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The 4th-Order Isotropic Tensor Function of a Symmetric 2nd-Order Tensor with Applications to Anisotropic Elasto-Plasticity

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

The effective elastic properties of polycrystals can vary significantly with their crystallographic texture [7]. Since a correlation of elastic and plastic properties has been proven (see [8] and references therein), a phenomenological modeling of the crystallographic texture induced elastic anisotropy is of importance in the context of both elasticity and plasticity. In the present paper an evolution equation for the effective elasticity tensors of aggregates of cubic crystals is specified by means of the theory of isotropic tensor functions. It is shown that constraints forced by the elastic symmetry on the micro scale simplify the phenomenological equations significantly.

1. Introduction

Notation: Linear mappings of 2nd-order tensors are written as $\mathbf{A} = \mathbb{C}[\mathbf{B}]$. The scalar product, the dyadic product, and the Euclidean norm are denoted by $\mathbf{A} \cdot \mathbf{B}$, $\mathbf{A} \otimes \mathbf{B}$, and $\|\mathbf{A}\| = (\mathbf{A} \cdot \mathbf{A})^{1/2}$, respectively. *Lin* denotes the set of all 2nd-oder tensors. *Sym* and *Orth* represent the sets of symmetric and proper orthogonal 2nd-order tensors.

Initially isotropic aggregates of crystalline grains show a texture-induced anisotropy of both their inelastic and elastic behavior when submitted to large inelastic deformations. The latter, however, is normally neglected, although experiments as well as numerical simulations clearly show a strong alteration of the elastic properties for certain materials. A source for such phenomena is a significant anisotropy of the corresponding physical property of the single crystals forming the aggregate. The main purpose of the present work is to derive the 4th-order isotropic tensor function of a symmetric 2nd-order tensor and to determine explicitly its irreducible part. This tensor function is necessary to formulate a phenomenological model for the evolution of the elastic properties polycrystals.

Generally, it is possible to decompose 4th-order elasticity tensors of arbitrary symmetry into a direct sum of orthogonal subspaces, on which the action of *Orth* is irreducible. The action of *Orth* on a vector space is said to be irreducible when there are no proper invariant subspaces. The harmonic decomposition has the form

$$\mathbb{C} = h_1\mathbb{P}_1^I + h_2\mathbb{P}_2^I + \mathbf{H}_1' \otimes \mathbf{I} + \mathbf{I} \otimes \mathbf{H}_1' + 4\mathbb{J}[\mathbf{H}_2'] + \mathbb{H}', \tag{1}$$

where

$$\mathbb{P}_1^I = \tfrac{1}{3}\mathbf{I} \otimes \mathbf{I}, \qquad \mathbb{P}_2^I = \mathbb{I} - \mathbb{P}_1^I, \qquad 4\mathbb{J}[\mathbf{A}] = (A_{im}\delta_{jn} + A_{in}\delta_{jm} + \delta_{im}A_{jn} + \delta_{in}A_{jm})\, \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_m \otimes \mathbf{e}_n \tag{2}$$

[12, 13, 5, 3]. $\mathbf{I}$ denotes the 2nd-order identity tensor and $\mathbb{I}$ represents the identity on symmetric 2nd-order tensors. The tensors $\mathbf{H}_1'$, $\mathbf{H}_2'$, and $\mathbb{H}'$ are irreducible, i.e. completely symmetric and traceless. A review concerning this representation is given in [6]. h_1 and h_2 are called the first and second isotropic parts; $\mathbf{H}_1'$ and $\mathbf{H}_2'$ are the first and second deviatoric parts; $\mathbb{H}'$ is the harmonic part. Irreducible 2nd-order tensors have five, and irreducible 4th-order tensors have nine independent components.

