On the symmetry identification for the multi-level models of polycrystalline materials

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Abstract. An approach to identify the elastic symmetry of anisotropic materials is considered and applied together with the multi-level constitutive models of polycrystals. By using the two-level model of elasto-visco-plasticity, the changes in the symmetry of the elasticity tensor for the representative volume element of a polycrystalline copper during inelastic deformation are studied. The two-link strain trajectories of the “simple shear – simple shear” type are analyzed and the problem of the compatibility of the properties under investigation with any symmetry classes is formulated and solved at various deformation stages.

1. Introduction
Physic-mechanical properties of materials are dependent on their microstructure so the control of its formation during different technological processes makes it possible to obtain components and structures with unique exploitation characteristics. During the large inelastic deformation of polycrystalline metals and alloys, the evolution of inner structure is especially influenced by the mechanisms related to the rotation of crystallites. The essentially inhomogeneous distribution of crystal lattice orientations (i.e. crystallographic texture) in such materials may results in the significant anisotropy of their macroscopic properties. Herewith, the establishing of the orthogonal transformations, with respect to which the constitutive equations are invariant plays an important role in different technical applications.

In this paper, with the help of a multi-level approach and crystal elasto-visco-plasticity, changes in the elastic properties of the representative volume element (RVE) of a polycrystalline copper during inelastic deformation along two-link trajectories are numerically investigated. The incompatibility of these properties with some special classes is analyzed at the various stages of the loading processes in question. The advantage of the designated approach is the possibility of the direct consideration of the material’s evolving microstructure, which allows the explicit determination of all macroscopic characteristics.

2. Elastic symmetry identification problem
Let us consider an anisotropic material, the elastic deformation of which is governed by the generalized Hooke’s law:

$$\sigma = \Pi : \epsilon,$$  \hspace{1cm} (1)
where $\sigma$ and $\epsilon$ are the Cauchy’s stress and the small strain (2-rank) tensors, respectively; $\Pi$ is the elasticity (4-rank) tensor. Depending on the symmetry group of $\Pi$, the material under examination can be assigned to some of the eight elastic symmetry classes [1]. It is of a certain interest to solve the symmetry identification problem (SIP) [2, 3], which is to form the hierarchy of the classes related to this tensor with a determined error.

The structure of a symmetry class allows us to represent its tensor, $\Pi^{(s)}$, where $s$ is the significator of the class in the framework of the accepted classification in the following form (hereinafter we adopt the summation convention for repeated indexes, which are not in the parentheses):

$$
\Pi^{(s)} = \Pi_\alpha \cdot O \ast K^{(s)}_\alpha.
$$

Here $\Pi_\alpha$ are arbitrary independent constants, $O$ is an orthogonal tensor, $K^{(s)}_\alpha$ are the linearly independent 4-rank tensors defined in the terms of some orthonormal basis, $\{l_i\}$ (hereinafter we associate this basis with the laboratory coordinate system) and the $\langle * \rangle$ operation is the Rayleigh product [4]. Equation (2) implies that the multi-dimensional matrix of $\Pi^{(s)}$ has the special form in the orthonormal basis, $\{k_i\}$, where $k_i = O \cdot l_i$, which is characteristic of the tensors from the same class. In this regard the specified basis can be termed canonical.

Let $\|\|_2$ be the Frobenius norm on the space of $r$-rank tensors. We call a quantity, $ME[\Pi^{(s)}, \Pi]$, such that $\|\Pi^{(s)} : \epsilon - \Pi : \epsilon\|_2 \leq ME[\Pi^{(s)}, \Pi]\|\epsilon\|_2$, holds for all $\epsilon$ the mismatch estimate (ME) for the approximation, $\Pi^{(s)}$, with respect to the tensor, $\Pi$. This estimate can be associated with the level of the maximal absolute error, which occurs in stresses determined by (1) when approximating the elasticity tensor by its symmetric analogue. Thus, it is possible to reduce the SIP for a given elasticity tensor to finding its approximation with the acceptable small value of the ME [3].

