_{22}$ (UP) (b) $h_{max}^D < L_{22}$ (UP) (c) $h_{min}^D < L_{22}$ (LO) (d) $h_{min}^D > L_{22}$ (LO).

$\{h_0^P(h_{max}), h_{max}\}$ (correspondingly: $\{h_0^P(h_{min}), h_{min}\}$). Note that for $h_{max} \to L_{22}$ one has $h^P \to \infty$, so the comparison material is incompressible.

Conclusions concerning the existence of a finite bound for the materials with constraints outlined for the V–R bounds are valid also for the H–S bounds.

As already discussed in the introduction the Hashin–Shtrikman bounds for random polycrystals have been provided for different crystal symmetries in Peselnick and Meister (1986), Watt (1965), Pham (2003), and Berryman (2005). An original outcome of the presented analysis is a new method of deriving these bounds that makes use of invariant decompositions of Hooke's tensors. This procedure enables specification of these estimates with use of invariants of a single crystal stiffness tensor independently of its symmetry group.

3. Self-consistent (SC) estimates

Self-consistent estimate of an overall behavior of polycrystal relies on Eshelby's solution (Eshelby, 1957) for the ellipsoidal inclusion embedded in the infinite medium. Here a single grain is considered as an inclusion while the medium has averaged, yet unknown, properties of a polycrystal. Following Hill's formulation of a SC procedure (Hill, 1965) one finds the following localization equation for local strain

$$\boldsymbol{\varepsilon} = \mathbb{A} \cdot \mathbf{E}, \quad \mathbb{A} = (\mathbb{L} + \mathbb{L}_*)^{-1} \circ (\bar{\mathbb{L}} + \mathbb{L}_*), \tag{63}$$

where $\mathbb{A}$ is a localization tensor and $\mathbb{L}_*$ is the Hill tensor which depends on the shape of inclusion and the averaged properties $\bar{\mathbb{L}}$. In this paper we consider the SC estimates for spherical grains. Therefore, we can show that equivalently

$$\bar{\mathbb{L}} = \langle \mathbb{L} \circ \mathbb{A} \rangle, \quad \langle \mathbb{A} \rangle = \mathbb{I}^S. \tag{64}$$

First equation is an implicit equation since $\mathbb{A}$ depends on $\bar{\mathbb{L}}$. Instead of (64) for derivation of $\bar{\mathbb{L}}$ the equivalent equation is utilized, namely

$$\langle (\bar{\mathbb{L}} - \mathbb{L}) \circ \mathbb{A} \rangle = \mathbb{O}. \tag{65}$$

where $\mathbb{O}$ is the Hooke's tensor with all components equal to zero. Another implicit formula for derivation of $\bar{\mathbb{L}}$ is obtained with analogy to (35), viz.:

$$\bar{\mathbb{L}} = \langle (\mathbb{L}(\phi^c) + \mathbb{L}_*(\bar{\mathbb{L}}))^{-1} \rangle^{-1} - \mathbb{L}_*(\bar{\mathbb{L}}). \tag{66}$$

Usually, one of the above formulae is solved numerically to find the SC estimate of the average properties of a polycrystal. An iterative procedure applied to solve the Eq. (66), in which $\mathbb{L}_*$ is calculated with use of approximation of $\bar{\mathbb{L}}$ from the previous iteration, with e.g. the Voigt upper bound being the starting value, leads to $\bar{\mathbb{L}}$ possessing the minor and major symmetries of Hooke's tensor (A.1).

In the case of macroscopic isotropy (no texture) and a spherical shape of grains the Hill tensor is specified by (36) and (37) with $\{h_0^P, h_0^D\}$ replaced by $\{\bar{h}^P, \bar{h}^D\}$. Introducing appropriate formulae into $\mathbb{A}$ one notices that the inversion present in the formula $(63)_2$ 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 material is volumetrically isotropic. Let us first consider this class of materials.

3.1. Volumetrically isotropic crystals

Substituting formulae (12) into $(63)_2$ the localization tensor is specified as

$$\mathbb{A}(\phi^c) = \frac{\bar{h}^P + h_*^P}{h^P + h_*^P} \mathbb{I}_P + \sum_{K=2}^{M} \frac{\bar{h}^D + h_*^D}{h_K + h_*^D} \mathbb{P}_K(\phi^c). \tag{67}$$

Substituting $\mathbb{A}$ specified above into (65) and performing averaging over the whole orientation space, we find that the SC estimates for $\bar{h}^P$ and $\bar{h}^D$ are obtained from the set of two scalar equations

$$\frac{\left(\bar{h}^P - h^P\right)\left(\bar{h}^P + h_*^P\right)}{h^P + h_*^P} = 0, \tag{68}$$

$$\left(\bar{h}^{\mathrm{D}}+h_*^{\mathrm{D}}\right)\sum_{K=2}^{M}\frac{(\bar{h}^{\mathrm{D}}-h_K)m_K}{h_K+h_*^{\mathrm{D}}}=0. \tag{69}$$

In view of positive definiteness of local and macroscopic constitutive tensors the first equation is fulfilled when

$$\bar{h}^{\mathrm{P}}=h^{\mathrm{P}} \tag{70}$$

consistently with the result of previous section. Substituting (37) into the second equation, one can reduce it to a polynomial equation of odd degree $2M-3$, which serves to obtain $\bar{h}^{\mathrm{D}}$. We look for $\bar{h}^{\mathrm{D}}$ among positive real roots of this polynomial. For example, for crystals of cubic symmetry we have $M=3$ and the well-known cubic equation is obtained (Kröner, 1958). It is important to note that the solution depends only on the values of local Kelvin's moduli and their multiplicity, thus the invariants of local elasticity tensor. Moreover, it should be stressed that knowledge about the multiplicity of Kelvin's moduli is not necessary - formally one can solve this equation as a 9-degree one setting all $m_K=1$:

$$\sum_{k=0}^{9}a_k\left(\bar{h}^{\mathrm{D}}\right)^k=0. \tag{71}$$

One can show that coefficients a_k depend then on the invariant h^{P} and other invariants of deviatoric part of elasticity tensor in a way which is independent of the ordering of the local Kelvin moduli (see B). Analysis of coefficients a_k leads to the conclusion that the polynomial (71) has always a single positive real root (for details see (Kowalczyk-Gajewska, 2009)). Consequently, the admissible solution exists and is unique.

For *incompressible* crystals one has $\bar{h}^{\mathrm{P}}\to\infty$. A SC estimate for the macroscopic shear modulus is obtained with use of the limit values for h_*^{P} and h_*^{D} specified by (41), where h_0^{D} is replaced by $\bar{h}^{\mathrm{D}}$, so Eq. (69) reduces to

$$5\bar{h}^{\mathrm{D}}\sum_{K=2}^{M}\frac{(\bar{h}^{\mathrm{D}}-h_K)m_K}{2h_K+3\bar{h}^{\mathrm{D}}}=0,\quad \sum_{K=2}^{M}m_K\leqslant 5. \tag{72}$$

This equation, under the assumptions $h_K>0$ and $\bar{h}^{\mathrm{D}}>0$, is equivalent to the polynomial equation of M-1 degree. One can prove that this polynomial has always exactly one real root which is positive. Consequently solution exists and is unique. Similarly like for volumetrically isotropic materials, this polynomial equation can be formulated with use of invariants of the local stiffness tensor (see B).