The symmetry group of $\mathbb{C}$ is the intersection of the symmetry groups of its harmonic and deviatoric parts [6]. As a result, a cubic crystal symmetry forces $\mathbf{H}_1' = \gamma_1\mathbf{I}$ and $\mathbf{H}_2' = \gamma_2\mathbf{I}$. From $\mathrm{tr}(\mathbf{H}_1') = 0$ and $\mathrm{tr}(\mathbf{H}_2') = 0$ one concludes $\gamma_1 = 0$ and $\gamma_2 = 0$, respectively. Therefore, the tensors $\mathbf{H}_1'$ and $\mathbf{H}_2'$ vanish and the harmonic decomposition of the single crystal stiffness reduces to

$$\mathbb{C} = h_1\mathbb{P}_1^I + h_2\mathbb{P}_2^I + \mathbb{H}'. \tag{3}$$

Only in the case of a cubic crystal symmetry the deviatoric parts $\mathbf{H}_1'$ and $\mathbf{H}_2'$ vanish.

The effective elastic properties can be determined by orientational or volume averages of the local elasticity tensors. Examples are the arithmetic, the geometric, or the harmonic average [2]. In what follows we consider aggregates of cubic crystals. The singlecrystalline grains are assumed to differ only by their crystallographic orientation. For the volume average of $\mathbb{C}$ remains only

$$\bar{\mathbb{C}} = h_1 \mathbb{P}_1^I + h_2 \mathbb{P}_2^I + \bar{\mathbb{H}}'. \tag{4}$$

Note that the volume average $\bar{\mathbb{H}}'$ of $\mathbb{H}'$ is irreducible. It is seen that a crystallographic texture evolution affects only the harmonic part of the stiffness. The same statement holds for the arithmetic mean [15] of local stiffnesses, the geometric mean [1, 9], and the harmonic mean [11] (see also [2]).

A simple phenomenological model for the texture induced elastic anisotropy is given by the following evolution equation

$$\frac{D}{Dt}\bar{\mathbb{H}}' = \|\mathbf{D}_p'\| \left(\mathbb{G}'(\mathbf{N}_p') - d(I_p)\bar{\mathbb{H}}'\right), \qquad \mathbf{N}_p' = \frac{\mathbf{D}_p'}{\|\mathbf{D}_p'\|}, \qquad I_p = \det(\mathbf{N}_p'), \tag{5}$$

where $\mathbf{D}_p'$ is the macroscopic plastic strain-rate which is deviatoric. All quantities are formulated with respect to the (Lagrangian) undistorted configuration, which is invariant under changes of the observer. $D(\cdot)/Dt$ denotes the material derivative. The plastic spin has not been taken into account in eqn (5). Furthermore, the driving term depends only on the direction $\mathbf{N}_p'$ of $\mathbf{D}_p'$. The main problem is to find the general representation of the function $\mathbb{G}'$, which has to be irreducible. In section 2 the general 4th-order isotropic tensor function of a symmetric 2nd-order tensor is derived by means of the theory of isotropic tensor functions of 2nd-order tensors ([17, 4], see also [10, 16, 14]). In section 3 the corresponding irreducible part is determined. It is shown that the condition of irreducibility simplifies the representation considerably.

2. The 4th-Order Isotropic Tensor Function of a Symmetric 2nd-Order Tensor

In what follows, we derive the representation of a general, not necessarily polynomial, 4th-order isotropic tensor function $\mathbb{G}$ of a symmetric 2nd-order tensor $\mathbf{A} \in Sym$. The tensor function $\mathbb{G}$ is required to exhibit the index symmetries of elasticity tensors, i.e. the major symmetry and the symmetry in the first and second pair of indices

$$\mathbf{M} \cdot \mathbb{G}[\mathbf{N}] = \mathbf{N} \cdot \mathbb{G}[\mathbf{M}], \qquad \mathbf{M} \cdot \mathbb{G}[\mathbf{N}] = \mathbf{M} \cdot \mathbb{G}[\mathbf{N}^T] = \mathbf{M}^T \cdot \mathbb{G}[\mathbf{N}] \qquad \forall \mathbf{M}, \mathbf{N} \in Lin. \tag{6}$$

The starting point is the irreducible representation of a (symmetric) 2nd-order isotropic tensor function of two symmetric 2nd-order tensors [17, 4]

$$\mathbf{G}(\mathbf{A}, \mathbf{B}) = \sum_{\alpha=0}^{7} g_\alpha \mathbf{G}_\alpha. \tag{7}$$