One should note that the “exact” ME is defined by the so-called operator norm, $\|\|_2$:

$$
\|\Pi^{(s)} - \Pi\| = \inf \|\Pi^{(s)} : \epsilon - \Pi : \epsilon\|_2,
$$

the minimization of which over the admissible sets of the tensors of the form (2) for different classes gives the solution of the SIP. Nevertheless, from the computational point of view, its upper bound, $\|\Pi^{(s)} - \Pi\|_2$ (i.e. the quantity defined by the Frobenius norm), is more convenient to use it as an object function. In the case when $K^{(s)}_\alpha$ are biorthonormal with respect to the total scalar product, the corresponding optimization problem can be formulated as follows:

$$
\text{Find } \tilde{O} \text{ such that } \sum_\alpha \left(\left(O^T \ast \Pi\right) \ast K^{(s)}_\alpha\right)^2 \rightarrow \max .
$$

In the general case, it is sufficient to consider the special orthogonal group of 2-rank tensors as the admissible set for the values of $\tilde{O}$. The solution, $\tilde{O}$, of the stated problem determines the orientation of the canonical basis of the tensor, $\Pi^{(s)} = \left(\tilde{O} \ast \left(O^* \ast K^{(s)}_\alpha\right)\right)\left(O \ast K^{(s)}_\alpha\right)$, which is the closest to $\Pi$ with respect to the Frobenius norm. As it can be seen, $\Pi^{(s)}$ is the orthogonal projection of $\Pi$ on the span of $\tilde{O} \ast K^{(s)}_\alpha$. It is worthy to remark that such projection preserves positive definiteness [5].

A canonical basis for a tensor from a symmetry class is not unique. In particular, the basis obtained from the canonical one by a transformation from the symmetry group of the given tensor is also canonical. Such fact allows us to reduce the admissible set of the problem (3) to tensors, with respect to which the special orthogonal group is defined as the union of the left cosets [6] in the symmetry group. Thus, in the framework of the proposed approach, optimization is not required to find the isotropic approximation and it is sufficient to consider only the orientation of the isotropy axis for the
transversal isotropic one. To describe this orientation, we shall use the angles, \((\theta, \phi)\), of the spherical coordinate system, which parameterize the component matrix of \(O\) in the problem (3) as follows:

\[
\{O_y\} = \begin{pmatrix}
\cos \theta \cos^2 \phi + \sin^2 \phi & (\cos \theta - 1) \cos \theta \sin \phi & \sin \theta \cos \phi \\
(\cos \theta - 1) \cos \phi \sin \phi & \cos \theta \sin^2 \phi + \cos^2 \phi & \sin \theta \sin \phi \\
-\sin \theta \cos \phi & -\sin \theta \sin \phi & \cos \theta 
\end{pmatrix}.
\]

As for other cases, the orientation of the canonical basis can be expressed e.g. by the Euler angles, \((\alpha, \beta, \gamma)\), in the form:

\[
\{O_y\} = \begin{pmatrix}
\cos \alpha \cos \beta \cos \gamma - \sin \alpha \sin \gamma & -\sin \alpha \cos \beta \cos \gamma - \cos \alpha \sin \beta \sin \gamma & \cos \alpha \sin \beta \\
\sin \alpha \cos \beta \cos \gamma + \cos \alpha \sin \gamma & \cos \alpha \cos \gamma - \sin \alpha \cos \beta \sin \gamma & \sin \alpha \sin \beta \\
-\sin \beta \cos \gamma & \sin \beta \sin \gamma & \cos \beta 
\end{pmatrix}.
\]

A symmetric approximation, \(\tilde{\Pi}^{(i)}\), obtained from the numerical solution of the problem (3) causes an absolute error with the exact upper estimate defined by \(\|\tilde{\Pi}^{(i)} - \Pi\|\). To characterize the relative error of \(\tilde{\Pi}^{(i)}\), we introduce the so-called relative mismatch estimate (RME) as \(RME^{(i)} = \|\Pi^{-1} \tilde{\Pi}^{(i)} - \Pi\|\), where \(\Pi^{-1}\) is the generalized inverse [2] tensor of \(\Pi\). It is simply to show that the introduced quantity satisfies \(\|\tilde{\Pi}^{(i)} : \varepsilon - \Pi : \varepsilon\| \leq RME^{(i)} \|\Pi : \varepsilon\|\) for all \(\varepsilon\).