3.2. Anisotropic crystals

Using spectral decompositions (42) and (43) and formulae (44) and (45) it is found

$$(\bar{\mathbb{L}}-\mathbb{L})\circ\mathbb{A}=\underbrace{\left(\hat{\bar{\mathbb{L}}}-\widehat{\mathbb{L}}\right)\circ\widehat{\mathbb{A}}}_{\widehat{\mathbb{R}}(\phi^c)}+\sum_{K=N+1}^{M}\underbrace{\frac{(\bar{h}^{\mathrm{D}}-h_K)\left(\bar{h}^{\mathrm{D}}+h_*^{\mathrm{D}}\right)}{h_K+h_*^{\mathrm{D}}}}_{\alpha_K}\mathbb{P}_K(\phi^c), \tag{73}$$

where

$$\widehat{\mathbb{A}}(\phi^c)=\left(\widehat{\mathbb{L}}(\phi^c)+\widehat{\mathbb{L}}_*(\phi^c)\right)^{-1}\circ\left(\hat{\bar{\mathbb{L}}}(\phi^c)+\widehat{\mathbb{L}}_*(\phi^c)\right), \tag{74}$$

$$\widehat{\mathbb{L}}^*(\phi^c)=\widehat{\mathbb{P}}(\phi^c)\circ\mathbb{L}_*=h_*^{\mathrm{P}}\mathbb{I}_{\mathrm{P}}+h_*^{\mathrm{D}}\widehat{\mathbb{P}}_{\mathrm{D}}(\phi^c), \tag{75}$$

$$\hat{\bar{\mathbb{L}}}(\phi^c)=\widehat{\mathbb{P}}(\phi^c)\circ\bar{\mathbb{L}}=\bar{h}^{\mathrm{P}}\mathbb{I}_{\mathrm{P}}+\bar{h}^{\mathrm{D}}\widehat{\mathbb{P}}_{\mathrm{D}}(\phi^c). \tag{76}$$

An inverse in (74) is the partial inverse. Harmonic decomposition of projectors $\mathbb{P}_K$, $(K=N+1,\dots M)$ and of the symmetric part of $\widehat{\mathbb{R}}(\phi^c)$:

$$\widehat{\mathbb{R}}^s(\phi^c)=\hat{\alpha}^{\mathrm{P}}\mathbb{I}_{\mathrm{P}}+\hat{\alpha}^{\mathrm{D}}\mathbb{I}_{\mathrm{D}}+\widehat{\mathbb{A}}^{\mu}(\phi^c)+\widehat{\mathbb{A}}^{\nu}(\phi^c)+\widehat{\mathbb{H}}(\phi^c) \tag{77}$$

are now performed. After averaging over the whole orientation space two scalar equations corresponding to (68) and (69) are obtained:

$$\widehat{\alpha}^{\mathrm{P}}=0,\quad \widehat{\alpha}^{\mathrm{D}}+\sum_{K=N+1}^{M}\alpha_K m_K=0. \tag{78}$$

Similarly as in the case of the H–S bounds, let us specify these equations for the materials in which $N=2$ and respective h_1 and h_2 are of multiplicity one. Introducing (53)–(56) into (74)–(76), after some algebra it is found that

$$\widehat{\alpha}^{\mathrm{P}}=\frac{\left(\bar{h}^{\mathrm{P}}+h_*^{\mathrm{P}}\right)\left((L_{12})^2+(\bar{h}^{\mathrm{P}}-L_{11})\left(h_*^{\mathrm{D}}+L_{22}\right)\right)}{\left(h_*^{\mathrm{P}}+L_{11}\right)\left(h_*^{\mathrm{D}}+L_{22}\right)-(L_{12})^2}, \tag{79}$$

$$\widehat{\alpha}^{\mathrm{D}}=\frac{\left(\bar{h}^{\mathrm{D}}+h_*^{\mathrm{D}}\right)\left((L_{12})^2+\left(h_*^{\mathrm{P}}+L_{11}\right)(\bar{h}^{\mathrm{D}}-L_{22})\right)}{\left(h_*^{\mathrm{P}}+L_{11}\right)\left(h_*^{\mathrm{D}}+L_{22}\right)-(L_{12})^2} \tag{80}$$

and Eq. (78) are equivalent to

$$(L_{12})^2+(\bar{h}^{\mathrm{P}}-L_{11})\left(h_*^{\mathrm{D}}+L_{22}\right)=0, \tag{81}$$

$$\frac{(L_{12})^2+\left(h_*^{\mathrm{P}}+L_{11}\right)(\bar{h}^{\mathrm{D}}-L_{22})}{\left(h_*^{\mathrm{P}}+L_{11}\right)\left(h_*^{\mathrm{D}}+L_{22}\right)-(L_{12})^2}+\sum_{K=3}^{M}\frac{(\bar{h}^{\mathrm{D}}-h_K)m_K}{h_K+h_*^{\mathrm{D}}}=0. \tag{82}$$

Due to relations (37), contrary to volumetrically isotropic materials, $\bar{h}^{\mathrm{P}}$ cannot be calculated independently of $\bar{h}^{\mathrm{D}}$.

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 **d** is specified as

$$\mathbf{d}=\pm\frac{1}{\sqrt{6}}(3\mathbf{m}\otimes\mathbf{m}-\mathbf{I}), \tag{83}$$

where **m** is the unit vector coaxial with the main axis of local symmetry. Formulae for SC estimates for these classes of single crystal anisotropy have been provided in Berryman (2005) in the form of implicit equations which are equivalent to (81) and (82). In Berryman (2005) the quantity denoted as G_{eff}^{V} is introduced which is called "uniaxial shear energy" per unit volume for an unit applied shear strain. It is easily verified that $2G_{\mathit{eff}}^{V}=L_{22}$.

3.3. Materials with constrained deformation

In this subsection the self-consistent estimates for *volumetrically isotropic* crystals with constrained deformation modes are studied. First, let us consider the case when the space of constrained 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 (70) for the overall bulk modulus is still valid. Substituting (18) and taking the limit for $h^*\to\infty$, Eq. (69) can be rewritten as follows

$$\frac{-m^*}{2\left(h^{\mathrm{P}}+3\bar{h}^{\mathrm{D}}\right)}+\sum_{K=3}^{M}\frac{(\bar{h}^{\mathrm{D}}-h_K)m_K}{w^K\left(h_K,h^{\mathrm{P}},\bar{h}^{\mathrm{D}}\right)}=0, \tag{84}$$

where

$$w^K(h_K,\bar{h}^{\mathrm{P}},\bar{h}^{\mathrm{D}})=4(\bar{h}^{\mathrm{D}})^2+3(\bar{h}^{\mathrm{P}}+2h_K)\bar{h}^{\mathrm{D}}+2h_K\bar{h}^{\mathrm{P}}. \tag{85}$$

Under assumptions that $\bar{h}^{\mathrm{D}}>0$ and $h_K>0$, this equation is equivalent to the polynomial equation of degree $2(M-2)$:

$$\sum_{K=3}^{M} 2\left(\bar{h}^{\mathrm{D}} - h_K\right)\left(h^{\mathrm{P}} + 3\bar{h}^{\mathrm{D}}\right) m_K \prod_{L=3(L\neq K)}^{M} w^L\left(h_L, \bar{h}^{\mathrm{P}}, \bar{h}^{\mathrm{D}}\right) - m^* \prod_{K=3}^{M} w^K\left(h_K, \bar{h}^{\mathrm{P}}, \bar{h}^{\mathrm{D}}\right) = 0. \tag{86}$$

Analysis of this polynomial leads to the conclusion that it has at least one positive real root as long as $m^* \leqslant 2$. In other words, *in the case of volumetrically isotropic material a finite SC estimate for the overall shear modulus exists as long as the dimension of a space of constrained deviatoric deformation modes is less than three*.

Now, let us consider *incompressible* materials in which additionally some subspace of deviatoric deformation modes is constrained. As it has been already shown, the overall bulk modulus is infinite in this case. Let us rewrite Eq. (72) as follows

$$5\bar{h}^{\mathrm{D}}\frac{(\bar{h}^{\mathrm{D}} - h^*)m^*}{2h^* + 3\bar{h}^{\mathrm{D}}} + 5\bar{h}^{\mathrm{D}}\sum_{K=3}^{M}\frac{(\bar{h}^{\mathrm{D}} - h_K)m_K}{2h_K + 3\bar{h}^{\mathrm{D}}} = 0, \quad \sum_{K=3}^{M} m_K \leqslant 4, \tag{87}$$

where as previously m^* denotes the dimension of the constrained subspace of deviatoric deformation modes (due to incompressibility, total dimension of the space of constrained deformation modes is $m^* + 1$). Now we take a limit of this equation for $h^* \to \infty$ and find the counterpart of polynomial Eq. (86),

$$\sum_{K=3}^{M} 2(\bar{h}^{\mathrm{D}} - h_K) m_K \prod_{L=3(L\neq K)} (2h_L + 3\bar{h}^{\mathrm{D}}) - m^* \prod_{K=3} (2h_K + 3\bar{h}^{\mathrm{D}}) = 0, \tag{88}$$

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 SC estimate for the overall shear modulus is finite only when the subspace of restricted deviatoric modes is one-dimensional*. It should be underlined that the above properties of the SC estimate have been proved without referring to the specific lattice symmetry.