The eight symmetric tensor generators $\mathbf{G}_\alpha$ are given by

$$\mathbf{I}, \mathbf{A}, \mathbf{A}^2, \mathbf{B}, \mathbf{AB} + \mathbf{BA}, \mathbf{A}^2\mathbf{B} + \mathbf{BA}^2, \mathbf{B}^2, \mathbf{AB}^2 + \mathbf{B}^2\mathbf{A}. \tag{8}$$

The g_α are general functions of the 10 invariants of the functional basis of $\mathbf{A}$ and $\mathbf{B}$

$$\begin{aligned} &\mathrm{tr}(\mathbf{A}), \mathrm{tr}(\mathbf{A}^2), \mathrm{tr}(\mathbf{A}^3), \mathrm{tr}(\mathbf{B}), \mathrm{tr}(\mathbf{B}^2), \mathrm{tr}(\mathbf{B}^3), \\ &\quad \mathrm{tr}(\mathbf{AB}), \mathrm{tr}(\mathbf{A}^2\mathbf{B}), \mathrm{tr}(\mathbf{AB}^2), \mathrm{tr}(\mathbf{A}^2\mathbf{B}^2). \end{aligned} \tag{9}$$

The representation (7) is called irreducible if the functional basis is irreducible and if none of the generators can be expressed as a linear combination of the other generators, formed with general functions g_α. A functional basis is called irreducible if none of its elements can be expressed as a single-valued function of the other elements [4]. This definition of irreducibility differs from the one applied when discussion the index symmetries of the tensor $\mathbb{H}'$.

The function $\mathbb{G}$ can be obtained by a linearization of $\mathbf{G}$ in $\mathbf{B}$

$$\mathbf{G}^{lin}(\mathbf{A}, \mathbf{B}) = \mathbb{G}(\mathbf{A})[\mathbf{B}]. \tag{10}$$

The linearized function $\mathbf{G}^{lin}$ reads

$$\mathbf{G}^{lin}(\mathbf{A}, \mathbf{B}) = g_0^{lin}\mathbf{I} + g_1^{lin}\mathbf{A} + g_2^{lin}\mathbf{A}^2 + g_3^{lin}\mathbf{B} + g_4^{lin}(\mathbf{AB} + \mathbf{BA}) + g_5^{lin}(\mathbf{A}^2\mathbf{B} + \mathbf{BA}^2). \tag{11}$$

After the linearization, the scalar functions $g_\alpha(\mathbf{A},\mathbf{B})$ can be expressed in terms of $\mathbf{B}$ and the new functions $g_{ij}(\mathbf{A})$ that are isotropic in $\mathbf{A}$

$$\begin{aligned} g_i^{lin} &= g_{i0}(\mathbf{A})\mathrm{tr}(\mathbf{B}) + g_{i1}(\mathbf{A})\mathrm{tr}(\mathbf{AB}) + g_{i2}(\mathbf{A})\mathrm{tr}(\mathbf{A}^2\mathbf{B}), \quad (i=0,1,2), \\ g_i^{lin} &= g_{i0}(\mathbf{A}), \quad (i=3,4,5). \end{aligned} \tag{12}$$

A direct calculation yields the following representation

$$\begin{aligned} \mathbb{G}(\mathbf{A}) &= (3g_{00}+g_{30})\,\mathbb{P}_1^I + g_{30}\mathbb{P}_2^I + g_{11}\mathbf{A}\otimes\mathbf{A} + g_{22}\mathbf{A}^2\otimes\mathbf{A}^2 + 2g_{40}\mathbb{J}[\mathbf{A}] + 2g_{50}\mathbb{J}[\mathbf{A}^2] \\ &+ g_{10}\mathbf{A}\otimes\mathbf{I} + g_{01}\mathbf{I}\otimes\mathbf{A} + g_{20}\mathbf{A}^2\otimes\mathbf{I} + g_{02}\mathbf{I}\otimes\mathbf{A}^2 \\ &+ g_{21}\mathbf{A}^2\otimes\mathbf{A} + g_{12}\mathbf{A}\otimes\mathbf{A}^2. \end{aligned} \tag{13}$$

