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An Isotropy Condition for Discrete Sets of Cubic Single Crystals

A tensorial and a scalar quantity describing the deviation from the isotropic elastic state is formulated for polycrystals. Furthermore an isotropy condition for discrete sets of cubic single crystals is expressed in terms of crystal orientations.

1. Introduction

In order to simplify the investigation and to handle the homogenization problem of polycrystalline metals in their elastic range analytically, the following assumptions are made: 1. the elastic behaviour is of cubic symmetry (e.g., Al, Cu, α-Fe); 2. the elastic behaviour of the aggregate is uniform; 3. the crystal orientations are constant within the grains; 4. the influence of the grain interaction, the grain boundaries, and the grain edges on the anisotropy of the macroscopic behaviour is negligible.

2. Elastic behaviour of cubic single crystals

The stress tensor $\mathbf{T}$ is given as a linear map of the strain tensor $\mathbf{E}$, and vice versa. The operators of this map - the forth-order stiffness Ξ^C and compliance tensor Π^C - are specified by the symmetry group $\mathcal{S}$ of the material being a subgroup of the orthogonal group *Orth*

$$\mathbf{T} = \Xi^C[\mathbf{E}], \qquad \mathbf{E} = \Pi^C[\mathbf{T}], \qquad \mathbf{H}^{\mathrm{T}}\Xi^C[\mathbf{E}]\mathbf{H} = \Xi^C[\mathbf{H}^{\mathrm{T}}\mathbf{E}\mathbf{H}], \qquad \forall \mathbf{H} \in \mathcal{S} \subseteq Orth. \tag{1}$$

For hyperelastic materials the elasticity tensors have the major symmetry $\Xi^C = \Xi^{C\,\mathrm{T}}$. Without loss of generality, the symmetry in the first and last pair of indices is assumed: $\Xi^C[\mathbf{E}] = \Xi^C[\mathbf{E}^{\mathrm{T}}]$, $\Xi^C[\mathbf{E}] = \Xi^C[\mathbf{E}]^{\mathrm{T}} \forall \mathbf{E}$. Because of the cubic symmetry there exist the following projector representations [3,4,1]

$$\Xi^C = \sum_{\alpha=1}^{3} \lambda_\alpha \Lambda_\alpha, \qquad \Pi^C = \sum_{\alpha=1}^{3} \frac{1}{\lambda_\alpha} \Lambda_\alpha, \qquad \Lambda_1 = \frac{1}{3}\mathbf{I} \otimes \mathbf{I}, \qquad \Lambda_2 = \Sigma - \Lambda_1, \qquad \Lambda_3 = \mathbf{I}^S - \Sigma. \tag{2}$$

$\mathbf{I}$ denotes the second-order identity tensor and $\mathbf{I}^S$ the symmetric part of the forth-order identity tensor. The anisotropic part Σ is given by the lattice vectors $\mathbf{g}_i$: $\Sigma = \sum_{i=1}^{3} \mathbf{g}_i \otimes \mathbf{g}_i \otimes \mathbf{g}_i \otimes \mathbf{g}_i$. The projectors Λ_α are idempotent $\Lambda_\alpha \Lambda_\alpha = \Lambda_\alpha$ and biorthogonal $\Lambda_\alpha \Lambda_\beta = \mathbf{0}$ $(\alpha \neq \beta)$. The eigenvalues of the stiffness tensor are determined by its components with respect to a CARTESIAN coordinate system as follows: $\lambda_1 = \Xi_{1111} + 2\Xi_{1122}$, $\lambda_2 = \Xi_{1111} - \Xi_{1122}$, $\lambda_3 = 2\Xi_{1212}$.

3. Elastic behaviour of the aggregate

TAYLOR's and SACHS' assumption of constant strain and stress fields, respectively, yield the most simple estimation of the elastic properties of the aggregate. The macroscopic elasticity tensors are then given as volume averages of the corresponding local fields and imply strict upper and lower bounds for the macroscopic strain energy density [6]

$$\Xi^V = \frac{1}{V}\int_V \Xi^C \mathrm{d}V, \qquad \Pi^R = \frac{1}{V}\int_V \Pi^C \mathrm{d}V. \tag{3}$$

In general, these volume averages are anisotropic. An estimation of the properties with the additional assumption of uniform distributed grain orientations follows by transforming the integrals (3) to the orientation space g and setting the orientation distribution function f equal to one [2]. If the orientation space is parametrized by EULER angles, one obtains with $\mathrm{d}V/V = f\mathrm{d}g = \sin(\Phi)\mathrm{d}\Phi\mathrm{d}\varphi_1\mathrm{d}\varphi_2/8\pi^2$

$$\Xi^{VI} = \frac{1}{8\pi^2}\int_g \Xi^C \sin(\Phi)\mathrm{d}\Phi\mathrm{d}\varphi_1\mathrm{d}\varphi_2, \qquad \Pi^{RI} = \frac{1}{8\pi^2}\int_g \Pi^C \sin(\Phi)\mathrm{d}\Phi\mathrm{d}\varphi_1\mathrm{d}\varphi_2. \tag{4}$$

The integration yields the well-known isotropic elasticity tensors, which imply strict bounds for the isotropic behaviour [8,7,5].