As it will be shown below the results concerning materials with the constrained deformation modes are very useful when considering the inelastic deformations of polycrystalline metals with an insufficient number of easy slip systems described by means of the viscoplastic regularization. The dimension m^* of the constrained subspace of deformation can be identified with $5 - i$, where i is the number of independent easy slip systems. Assume that inelastic deformation takes 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 (Hutchinson, 1976)

$$\dot{\boldsymbol{\varepsilon}}^v = \dot{\gamma}_0 \sum_{r=1}^{N} \left|\frac{\tau^r}{\tau_c^r}\right|^{n-1} \frac{\tau^r}{\tau_c^r}\mathbf{P}^r, \tag{89}$$

in which $\dot{\gamma}_0$ is a reference slip rate, τ^r, τ_c^r are the resolved shear stress on the slip system r and the corresponding critical shear stress, where

$$\tau^r = \boldsymbol{\sigma} \cdot \mathbf{P}^r, \quad \mathbf{P}^r = \frac{1}{2}(\mathbf{m}^r \otimes \mathbf{n}^r + \mathbf{n}^r \otimes \mathbf{m}^r). \tag{90}$$

Two unit vectors $\mathbf{m}^r$ and $\mathbf{n}^r$ define the slip system denoting slip direction and normal to the slip plane, respectively. Usually exponent n much higher than one is used in modeling of viscoplastic response of polycrystalline metals, e.g. for successful predictions of texture evolution in fcc metals $n \approx 100$ has been identified as a relevant value (Havner, 2008) and $n \approx 20$ is used in the simulations by the VPSC code for low symmetry crystals (Lebensohn and Tomé, 1993; Agnew et al., 2001; Proust et al., 2009). However, although the linear case $n = 1$ studied in this paper is of limited practical applicability, it is important for the qualitative analysis and verification of the homogenization scheme (Lebensohn et al., 2004). It can be shown that some properties of the solution for the linear case can be transferred to the non-linear case (Nebozhyn et al., 2000; Nebozhyn et al., 2001). Derivation of bounds and self-consistent estimates for $n > 1$ requires an appropriate linearization of a problem and estimates are found numerically by discretization of the orientation space, e.g. (Hutchinson, 1976; Nebozhyn et al., 2001; Bornert et al., 2001). The overall flow stress depends on a loading scheme. In these calculations knowledge about the analytical solutions for the linear case is beneficial from the point of view of verification of the applied numerical scheme. Moreover, it provides good initial approximation of a solution needed within the computational procedure.

Note that the constitutive relation (89) can be also applied when describing steady creep of polycrystalline metals and other materials at temperatures above one third of the melting temperature. The applicable values of n are then between 3 and 8 (Hutchinson, 1976).

For $n = 1$ the local linear viscous relation has the form

$$\dot{\boldsymbol{\varepsilon}}^v = \mathbb{M}^v \cdot \boldsymbol{\sigma}, \quad \mathbb{M}^v = \dot{\gamma}_0 \sum_{r=1}^{N} \frac{1}{\tau_c^r}\mathbf{P}^r \otimes \mathbf{P}^r. \tag{91}$$

The number N and geometry of slip systems depend on the geometry of crystallographic lattice of a single crystal. Clearly, material described by (91) is incompressible. The overall constitutive relation for random polycrystal can be written as (Perzyna, 1963; Hutchinson, 1976)

$$\dot{\mathbf{E}}^v = \frac{1}{\bar{h}^{\mathrm{D}}}\mathbb{I}_{\mathrm{D}} \cdot \boldsymbol{\Sigma} = \frac{3\dot{\gamma}_0}{2\bar{\sigma}_Y}\mathbb{I}_{\mathrm{D}} \cdot \boldsymbol{\Sigma}, \tag{92}$$

where $\bar{\sigma}_Y$ is the reference flow stress.

In the case of metals and alloys of high specific strength the group of easy slip systems usually does not fulfill the Taylor condition. In Nebozhyn et al. (2000) and Nebozhyn et al. (2001), on the basis of the analysis of the variational SC estimates for random power-law polycrystals with reduced number $1 < i < 5$ of independent easy slip systems, it has been found that the overall flow stress follows the scaling law of the form

$$\bar{\sigma}_Y \sim (\rho_{hard})^{\frac{4-i}{2}}, \tag{93}$$

where $\rho_{hard} = \tau_c^{hard}/\tau_c^{easy}$. This law is independent of the exponent n. Before analyzing the examples we will show that such scaling law can be easily deduced from the analytic formula (72) for linear polycrystals.

Assume the crystal with easy and hard categories of slip modes and with the critical shear stress for the hard modes much higher than for the easy ones. For the purpose of the analysis of a scaling law, without introducing significant approximations, the local viscous compliance (91) can be written as

$$\mathbb{M}^v = \frac{1}{h_{easy}}\mathbb{P}_2 + \frac{1}{h_{hard}}\mathbb{P}_3, \tag{94}$$

where m_2 – multiplicity of $\mathcal{P}_2$ – is equal to i in the scaling law (93) while the viscous moduli h_{easy} and h_{hard} are algebraic functions of $\dot{\gamma}_0$ and the critical shear stresses τ_c^{hard} and τ_c^{easy} (see Table 1 in the next section for an example). Projectors $\mathbb{P}_K$ $(K = 2, 3)$ depend on crystal symmetry and fulfill (14). For such specification of $\mathbb{M}^v$ the Eq. (72) reduces to the following square equation

$$3\bar{h}^2 + \underbrace{(\eta(i-3) + 2 - i)}_{b(\eta,i)}\bar{h} - 2\eta = 0, \tag{95}$$

where $\bar{h} = \frac{\bar{h}^{\mathrm{D}}_{\mathrm{SC}}}{h_{easy}}$, $\eta = \frac{h_{hard}}{h_{easy}}$, $i = m_2$, with the positive root

$$\bar{h} = \frac{-b(\eta,i)}{6} + \frac{|b(\eta,i)|}{6}\underbrace{\sqrt{1+\frac{24\eta}{b(\eta,i)^2}}}_{f(\eta,i)}. \tag{96}$$

For $i \neq 3$ the function $f(\eta,i)$ can be expanded into a power series around $1/\eta \to 0$. These expansions introduced into (96), after neglecting terms of order $1/\eta^2$ and smaller, lead to the following approximation of $\bar{h}$ for high values of η

$$\bar{h} \approx \begin{cases} \frac{2}{3}(\eta+1) & \text{for} \quad i=1, \\ \frac{1}{3}\eta+2 & \text{for} \quad i=2, \\ 2 & \text{for} \quad i=4. \end{cases} \tag{97}$$

For $i = 3$ formula (96) reduces to

$$\bar{h} = \frac{1}{6}\left(1+\sqrt{1+24\eta}\right) \sim \sqrt{\eta}. \tag{98}$$

It is seen that the scaling law proposed in Nebozhyn et al. (2001) is confirmed by the above analytical derivations. Moreover, the above result provides additional information. First, we observe that the scaling law for $i = 1$ is the same as for $i = 2$. Second, the linear approximation of $\bar{h}$ for $i = 1, 2$ is provided and the finite limit value for $i = 4$ is specified. The quality of linear approximations for $i = 1, 2$ is illustrated in Fig. 3.

