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On the construction of anisotropic polyconvex energy densities

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In this contribution we propose a general framework for the construction of polyconvex energies for arbitrary anisotropy classes. The main idea is the introduction of an anisotropic metric reflecting the material symmetry of the underlying crystal.

1 Introduction

In large strain elasticity the existence of minimizers is guaranteed if the variational functional to be minimized is sequentially weakly lower semicontinuous (s.w.l.s.) and coercive. Therefore, polyconvex functions which are always s.w.l.s. are usually considered, see [1]. For isotropic materials there exists a wide range of constitutive functions that satisfy the polyconvexity requirement. The construction of transversely isotropic and orthotropic energy functions has been already proposed in [4,5]. Further extensions and case studies are given in [2] and [3]. The main goal of this contribution is to provide a new method for the construction of polyconvex energies for arbitrary anisotropy classes. Our idea is the introduction of an anisotropic metric encoding the anisotropies of the underlying crystal.

2 Anisotropic Metrics

In hyperelasticity the considered boundary value problem is governed by the free energy function ψ, which is assumed to be a function of the objective right Cauchy-Green tensor $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$, where $\boldsymbol{F}$ is the deformation gradient. The principle of material symmetry requires

$$\psi(\boldsymbol{C}) = \psi(\boldsymbol{Q}\boldsymbol{C}\boldsymbol{Q}^T) \quad \forall\, \boldsymbol{Q} \in \mathcal{G} \subset SO(3), \tag{1}$$

where $\mathcal{G}$ denotes the corresponding material symmetry group and $SO(3)$ is the special orthogonal group. The main idea of the proposed concept is based on the introduction of an anisotropic metric $\boldsymbol{G}$, which reflects the symmetry properties of the considered crystal class. Thus $\boldsymbol{G}$ is per definition symmetric and positive definite. We focus on functional bases for the free energy functions in terms of the powers of the traces of the right Cauchy-Green tensor. Therefore we have to ensure

$$\boldsymbol{C} : \boldsymbol{G} = \boldsymbol{Q}\boldsymbol{C}\boldsymbol{Q}^T : \boldsymbol{G} = \boldsymbol{C} : \boldsymbol{Q}^T\boldsymbol{G}\boldsymbol{Q} \quad \rightarrow \quad \boldsymbol{G} = \boldsymbol{Q}\boldsymbol{G}\boldsymbol{Q}^T \quad \forall\, \boldsymbol{Q} \in \mathcal{G} \subset SO(3), \tag{2}$$

i.e., $\boldsymbol{G}$ has to be invariant with respect to transformations which are elements of the material symmetry group. A possible functional basis of polyconvex invariants is, e.g.,

$$I_1 = \mathrm{tr}\boldsymbol{C}, \quad I_2 = \mathrm{tr}[\mathrm{Cof}\boldsymbol{C}], \quad I_3 = \det\boldsymbol{C}, \quad J_4 = \mathrm{tr}[\boldsymbol{C}\boldsymbol{G}], \quad J_5 = \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{G}]. \tag{3}$$

The polyconvexity of these invariants is proved in [1,4,5,6]. In general, the free energy function is assumed to be of the type

$$\psi^{aniso} = \sum_{r=1}^{n}\sum_{j=1}^{m} \xi_{rj}\left[\frac{1}{\alpha_{rj}+1}\frac{1}{(g_j)^{\alpha_{rj}}}(J_{4j})^{\alpha_{rj}+1} + \frac{1}{\beta_{rj}+1}\frac{1}{(g_j)^{\beta_{rj}}}(J_{5j})^{\beta_{rj}+1} + \frac{g_j}{\gamma_{rj}}(I_3)^{-\gamma_{rj}}\right], \tag{4}$$

where the relations $g_j := \mathrm{tr}\boldsymbol{G}_j$, $J_{4j} = \mathrm{tr}[\boldsymbol{C}\boldsymbol{G}_j]$, $J_5 = \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{G}_j]$ are used and we introduced m-different metrics $\boldsymbol{G}_j$ satisfying (2). The free energy function ψ^{aniso} is polyconvex if the conditions

$$\alpha_{rj}, \beta_{rj}, \xi_{rj} \geq 0 \quad \text{and} \quad \gamma_{rj} \geq -\frac{1}{2} \tag{5}$$