From the requirement $(6)_1$ one concludes

$$g_{10}=g_{01}, \qquad g_{20}=g_{02}, \qquad g_{12}=g_{21}. \tag{14}$$

As a result, the 4th-order isotropic tensor function $\mathbb{G}$ reads

$$\begin{aligned} \mathbb{G}(\mathbf{A}) &= \textstyle\sum_{\alpha=1}^{9} G_\alpha(\mathbf{A})\mathbb{G}_\alpha(\mathbf{A}) \\ &= (3g_{00}+g_{30})\,\mathbb{P}_1^I + g_{30}\mathbb{P}_2^I + g_{11}\mathbf{A}\otimes\mathbf{A} + g_{22}\mathbf{A}^2\otimes\mathbf{A}^2 + 2g_{40}\mathbb{J}[\mathbf{A}] + 2g_{50}\mathbb{J}[\mathbf{A}^2] \\ &+ g_{10}\left(\mathbf{A}\otimes\mathbf{I}+\mathbf{I}\otimes\mathbf{A}\right) + g_{20}\left(\mathbf{A}^2\otimes\mathbf{I}+\mathbf{I}\otimes\mathbf{A}^2\right) \\ &+ g_{21}\left(\mathbf{A}^2\otimes\mathbf{A}+\mathbf{A}\otimes\mathbf{A}^2\right). \end{aligned} \tag{15}$$

3. The Irreducible Part of the 4th-Order Isotropic Tensor Function of a Symmetric 2nd-Order Tensor

As mentioned before, an irreducible 4th-order tensor is symmetric and traceless with respect to every pair of indices. In this section we present the irreducible part $\mathbb{G}'$ of the function $\mathbb{G}$ (see (13)) by employing the procedure suggested by [5]. The irreducible part of a 4th-order tensor function $\mathbb{G}$ is given by

$$\mathbb{G}' = \frac{1}{3}\langle\mathbb{G}\rangle - \frac{1}{21}\{\hat{\mathbf{H}}\otimes\mathbf{I}\} + \frac{1}{105}\mathrm{tr}(\hat{\mathbf{H}})\langle\mathbf{I}\otimes\mathbf{I}\rangle, \tag{16}$$

where

$$\hat{\mathbf{H}} = G_{iikl}\mathbf{e}_k\otimes\mathbf{e}_l + 2G_{ikil}\mathbf{e}_k\otimes\mathbf{e}_l. \tag{17}$$

$\{\mathbf{e}_k\}$ represents an orthonormal basis. The bracket formulae is defined by $(\mathbf{A},\mathbf{B}\in Sym)$

$$\begin{aligned} \langle A_{ij}A_{kl}\rangle &= A_{ij}A_{kl} + A_{ik}A_{jl} + A_{il}A_{kj}, \\ \{A_{ij}B_{kl}\} &= A_{ij}B_{kl} + A_{ik}B_{jl} + A_{il}B_{kj} + B_{ij}A_{kl} + B_{ik}A_{jl} + B_{il}A_{kj}. \end{aligned} \tag{18}$$

Note, that $\mathbb{G}$ has the major symmetric. Therefore, $\langle G_{ijkl}\rangle = G_{ijkl}+G_{ikjl}+G_{ilkj}$. All components of $\mathbb{G}'$ are linear functions of the components of $\mathbb{G}$.

Inspection of eqn (15) shows that only the following three of the nine 4th-order tensor generators contain non-vanishing irreducible parts

$$\mathbb{G}_3(\mathbf{A}) = \mathbf{A}\otimes\mathbf{A}, \qquad \mathbb{G}_4(\mathbf{A}) = \mathbf{A}^2\otimes\mathbf{A}^2, \qquad \mathbb{G}_9(\mathbf{A}) = \mathbf{A}^2\otimes\mathbf{A}+\mathbf{A}\otimes\mathbf{A}^2, \tag{19}$$