Let us now compare the SC estimate specified by (96) with the V–R bounds, with the H–S bounds and with the Hill's estimates resulting from these bounds, namely

$$\bar{h}^{\mathrm{D}}_{\text{H-VR}} = \frac{1}{2}\left(\bar{h}^{\mathrm{D}}_{\mathrm{LO}} + \bar{h}^{\mathrm{D}}_{\mathrm{UP}}\right), \quad \bar{h}^{\mathrm{D}}_{\text{H-HS}} = \frac{1}{2}\left(\bar{h}^{\mathrm{D}}_{\text{LO-HS}} + \bar{h}^{\mathrm{D}}_{\text{UP-HS}}\right). \tag{99}$$

In Fig. 4 this comparison is performed subsequently for $i = 1, 2, 3, 4$ and large and moderate values of η. Analysis of figures leads to the following conclusions:

- For one independent easy slip system the self-consistent estimate is close to the H–S upper bound and is larger than both Hill's estimates.
- For two independent easy slip systems the SC estimate is close to, though higher than, Hill's estimate obtained for the V–R bounds.
- For three independent slip systems and moderate values of η the SC estimate is well approximated by Hill's estimate resulting from H–S bounds. However, for high values of η it strongly deviates from other estimates and bounds lying between Hill's estimates and the H–S lower bound
- As it has been demonstrated above, for four independent slip systems the SC estimate for $\eta \to \infty$ tends to a finite value, thus it is the closest to the lower H–S bound.

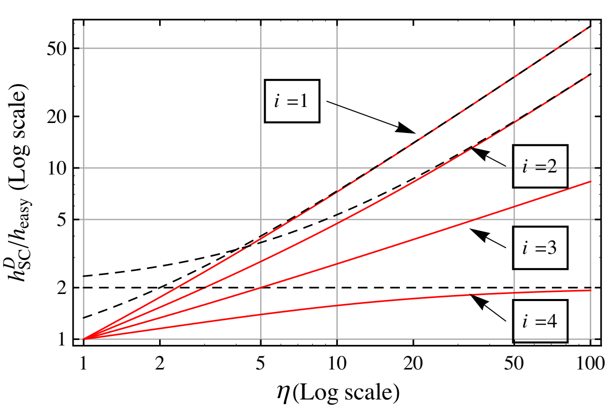

Fig. 3. SC estimate of viscous $\bar{h}^{\mathrm{D}}_{\mathrm{SC}}$ for random polycrystal with reduced number i of independent easy slip systems – exact solutions (continuous line) and approximate ones (dashed line) for large values of $\eta = h_{hard}/h_{easy}$.

3.4. Materials with unsustained stresses

In this subsection volumetrically isotropic crystals with unsustained deviatoric stresses are considered. In order to formulate the condition for existence of a non-zero SC estimate of $\bar{h}^{\mathrm{D}}$ for random polycrystal composed of such crystallites, the polynomial Eq. (71) will be used. Observe that for the established m denoting the dimension of the subspace of unsustained deviatoric stresses ($m \leqslant 5$) one has

$$J_K = 0 \quad \text{for} \quad K = 6 - I, \quad \text{where} \quad I = 1, \ldots, m^*. \tag{100}$$

Using the above relations to find α_k specified by (B.1) and analyzing the resulting polynomial equation, we find that it has a non-zero positive solution for $\bar{h}^{\mathrm{D}}$ if $m \leqslant 2$. If hydrostatic stress states are unsustained ($h^{\mathrm{P}} = \bar{h}^{\mathrm{P}} \to 0$) then the SC estimate of shear modulus is non-zero if $m \leqslant 1$. In the case of incompressible crystals ($h^{\mathrm{P}} = \bar{h}^{\mathrm{P}} \to \infty$) we explore the polynomial Eq. (B.2) and we find that $\bar{h}^{\mathrm{D}}$ is non-zero when $m \leqslant 2$. The latter case corresponds to incompressible steady creep of crystals with one category of slip systems much easier to initiate than remaining ones. A number m is then identified with the number of independent slip systems within the easy category. A good example of such crystal is magnesium for which the basal slip is much easier to initiate than remaining slip systems. There are two independent basal slip systems for magnesium, so in this case $m = 2$. Consequently, a non-zero SC estimate of an overall flow stress will be found for a random polycrystal even if $\tau_c^{basal} \to 0$ (see the next section).

In order to study in more detail the consequences of the above results let us study a volumetrically isotropic crystal for which one deviatoric Kelvin modulus h_K is much smaller than the others. For such crystal the stiffness tensor can be approximately written in the form

$$\mathbb{L} = h^{\mathrm{P}}\mathbb{I}_P + h_{easy}\mathbb{P}_2 + h_{hard}\mathbb{P}_3, \tag{101}$$

where multiplicity of h_{easy} is denoted by m, $\mathbb{P}_K$ depend on crystal symmetry and fulfill (14). For such $\mathbb{L}$ the Eq. (69) reduces to

$$4\bar{h}^3 - [2\xi(m-3) - 2(m-2) - 3\mu]\bar{h}^2 - [\xi(6+\mu(m-2)) \\ +\mu(3-m)]\bar{h} - 2\xi\mu = 0, \tag{102}$$

where $\bar{h} = \bar{h}^{\mathrm{D}}_{\mathrm{SC}}/h_{hard}$, $\xi = h_{easy}/h_{hard} < 1$ and $\mu = h^{\mathrm{P}}/h_{hard}$. When $\xi \to 0$ this equation reduces to

$$\bar{h}\left[4\bar{h}^2 + (2(m-2)+3\mu)\bar{h} - \mu(3-m)\right] = 0 \tag{103}$$

and the non-zero solution is found from the square equation above only for $m = 1$ and $m = 2$, namely

$$\bar{h}_{m=1} = \frac{1}{8}\left(2 - 3\mu + \sqrt{4+20\mu+9\mu^2}\right), \tag{104}$$

$$\bar{h}_{m=2} = \frac{1}{8}\left(-3\mu + \sqrt{16\mu+9\mu^2}\right). \tag{105}$$

When $\mu \to \infty$, so when the material is incompressible, using (72) or taking the limit of Eq. (103), we find

$$\bar{h}^{\mu\to\infty}_{m=1} = \frac{2}{3}, \quad \bar{h}^{\mu\to\infty}_{m=2} = \frac{1}{3}. \tag{106}$$

Finally, when $\mu \to 0$, so when the hydrostatic stress states are unsustained, a non-zero $\bar{h}$ is obtained only for $m = 1$, namely

$$\bar{h}^{\mu\to 0}_{m=1} = \frac{1}{2}. \tag{107}$$

The results are illustrated in Fig. 5, where we present dependence of $\bar{h}$ on μ. In Fig. 6 the values of the overall Poisson ratio corresponding