The isotropic bounds (4) solve the minimum problems $\| \boldsymbol{\Xi}^C - \boldsymbol{\Xi}^I \| \to \min$ and $\| \boldsymbol{\Pi}^C - \boldsymbol{\Pi}^I \| \to \min$ with $\boldsymbol{\Xi}^I$ and $\boldsymbol{\Pi}^I$ isotropic forth-order tensors and $\| \boldsymbol{\Xi} \| := (\Xi_{ijkl}\Xi_{ijkl})^{1/2}$. This result is straight-forward if the projector representation of the isotropic elastic law is used, e.g., in terms of stiffnesses

$$\| \boldsymbol{\Xi}^{C,V} - \lambda_1 \boldsymbol{\Lambda}_1^I - \lambda_2 \boldsymbol{\Lambda}_2^I \| \to \min \qquad \Rightarrow \qquad \lambda_1 = \frac{1}{3}\Xi_{iikk}, \ \lambda_2 = \frac{1}{5}\left(\Xi_{ikki} - \frac{1}{3}\Xi_{iikk}\right). \tag{5}$$

The isotropic projectors are given by $\boldsymbol{\Lambda}_1^I = \frac{1}{3}\mathbf{I} \otimes \mathbf{I}$ and $\boldsymbol{\Lambda}_2^I = \mathbf{I}^S - \boldsymbol{\Lambda}_1^I$. The isotropic estimations by Voigt and Reuss represent the isotropic elastic laws nearest to both the single crystal law (1) and the volume averages (3). This interpretation motivates the use of the Frobenius norm to formulate equivalent scalar measures.

4. Isotropy condition

For aggregates consisting of a finite number of cubic single crystals with arbitrary size, the difference of the anisotropic and isotropic averages can be expressed as (V: volume of the aggregate, V^α: volume with the orientation $\mathbf{g}_i^\alpha$, $v^\alpha = V^\alpha / V$)

$$\boldsymbol{\Xi}^V - \boldsymbol{\Xi}^{VI} = \| \boldsymbol{\Xi}^C - \boldsymbol{\Xi}^{VI} \| \boldsymbol{\Delta}, \qquad \boldsymbol{\Pi}^R - \boldsymbol{\Pi}^{RI} = \| \boldsymbol{\Pi}^C - \boldsymbol{\Pi}^{RI} \| \boldsymbol{\Delta}, \tag{6}$$

with

$$\boldsymbol{\Delta} = \frac{\sqrt{30}}{30}\left(\mathbf{I} \otimes \mathbf{I} + 2\mathbf{I}^S - 5\sum_{\alpha=1}^{N} v^\alpha \sum_{k=1}^{3} \mathbf{g}_k^\alpha \otimes \mathbf{g}_k^\alpha \otimes \mathbf{g}_k^\alpha \otimes \mathbf{g}_k^\alpha\right). \tag{7}$$

The difference of the averages is influenced on the one hand by the degree of anisotropy of the single crystals through, e.g., $\| \boldsymbol{\Xi}^C - \boldsymbol{\Xi}^{VI} \|$, and on the other hand by the orientation distribution in form of the tensor $\boldsymbol{\Delta}$. This representation implies the isotropy condition in terms of the N crystal orientations: $\boldsymbol{\Delta} = \mathbf{0}$. With the proper orthogonal tensor $\mathbf{Q}^\alpha = \mathbf{g}_i^\alpha \otimes \mathbf{e}_i$ follows an equivalent formulation

$$\Delta_{ijkl} = 0 \qquad \Leftrightarrow \qquad \sum_{\alpha=1}^{N} v^\alpha \sum_{k=1}^{3} Q_{ik}^\alpha Q_{jk}^\alpha Q_{mk}^\alpha Q_{nk}^\alpha = \frac{1}{5}\left(\delta_{ij}\delta_{mn} + \delta_{im}\delta_{jn} + \delta_{in}\delta_{jm}\right). \tag{8}$$

The right hand side of eqn. (8) represents a special case of the general isotropic forth-order tensor. The norm $\| \boldsymbol{\Delta} \|$ is equal to one for a single orientation, equal to zero for a uniform orientation distribution, and in the interval $(0,1)$ otherwise. $\| \boldsymbol{\Delta} \|$ can be interpreted as material independent measure for the anisotropy of the aggregate within the class of f.c.c. polycrystals. Exact and approximate solutions of eqn. (8) can be used as input data for simulations of the inelastic behaviour by means of representative volume elements.

5. References

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