which are given by

$$\begin{aligned} \mathbb{G}_3'(\mathbf{A}) &= \tfrac{1}{3}\langle\mathbf{A}\otimes\mathbf{A}\rangle - \tfrac{1}{21}\left(\mathrm{tr}(\mathbf{A})\{\mathbf{A}\otimes\mathbf{I}\} + 2\{\mathbf{A}^2\otimes\mathbf{I}\}\right) + \tfrac{1}{105}\left(\mathrm{tr}(\mathbf{A})^2 + 2\mathrm{tr}(\mathbf{A}^2)\right)\langle\mathbf{I}\otimes\mathbf{I}\rangle, \\ \mathbb{G}_4'(\mathbf{A}) &= \mathbb{G}_3'(\mathbf{A}^2), \\ \mathbb{G}_9'(\mathbf{A}) &= \tfrac{1}{3}\{\mathbf{A}^2\otimes\mathbf{A}\} - \tfrac{1}{21}\left(\mathrm{tr}(\mathbf{A}^2)\{\mathbf{A}\otimes\mathbf{I}\} + \mathrm{tr}(\mathbf{A})\{\mathbf{A}^2\otimes\mathbf{I}\} + 4\{\mathbf{A}^3\otimes\mathbf{I}\}\right) \\ &+ \tfrac{2}{105}\left(\mathrm{tr}(\mathbf{A})\mathrm{tr}(\mathbf{A}^2) + 2\mathrm{tr}(\mathbf{A}^3)\right)\langle\mathbf{I}\otimes\mathbf{I}\rangle. \end{aligned} \tag{20}$$

If the tensor $\mathbf{A}$ is replaced by the direction $\mathbf{N}' = \mathbf{A}'/||\mathbf{A}'||$ of its deviatoric part $\mathbf{A}' = \mathbf{A} - \mathrm{tr}(\mathbf{A})\mathbf{I}/3$, then, the generators read

$$\mathbb{G}_1'(\mathbf{N}') = \frac{1}{3}\langle \mathbf{N}' \otimes \mathbf{N}' \rangle - \frac{2}{21}\{\mathbf{N}'^2 \otimes \mathbf{I}\} + \frac{2}{105}\mathrm{tr}(\mathbf{N}'^2)\langle \mathbf{I} \otimes \mathbf{I} \rangle, \tag{21}$$

$$\mathbb{G}_2'(\mathbf{N}') = \frac{1}{3}\langle \mathbf{N}'^2 \otimes \mathbf{N}'^2 \rangle - \frac{1}{21}\left(\mathrm{tr}(\mathbf{N}'^2)\{\mathbf{N}'^2 \otimes \mathbf{I}\} + 2\{\mathbf{N}'^4 \otimes \mathbf{I}\}\right) + \frac{1}{105}\left(\mathrm{tr}(\mathbf{N}'^2)^2 + 2\mathrm{tr}(\mathbf{N}'^4)\right)\langle \mathbf{I} \otimes \mathbf{I} \rangle, \tag{22}$$

$$\mathbb{G}_3'(\mathbf{N}') = \frac{1}{3}\{\mathbf{N}'^2 \otimes \mathbf{N}'\} - \frac{1}{21}\left(\mathrm{tr}(\mathbf{N}'^2)\{\mathbf{N}' \otimes \mathbf{I}\} + 4\{\mathbf{N}'^3 \otimes \mathbf{I}\}\right) + \frac{4}{105}\mathrm{tr}(\mathbf{N}'^3)\langle \mathbf{I} \otimes \mathbf{I} \rangle. \tag{23}$$

Since $\mathbf{N}'$ is traceless and normalized, the three functions G_1, G_2, and G_3 depend on the only non-constant principal invariant $\det(\mathbf{N}')$ of $\mathbf{N}'$. As a result, $\mathbb{G}'(\mathbf{N}')$ reads

$$\mathbb{G}'(\mathbf{N}') = G_3(I)\mathbb{G}_3'(\mathbf{N}') + G_4(I)\mathbb{G}_4'(\mathbf{N}') + G_9(I)\mathbb{G}_9'(\mathbf{N}'), \qquad I = \det(\mathbf{N}'). \tag{24}$$

Within the presented evolution equation (5), the four scalar functions $G_3(I_p)$ $G_4(I_p)$, $G_9(I_p)$, and $d(I_p)$ which depend on the scalar $I_p = \det(\mathbf{N}_p')$ remain to be identified.

4. Conclusions

The theory of isotropy tensor functions of 2nd-order tensors is applied in order to formulate evolution equation of 4th-order elasticity tensors. The general representation theorem of a 4th-order isotropic tensor function of a symmetric tensor is derived. The irreducible part of this representation is determined explicitly. It is shown that the consideration of constraints given by the elastic symmetry on the micro scale simplifies the phenomenological equation significantly.

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