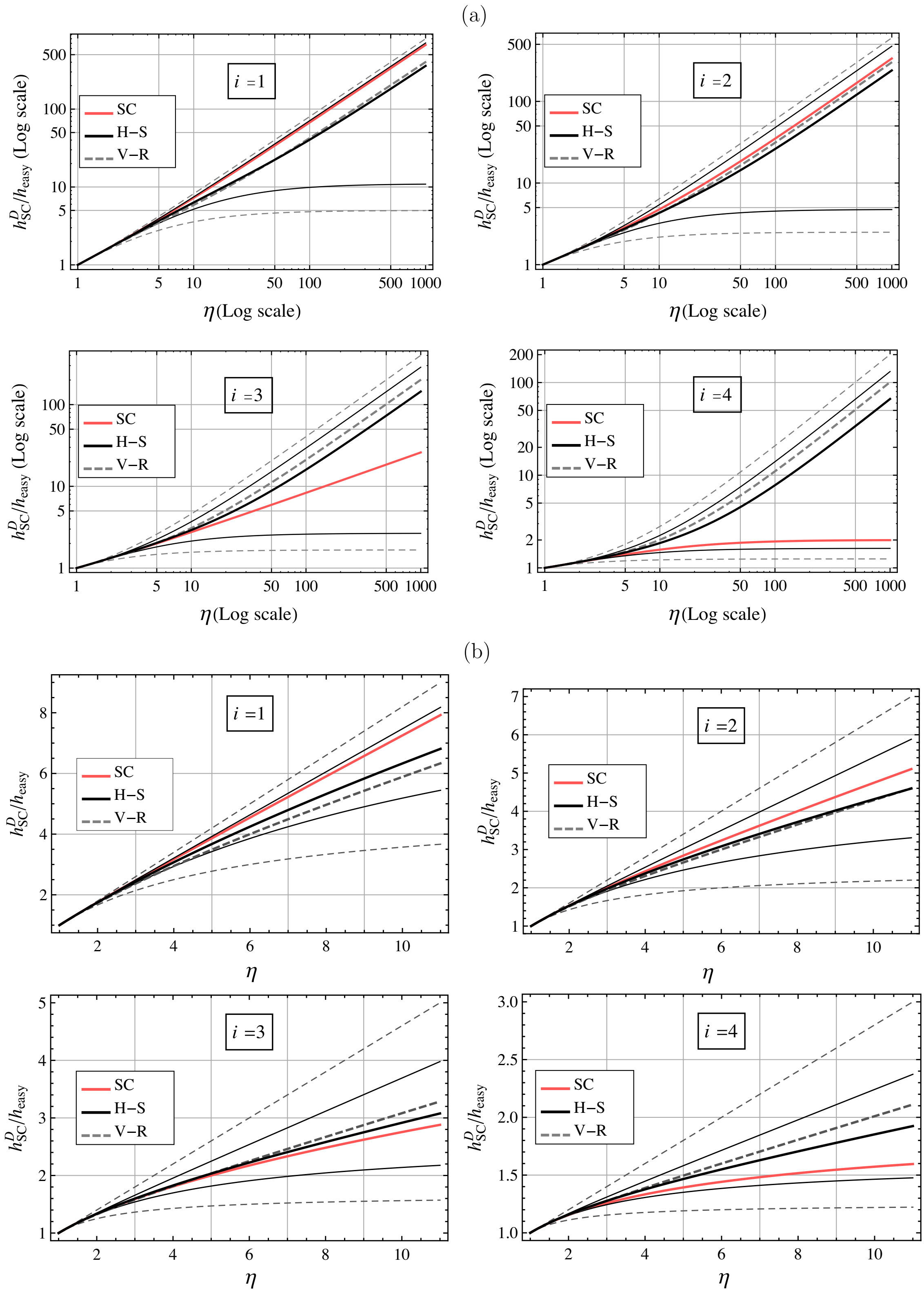

Fig. 4. Comparison of bounds and Hill's estimates to the SC estimate of viscous $\bar{h}^{D}_{SC}$ for random polycrystal with reduced number i of independent easy slip systems for large (a) and moderate (b) values of $\eta = h_{hard}/h_{easy}$.

to the obtained SC estimates and the upper H–S bound of overall bulk and shear moduli are presented. We observe that the Poisson ratio $\bar{\nu}_{SC}$ is negative for $\mu < 1/7$ in the case of $m = 1$ and for $\mu < 4/7$ in the case of $m = 2$.

In Fig. 7 the effective Poisson ratio for $\bar{h}^{D}_{SC}$ results from the solution of the Eq. (102) for different values of μ and ξ as well as $m = \{1, 2, 3, 4\}$. In Fig. 7 the line corresponding to $\bar{\nu} = 0$ has been

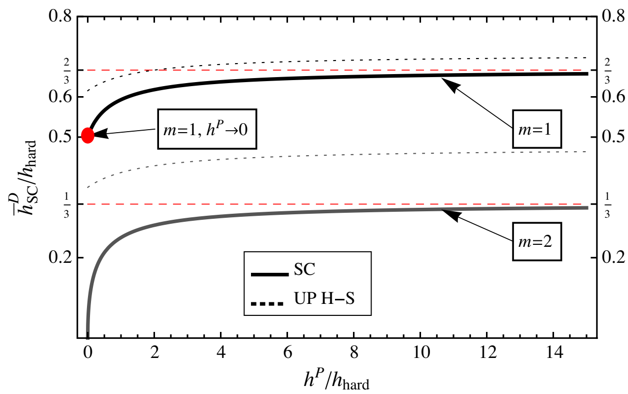

Fig. 5. SC estimate and the upper H–S bound of the overall shear modulus for the random volumetrically isotropic polycrystal with unsustained stresses; m–multiplicity of the deviatoric Kelvin modulus h_{easy}.

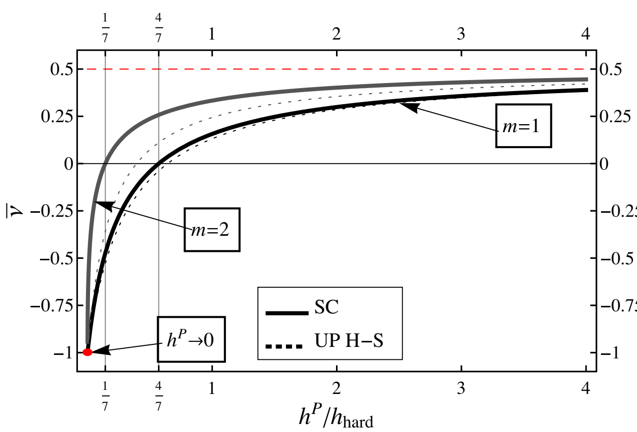

Fig. 6. The overall Poisson's ratio for random volumetrically isotropic polycrystal with unsustained stresses obtained with use of the SC estimate or the H–S upper bound for overall stiffness; m–multiplicity of the deviatoric Kelvin modulus $h_{easy} \to 0$.

distinguished. Note that this line always lies in the regime for which $h_{easy} \leqslant h^P = \bar{h}^P \leqslant h_{hard}$.

4. Examples

In this section we demonstrate the applicability of the derived results to the analysis of linear viscous flow (i.e. steady creep) for materials with hcp lattice symmetry and validation of the self-consistent homogenization procedure. Following (Lebensohn et al., 2004) we consider Ice-type and Zr-type crystals and additionally Mg-type crystals. The first two examples represent incompressible crystals with constrained deformation while the last example represents an incompressible crystal with unsustained stresses. The relevant slip systems are:

- three basal slip systems $\{0001\}\langle 11\bar{2}0\rangle$,
- three prismatic slip systems $\{10\bar{1}0\}\langle 11\bar{2}0\rangle$,
- first-order pyramidal $\langle c+a\rangle$ slip systems $\{10\bar{1}\bar{1}\}\langle 11\bar{2}3\rangle$,
- second-order pyramidal $\langle c+a\rangle$ slip systems $\{11\bar{2}2\}\langle 11\bar{2}3\rangle$.

Denoting by τ_c^{bas}, τ_c^{prism}, $\tau_c^{pyr.I}$ and $\tau_c^{pyr.II}$ the resolved critical shear stresses under which subsequent modes are initiated, we assume the following relation between their values for the considered materials:

Table 1
Local viscous moduli in $[\tau_c^{bas}/\dot{\gamma}_0]$ for selected hcp materials (i–number of independent easy slip systems).

	Ice	Zr	Mg
h_2	$\frac{(1+d^2)^2}{9d^2}\rho$	$\frac{(3+7d^2+4d^4)}{54d^2}\rho$	$\frac{(1+d^2)^2}{9d^2}$
$h_2^{\rho\to\infty}$	∞	∞	
h_3	$\frac{4(1+d^2)^2}{3(1+4d^2+d^4)}\rho$	$\frac{4(3+7d^2+4d^4)\rho}{3(3+7d^2+4d^4)\rho+16d^2}$	$\frac{4(1+d^2)^2}{3(1+4d^2+d^4)}$
$h_3^{\rho\to\infty}$	∞	$4/3$	
h_4	$\frac{4(1+d^2)^2\rho}{3(2(1-d^2)^2+(1+d^2)^2\rho)}$	$\frac{4(3+7d^2+4d^4)\rho}{3(4(3-6d^2+4d^4)+(3+7d^2+4d^4)\rho)}$	$\frac{4(1+d^2)^2}{3(2(1-d^2)^2+(1+d^2)^2\rho)}$
$h_4^{\rho\to\infty}$	$4/3$	$4/3$	0
i	2	4	2

- For ice-type crystals $\tau_c^{prism} = \tau_c^{pyr.II} = \rho\tau_c^{bas}$, $\tau_c^{pyr.I} \to \infty$ and the lattice parameter $c/a = 1.629$.
- For Zr-type crystals $\tau_c^{prism} = \tau_c^{bas}$, $\tau_c^{pyr.I} = \rho\tau_c^{bas}$, $\tau_c^{pyr.II} \to \infty$ and the lattice parameter $c/a = 1.593$.
- For Mg-type crystals $\tau_c^{prism} = \tau_c^{pyr.II}$, $\tau_c^{bas} = 1/\rho\tau_c^{pyr.II}$, $\tau_c^{pyr.I} \to \infty$ and the lattice parameter $c/a = 1.624$.