3. Numerical experiment

By using the two-level constitutive model of elasto-visco-plasticity [7], a numerical investigation on elastic symmetry changes during inelastic deformation was performed for the RVE of a polycrystalline copper. A single realization of the aggregate of 1000 crystallites with initially uniform orientation distribution was examined. The analysis was focused on the kinematic two-link strain trajectories of the type “simple shear – simple shear” with the constant velocity gradients of the following forms.

Stage I: \(\nabla v_i = 5 \times 10^{-4} (11_1 - 11_2 + 11_3 - 11_4)\).

Stage II: \(\nabla v_h = 5 \times 10^{-4} (11_1 - \cos^2 \psi 11_2 - \sin^2 \psi 11_3 \cos \psi (11_2 - 11_1) + \sin \psi (11_3 - 11_1) - \cos \psi \sin \psi (11_3 + 11_1)).\)

The value of the parameter, \(\psi\), was varied from 0° to 180°. Each stage was followed by an elastic unloading down to zero macroscopic stress. The time durations of the active loadings are \(T_{l,h} = 2000\) s. Let us note that the process according to the provided scheme corresponds to the two consecutive stages of equal channel angular pressing with the channels intersection angle of 90° and the rotation of the sample around its axis by the angle, \(\psi\), before the second route.

4. Results

The direct pole figures (DPFs) for the polycrystalline aggregate in different configurations are shown in figure 1 (hereinafter the value of \(\varepsilon\) is equal to the accumulated effective strain). The considered cases show the requirement of the significant inhomogeneity by the crystallites’ orientation distribution.
The plot presented in figure 2a describes the changes in $\overline{RME}^{(s)}$ of the aggregate elastic properties with respect to some symmetry classes during the Stage I. In figure 2b, the same quantity is plotted for the final configurations of the Stage II in dependence on $\psi$. All outcomes of the process demonstrate the amplification of the elastic properties non-conformance with the classes under consideration compared to the initial configuration.

One should note that, in some cases, the RMEs are not strictly increasing during the Stage II as shown e.g. in figure 3a, where the values of $\overline{RME}^{(iso)}$ (in the isotropy class) are provided for different $\psi$. The curves interpolating the dependence of the same quantity on this angle at various moments of the Stage 2 are plotted in figure 3b. As it is easy to see, the curves have pronounced minima at $\psi = 90^\circ$, near which the changes in $\overline{RME}^{(iso)}$ are not monotonic.

Figures 4-6 show the orientations of the canonical bases of the optimal symmetric approximations obtained for the aggregate in some configurations. At each plot, the family of the points refers to parameters of the orientation tensors, (4) or (5), differing from each other by a transformation from the related symmetry group. In the case of orthotropic approximations, the provided orientations are associated with the longitudinal elastic moduli in the non-increasing order.
Figure 3. RMEs of the aggregate elastic properties in the isotropy class:
a) different variants of the Stage II; b) various moments of the Stage II.

Figure 4. Orientations of the canonical bases
for the optimal transversal isotropic approximations of the aggregate elasticity tensor:
a) initial and final configurations of the Stage I; b) final configurations of the variants of the Stage II.

Figure 5. Orientations of the canonical bases
for the optimal cubic approximations of the aggregate elasticity tensor:
a) initial and final configurations of the Stage I; b) final configurations of the variants of the Stage II.
Figure 6. Orientations of the canonical bases for the optimal orthotropic approximations of the aggregate elasticity tensor: a) initial and final configurations of the Stage I; b) final configurations of the variants of the Stage II.

5. Conclusion
In this work, an approach to solve the SIP for anisotropic materials is considered in application to multi-level-modeling. An investigation on changes in the elastic symmetry of the RVE of a polycrystalline copper during inelastic deformation is performed with the help of a two-level model of crystal elasto-visco-plasticity. Kinematic two-link strain trajectories of a special form are analyzed. The used approach is based on the approximation of the macroscopic elasticity tensor by the tensors of various symmetry types, which minimize some upper estimate of the residual norm in the generalized Hooke’s law. As a result, it is possible to form the hierarchy of the symmetry classes, which the material in given configurations can be related to (by its elastic properties) with a known error.

Acknowledgments
The work was supported by the Russian Foundation for Basic Research (grants No. 17-41-590694-p_a, No. 17-01-00379-a).

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