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hold. Furthermore, ψ^{aniso} is coercive which is a sufficient condition together with the polyconvexity condition in order to guarantee the existence of minimizers. The proof of coercivity is presented in detail in [6]. The second Piola-Kirchhoff stresses are given by the well-known relation $\boldsymbol{S} = 2\partial_{\boldsymbol{C}}\psi^{aniso}$, with

$$\boldsymbol{S} = 2\sum_{r=1}^{n}\sum_{j=1}^{m}\xi_{rj}\left[(-g_j I_3^{-\gamma_{rj}} + \frac{1}{(g_j)^{\beta_{rj}}}J_{5j}^{\beta_{rj}+1})\boldsymbol{C}^{-1} + \frac{1}{(g_j)^{\alpha_{rj}}}J_{4j}^{\alpha_{rj}}\boldsymbol{G}_j - \frac{1}{(g_j)^{\beta_{rj}}}J_{5j}^{\beta_{rj}}I_3\boldsymbol{C}^{-1}\boldsymbol{G}_j\boldsymbol{C}^{-1}\right] . \quad (6)$$

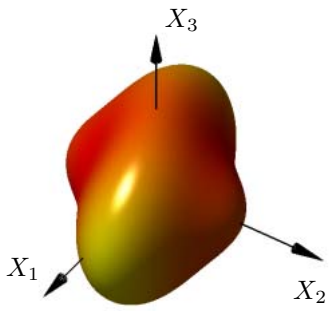
At the natural state $\boldsymbol{C} = \mathbf{1}$ the stress free reference configuration condition $\boldsymbol{S}(\boldsymbol{C} = \mathbf{1}) = \mathbf{0}$ is automatically satisfied.

3 Anisotropic Moduli–Fitting to Referential Data

In order to approximate the phenomenological responses of real anisotropic materials with the above mentioned anisotropic polyconvex functions we have to fit the fourth-order elasticity tensor $\mathbb{C} = 4\partial_{\boldsymbol{C}\boldsymbol{C}}\psi^{aniso}$ near the natural state to some available data. Hence, we identify the material parameters by comparing the calculated tangent moduli with experimental data based moduli given in the classical representation. In detail, the fitting of moduli is done by minimizing the error function

$$e = \frac{\| \mathbb{C}^{(V)comp} - \mathbb{C}^{(V)exp} \|}{\| \mathbb{C}^{(V)exp} \|} , \quad (7)$$

where $\mathbb{C}^{(V)comp} \in \mathbb{R}^{6\times 6}$ denotes the computed tangent moduli at the natural state, i.e., $\mathbb{C}^{(V)comp} := 2\partial_{\boldsymbol{C}}\boldsymbol{S}|_{\boldsymbol{C}=\mathbf{1}}$, and is considered in Voigt notation. Here we approximate the elasticity moduli at the natural state of a monoclinic crystalline solid and adjust the parameters appearing in (4) for $r = j = 3$.



$$\mathbb{C}^{(V)exp} = \begin{bmatrix} 234.4 & 70.7 & 62.6 & 21.4 & 0 & 0 \\ & 185.8 & 68.5 & 9.8 & 0 & 0 \\ & & 181.3 & 9.4 & 0 & 0 \\ & & & 51.0 & 0 & 0 \\ & sym. & & & 47.4 & 7.7 \\ & & & & & 69.2 \end{bmatrix}$$

Fig. 1 Monoclinic material Aegirite: characteristic surface of Young's modulus, elasticities [GPa].

For Aegirite we obtain with $\boldsymbol{G}_1 = \mathrm{diag}(1, 1, 1)$ and the monoclinic metric tensors

$$\boldsymbol{G}_2^m = \begin{bmatrix} 2.530 & 0.433 & 0 \\ 0.433 & 0.676 & 0 \\ 0 & 0 & 1.976 \end{bmatrix}, \quad \boldsymbol{G}_3^m = \begin{bmatrix} 2.218 & -0.228 & 0 \\ -0.228 & 0.218 & 0 \\ 0 & 0 & 2.596 \end{bmatrix} \quad (8)$$

a relative error $e \approx 1.62\%$.

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