Following Lebensohn et al., 2004 the nomenclature Ice-*type*, Zr-*type* and Mg-*type* is used to indicate that, as discussed above, $n = 1$ is not valid exponent for these materials, i.e. $n = 3$ is usually identified for steady creep of ice, while n around 20 is used in modeling of inelastic response of Mg and Zr alloys with use of the the VPSC model. However, as concerns $\rho = \tau_c^{hard}/\tau_c^{easy}$ the assumed differentiation between slip system categories in general follows the values established on the basis of experiments, see for example (Agnew et al., 2001; Proust et al., 2009) for Mg-alloys or (Fundenberger et al., 1997; Castelnau et al., 2001) for Zr-alloys.[4] As concerns ice, in many papers only basal slip is assumed to be active ($\rho \to \infty$) or if other slip systems are considered they have much higher critical shear stress, c.f. (Morland and Staroszczyk, 2009).

In the case of linear viscous flow of hcp material the compliance tensor $\mathbb{M}^v$ exhibits transversal isotropy, namely

$$\mathbb{M}^v = \frac{1}{h_2(\rho, c/a)}\mathbb{P}_2 + \frac{1}{h_3(\rho, c/a)}\mathbb{P}_3 + \frac{1}{h_4(\rho, c/a)}\mathbb{P}_4$$
$$m_2 = 1,\ m_3 = m_4 = 2, \tag{108}$$

where transversely isotropic projectors $\mathbb{P}_K$ are specified as for the volumetrically isotropic material (see e.g. (Rychlewski, 1995; Kowalczyk-Gajewska and Ostrowska-Maciejewska, 2009)). Local Kelvin moduli h_k are specified in Table 1, together with the limit case when $\rho \to \infty$.

In Fig. 8 bounds and estimates for an overall flow stress for ice-type and Zr-type random polycrystals are presented. In agreement with the theoretical analysis presented in previous sections, with increasing value of ρ:

- for ice-type polycrystals the SC estimate of an overall flow stress tends to infinity being close to the Hill estimate based on the V–R bounds,
- for Zr-type polycrystal the SC estimate saturates at finite value similarly to the lower bounds.

The question is if this result, proven for arbitrary lattice symmetry in Section 3.3, indicates limitation of the SC method

[4] It should be noted that, contrary to the example studied in Lebensohn et al. (2004), it is observed for zirconium that the basal slip is usually less easy to initiate than prismatic slip.

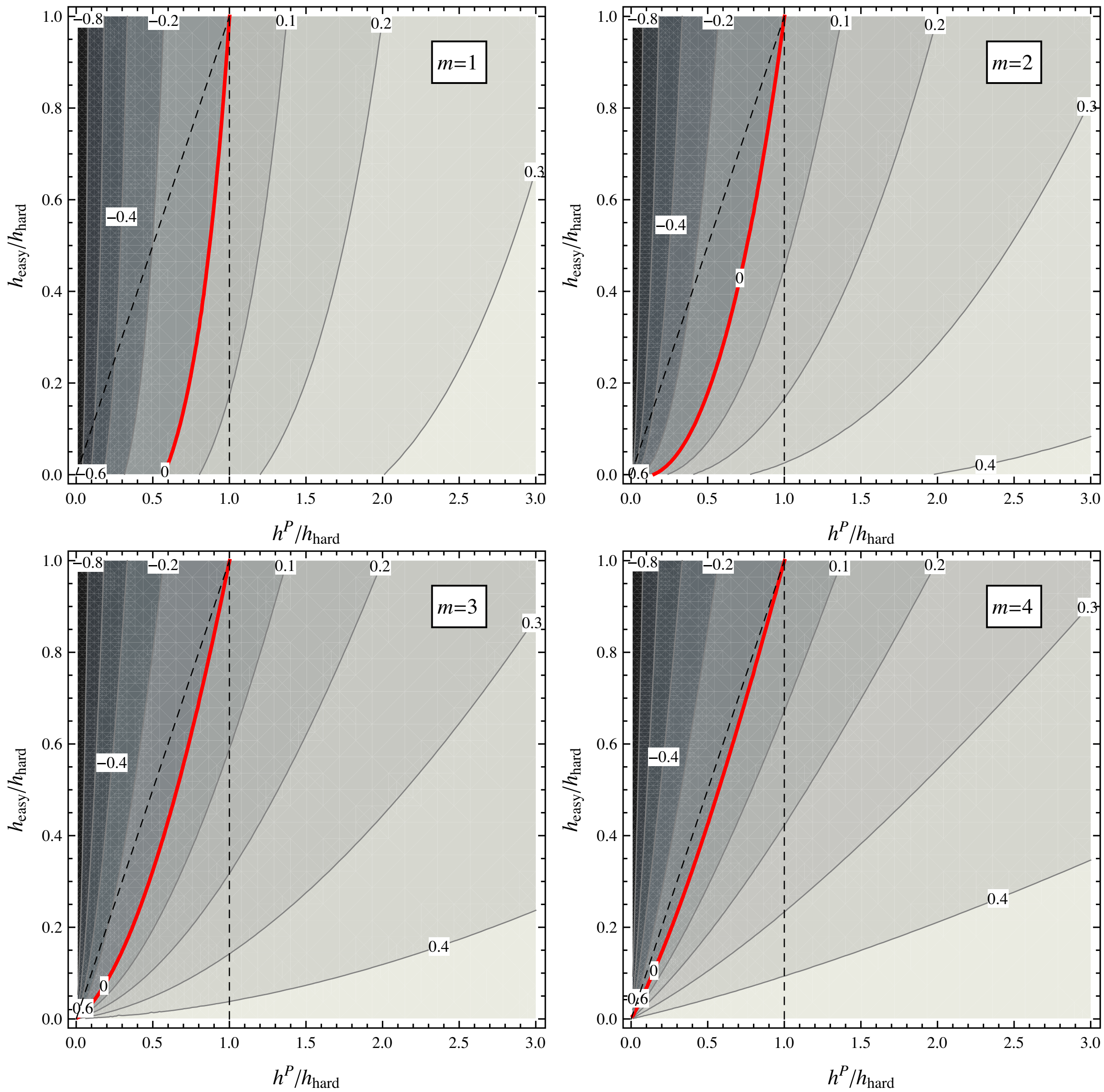

Fig. 7. Self-consistent estimate of effective Poisson's ratio for random volumetrically isotropic polycrystal with stiffness tensor specified by (101); m–multiplicity of the deviatoric Kelvin modulus h_{easy}.

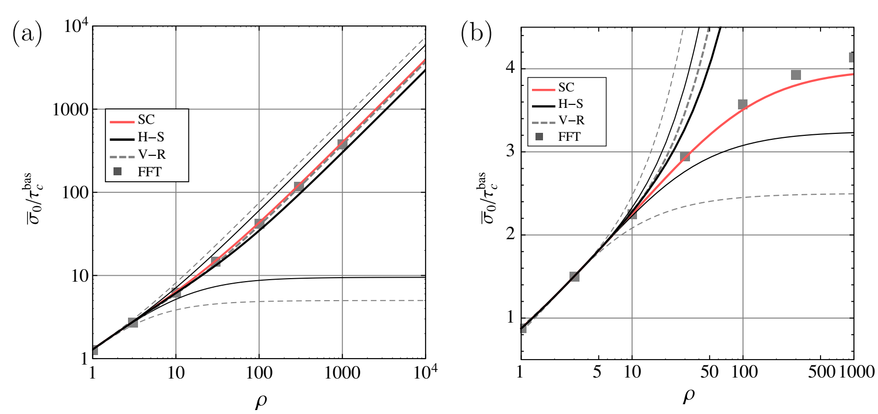

Fig. 8. Bounds, corresponding Hill's estimates as well as the SC estimate of the overall flow stress for random polycrystal: (a) Ice-type polycrystal, (b) Zr-type polycrystal.

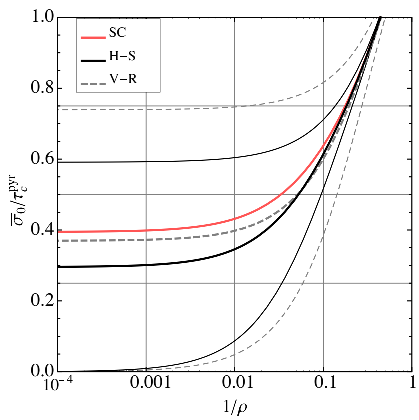

Fig. 9. Bounds, corresponding Hill's estimates as well as the SC estimate of the overall flow stress for Mg-type random polycrystal.

applied to materials with an insufficient number of independent easy slip systems or represents their real behavior. Although a definite answer to this question is not yet established, some support for the latter possibility can be found in Lebensohn et al. (2004), where the relevant results of numerical simulations employing the Fast Fourier Transforms (FFT) for assembles of random aggregates of such crystals have been reported. These results are depicted in Fig. 8 by large squares. They are in very good quantitative agreement with the SC estimate for both materials, which indicates validity of this method for estimating the overall properties of polycrystalline materials. Note that the existence of the finite SC estimate for hcp random polycrystals with only four independent slip systems has been already noticed by Hutchinson (1977). He also suggested that such approximation could be valid for real hcp materials.

In Fig. 9 the bounds and estimates of an overall flow stress for a Mg-type random polycrystal as functions of $1/\rho$ are presented. It is seen that, in agreement with the theoretical study, a nonzero flow stress for random polycrystal is predicted, even though locally basal slip is initiated under resolved shear stress tending to zero ($1/\rho \to 0$).

5. Conclusions

In this paper, using the method proposed in Kowalczyk-Gajewska (2009), bounds and SC estimates on overall properties of polycrystalline materials of arbitrary anisotropy have been studied. Linear constitutive laws have been considered for which the material properties are represented by fourth-order Hooke's tensors.

With use of the spectral and harmonic decompositions of Hooke's tensors, new expressions for H–S bounds and SC estimates have been derived for random polycrystals composed of elements of arbitrary anisotropy. For a wide class of anisotropic crystals corresponding formulae for SC estimates have been provided in the form of polynomial equations with coefficients depending on the invariants of a local stiffness tensor. Incompressible materials and materials with constrained deformation modes or with unsustained stress modes have been considered.

It should be noted that the spectral and harmonic decompositions of Hooke's tensors are relatively new mathematical tools (Rychlewski, 1983; Cowin and Mehrabadi, 1995; Forte and Vianello, 1996; Rychlewski, 2000). Their simultaneous application, first, to the analysis of the stiffness/compliance tensors and then, to bounds and estimates of overall properties of polycrystalline materials seems to be not known in the literature. The use of invariants of fourth-order tensors resulting from the decompositions employed allows us to demonstrate that the existence of a finite SC estimate for an overall shear modulus for random polycrystal depends on the dimension of a subspace of constrained deviatoric deformation. It has been shown that the above property of SC scheme is important for the case of linear viscous polycrystals of low symmetry with an insufficient number of easy slip systems. This original analytical result indicates that the crystal should have at least four independent slip systems in order to have a finite self-consistent estimate of an overall flow stress. It is the counterpart of the well-known Taylor condition. Similarly, it has been demonstrated that the existence of a non-zero shear modulus for random polycrystal with unsustained stress modes depends on the dimension of a subspace of unsustained stresses.

Acknowledgement

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Appendix A. Invariant decompositions of Hooke's tensors

A.1. Spectral decomposition

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

$$T_{ijkl} = T_{jikl} = T_{ijlk} = T_{klij}. \tag{A.1}$$

The last internal symmetry in (A.1) is called a major symmetry. Since in the same time Hooke's tensor is a symmetric second-order tensor in six-dimensional Euclidean space the spectral theorem can be applied to such tensor (Rychlewski, 1983; Mehrabadi and Cowin, 1990), *viz.*

$$\mathbb{T} = \sum_{K=1}^{M} T_K \mathbb{P}_K, \tag{A.2}$$

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

$$\mathbb{P}_K \circ \mathbb{P}_L = \begin{cases} \mathbb{P}_K & \text{if} \quad K = L \\ \mathbb{O} & \text{if} \quad K \neq L \end{cases}, \quad \sum_{K=1}^{M} \mathbb{P}_K = \mathbb{I}^S. \tag{A.3}$$

If T_K is an eigenvalue of multiplicity m_K then the corresponding projector may be specified in the form

$$\mathbb{P}_K = \sum_{i=1}^{m_K} \boldsymbol{\omega}_i \otimes \boldsymbol{\omega}_i, \tag{A.4}$$

where $\{\boldsymbol{\omega}_i\}, i = 1, \ldots, m_K$ constitute basis in the corresponding m_K-dimensional eigen-subspace of second-order tensors. It should be stressed that decomposition (A.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 Rychlewski (1983), Rychlewski (1995), Cowin and Mehrabadi (1995), Chadwick et al. (2001), and Kowalczyk-Gajewska and Ostrowska-Maciejewska (2004a, 2009).

A.2. Harmonic decomposition

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

$$\mathbb{T} = \underbrace{h^{\mathrm{P}}\mathbb{I}_{\mathrm{P}} + h^{\mathrm{D}}\mathbb{I}_{\mathrm{D}}}_{\text{the isotropic part}} + \underbrace{\mathbb{A}^{\mu} + \mathbb{A}^{\nu} + \mathbb{H}}_{\text{the anisotropic part}}, \tag{A.5}$$

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

$$\mathbb{I}_{\mathrm{P}} = \frac{1}{3}\mathbf{I}\otimes\mathbf{I}, \quad \mathbb{I}_{\mathrm{D}} = \mathbb{I}^S - \frac{1}{3}\mathbf{I}\otimes\mathbf{I} \tag{A.6}$$

and two scalars h^{P} and h^{D}. Second two parts are specified as linear functions of two second-order deviators $\boldsymbol{\phi}$ and $\boldsymbol{\rho}$, namely[5]

$$\mathbb{A}^{\mu}(\boldsymbol{\phi}) = \mathbf{I}\otimes\boldsymbol{\phi} + \boldsymbol{\phi}\otimes\mathbf{I}, \tag{A.8}$$

$$\mathbb{A}^{\nu}(\boldsymbol{\rho}) = \frac{1}{2}[\mathbf{I}\otimes\boldsymbol{\rho} + \boldsymbol{\rho}\otimes\mathbf{I}]^{T(23)+T(24)} - \frac{2}{3}[\mathbf{I}\otimes\boldsymbol{\rho} + \boldsymbol{\rho}\otimes\mathbf{I}] \tag{A.9}$$

where $T^{T(23)+T(24)}_{ijkl} \equiv T_{ikjl} + T_{ilkj}$ and $\mathbb{H}$ is totally symmetric and traceless. This decomposition enables the following one to one correspondence

$$\mathbb{T} \leftrightarrow \left(h^{\mathrm{P}}, h^{\mathrm{D}}, \boldsymbol{\phi}, \boldsymbol{\rho}, \mathbb{H}\right). \tag{A.10}$$

Scalars are calculated as follows

$$h^{\mathrm{P}} = \frac{1}{3}\mathbf{I}\cdot\mathbb{T}\cdot\mathbf{I}, \quad h^{\mathrm{D}} = \frac{1}{5}(\mathrm{Tr}\mathbb{T} - h^{\mathrm{P}}), \quad h^{\mathrm{P}} = \frac{1}{3}T_{iikk}, \quad \mathrm{Tr}\mathbb{T} = T_{ikik}, \tag{A.11}$$

while second-order deviators are calculated with use of the so-called Novozhilov's deviators $\boldsymbol{\mu}_{\mathrm{D}}$ and $\boldsymbol{\nu}_{\mathrm{D}}$, namely

$$\boldsymbol{\phi} = \frac{1}{3}\boldsymbol{\mu}_{\mathrm{D}}, \quad \boldsymbol{\rho} = \frac{2}{7}(3\boldsymbol{\nu}_{\mathrm{D}} - 2\boldsymbol{\mu}_{\mathrm{D}}), \tag{A.12}$$

where $\boldsymbol{\mu}_{\mathrm{D}}$ and $\boldsymbol{\nu}_{\mathrm{D}}$ are deviators of the following tensors

$$\boldsymbol{\mu} = \mathbb{T}\cdot\mathbf{I}, \quad \boldsymbol{\nu} = \mathbb{T}^{T(23)}\cdot\mathbf{I}, \quad \mu_{ij} = T_{ijkk}, \quad \nu_{ij} = T_{ikjk}. \tag{A.13}$$

The symmetry group of the tensor $\mathbb{T}$ is a product of symmetry groups of the tensors $\boldsymbol{\phi}$, $\boldsymbol{\rho}$ (or equivalently of $\boldsymbol{\mu}_{\mathrm{D}}, \boldsymbol{\nu}_{\mathrm{D}}$) and $\mathbb{H}$.

Because projectors $\mathbb{P}_K$ of the spectral decomposition of $\mathbb{T}$ are fourth-order Hooke's tensors the harmonic decomposition (A.5) of them can be performed, namely

$$\mathbb{P}_K = \eta^{\mathrm{P}}_K\mathbb{I}_{\mathrm{P}} + \eta^{\mathrm{D}}_K\mathbb{I}_{\mathrm{D}} + \mathbb{A}^{\mu}_K + \mathbb{A}^{\nu}_K + \mathbb{H}_K, \tag{A.14}$$

where specifically

$$\eta^{\mathrm{P}}_K = \frac{1}{3}\mathbf{I}\cdot\mathbb{P}_K\cdot\mathbf{I}, \quad \eta^{\mathrm{D}}_K = \frac{1}{5}(m_K - \eta^{\mathrm{P}}_K), \quad \mathbb{A}^{\mu}_K = \mathbb{A}^{\mu}(\boldsymbol{\mu}_{\mathrm{D}K}), \quad \mathbb{A}^{\nu}_K = \mathbb{A}^{\nu}(\boldsymbol{\nu}_{\mathrm{D}K}) \tag{A.15}$$

and m_K is the multiplicity of the corresponding modulus h_K. One should note the following identities:

$$\sum_{K=1}^{M}\mathbb{P}_K = \mathbb{I}^S \Rightarrow \sum_{K=1}^{M}\eta^{\mathrm{P}}_K = 1, \quad \sum_{K=1}^{M}\eta^{\mathrm{D}}_K = 1, \quad \sum_{K=1}^{M}m_K = 6, \tag{A.16}$$

where $0 \leqslant \eta^{\mathrm{P}}_K \leqslant 1, 0 \leqslant \eta^{\mathrm{D}}_K \leqslant 1$ and

$$\sum_{K=1}^{M}\mathbb{A}^{\mu}_K = \mathbb{O}\left(\sum_{K=1}^{M}\boldsymbol{\mu}_{\mathrm{D}K} = \mathbf{0}\right), \quad \sum_{K=1}^{M}\mathbb{A}^{\nu}_K = \mathbb{O}\left(\sum_{K=1}^{M}\boldsymbol{\nu}_{\mathrm{D}K} = \mathbf{0}\right), \quad \sum_{K=1}^{M}\mathbb{H}_K = \mathbb{O}. \tag{A.17}$$

[5] As shown by Rychlewski (2000) there are infinitely many possible definitions of $\mathbb{A}^{\mu}$ and $\mathbb{A}^{\nu}$, while their sum remains the same for the considered tensor $\mathbb{T}$. All of them have the form

$$\mathbb{A}^{\alpha} = \aleph^{\alpha} \times (\mathbf{I}\otimes\mathbf{a}^{\alpha} + \mathbf{a}^{\alpha}\otimes\mathbf{I}), \tag{A.7}$$

where $\aleph^{\alpha}$ are independent permutation operations while $\mathbf{a}^{\alpha}$ are some second-order deviators depending on Novozhilov's tensors deviators.

The form of decomposition (A.5) is based on the presentations in Rychlewski (2000), Rychlewski (2001b). Different definitions of $\mathbb{A}^{\mu}$ and $\mathbb{A}^{\nu}$ have been utilized in Forte and Vianello (1996). This relatively new mathematical tool proved to be useful when analyzing symmetry groups of elastic materials (Forte and Vianello, 1996), finding the basis of invariants for Hooke's tensor (Boehler et al., 1994) or identification of anisotropic properties of biological materials (Piekarski et al., 2004).

Appendix B. Polynomial equations for self-consistent estimates of shear modulus for volumetrically isotropic materials

The crystal bulk modulus h^{P} and the following functions of deviatoric Kelvin modulae

$$\begin{aligned}
&J_1 = h_2 + h_3 + h_4 + h_5 + h_6 > 0,\\
&J_2 = h_2h_3 + h_2h_4 + \cdots + h_5h_6 > 0,\\
&J_3 = h_2h_3h_4 + h_2h_3h_5 + \cdots + h_4h_5h_6 > 0,\\
&J_4 = h_2h_3h_4h_5 + h_2h_3h_4h_6 + \cdots + h_3h_4h_5h_6 > 0,\\
&J_5 = h_2h_3h_4h_5h_6 > 0
\end{aligned}$$

are invariants of a local $\mathbb{L}$ for the volumetrically isotropic material which are independent of the ordering of h_K and can be calculated without performing the spectral decomposition. The coefficients α_k of the polynomial Eq. (71) for a self-consistent estimate of an overall shear modulus $\bar{h}^{\mathrm{D}}$ are specified with use of the above invariants as follows

$$\begin{aligned}
&\alpha_0 = -16J_5h_P^4 < 0,\\
&\alpha_1 = -h_P^3(192J_5 + 16J_4h_P) < 0,\\
&\alpha_2 = -h_P^2\left(864J_5 + 160J_4h_P + 12J_3h_P^2\right) < 0,\\
&\alpha_3 = -h_P\left(1728J_5 + 576J_4h_P + 88J_3h_P^2\right) < 0,\\
&\alpha_4 = -\left(1296J_5 + 864J_4h_P + 204J_3h_P^2 - 36J_2h_P^3 - 27J_1h_P^4\right),\\
&\alpha_5 = -\left(432J_4 + 144J_3h_P - 204J_2h_P^2 - 216J_1h_P^3 - 81h_P^4\right),\\
&\alpha_6 = 352J_2h_P + 576J_1h_P^2 + 432h_P^3 > 0,\\
&\alpha_7 = 192J_2 + 640J_1h_P + 864h_P^2 > 0,\\
&\alpha_8 = 256J_1 + 768h_P > 0,\\
&\alpha_9 = 256.
\end{aligned} \tag{B.1}$$

We have proved in Kowalczyk-Gajewska (2009) that Eq. (71) has always a unique positive solution.

The 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 modulae $h_K, K = 2, \ldots, 6$. It has the following form

$$81\bar{h}_D^5 + 27J_1\bar{h}_D^4 - 12J_3\bar{h}_D^2 - 16J_4\bar{h}_D - 16J_5 = 0. \tag{B.2}$$

This equations has a single positive real root.

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