UNIVERSITÄT
DUISBURG
ESSEN

Faculty of Engineering
Department of Civil Engineering
Institute of Mechanics
Prof. Dr.-Ing. habil. J. Schröder

Construction of Anisotropic Polyconvex Energies on the Basis of Crystallographic Motivated Structural Tensors

Motivation

- For the description of isotropic as well as for transversely isotropic and orthotropic material behavior energy functions that are polyconvex already exist.
- The main goal is to provide a new method for the construction of anisotropic polyconvex hyperelastic models for arbitrary anisotropy classes.
- Basic literature: Ball [1], Schröder & Neff [3,4], Schröder, Neff & Ebbing [5].
- A priori stress-free reference configuration: Itskov & Aksel [2].

Polyconvex Energy Functions for Arbitrary Anisotropy

–Anisotropy: The principle of material symmetry requires

$$\psi(\boldsymbol{C}) = \psi(\boldsymbol{Q}\boldsymbol{C}\boldsymbol{Q}^T) \quad \forall \quad \boldsymbol{Q} \in \mathcal{G} \subset \mathrm{O}(3).$$

Introduction of an anisotropic metric tensor

$$\boldsymbol{G} := \boldsymbol{H}\boldsymbol{H}^T,$$

which is per defintion symmetric and positive definite. $\boldsymbol{G}$ reflects the symmetry properties of the underlying crystal class, i.e.

$$\boldsymbol{G} = \boldsymbol{Q}\boldsymbol{G}\boldsymbol{Q}^T \quad \forall \quad \boldsymbol{Q} \in \mathcal{G} \subset \mathrm{O}(3)$$

must hold. Thus, energy functions in terms of the scalar products

$$\boldsymbol{C}\cdot\boldsymbol{G} = \boldsymbol{Q}\boldsymbol{C}\boldsymbol{Q}^T\cdot\boldsymbol{G} = \boldsymbol{C}\cdot\boldsymbol{Q}^T\boldsymbol{G}\boldsymbol{Q} \quad \forall\, \boldsymbol{Q} \in \mathcal{G}$$

automatically satisfy the principle of material symmetry.

Representation of metric tensors, e.g.:
Monoclinic system, $\boldsymbol{G}^m \in \mathcal{G}^m$: Triclinic system, $\boldsymbol{G}^a \in \mathcal{G}^a$:

$$\boldsymbol{G}^m = \begin{bmatrix} a & d & 0 \\ d & b & 0 \\ 0 & 0 & c \end{bmatrix}, \qquad \boldsymbol{G}^a = \begin{bmatrix} a & d & e \\ d & b & f \\ e & f & c \end{bmatrix}.$$

The parameters a, b, c and d are additional material parameters.

–Polyconvexity: Anisotropic invariants

$$J_4 = \boldsymbol{C}\cdot\boldsymbol{G} \quad \text{and} \quad J_5 = \mathrm{cof}\boldsymbol{C}\cdot\boldsymbol{G}$$

are polyconvex.

Proof: $(\boldsymbol{C}\cdot\boldsymbol{G})^k = \langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{F}\boldsymbol{H}\rangle^k, \forall\, k \geq 1$:

$$\begin{aligned} D_F^2(\langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{F}\boldsymbol{H}\rangle^k)\,.(\boldsymbol{\xi},\boldsymbol{\xi}) &= 2k \parallel \boldsymbol{F}\boldsymbol{H} \parallel^{2k-2} \parallel \boldsymbol{\xi}\boldsymbol{H} \parallel^2 \\ &+4k(k-1) \parallel \boldsymbol{F}\boldsymbol{H} \parallel^{2k-4} \\ &\langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{\xi}\boldsymbol{H}\rangle^2 \geq 0. \end{aligned}$$

Generic anisotropic polyconvex coercive free energy function

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

with $g_j = \mathrm{tr}\boldsymbol{G}_j$, $J_{4j} = \boldsymbol{C}\cdot\boldsymbol{G}_j$, $J_{5j} = \mathrm{cof}\boldsymbol{C}\cdot\boldsymbol{G}_j$ and $\alpha_{rj}, \beta_{rj}, \xi_{rj} \geq 0, \gamma_{rj} \geq -\frac{1}{2}$. Proof of coercivity: see [5].
Second Piola-Kirchhoff stresses

$$\begin{aligned} \boldsymbol{S} = & \sum_{r=1}^{n}\sum_{j=1}^{m} 2\xi_{rj} \Bigg[(-g_j I_3^{-\gamma_{rj}} + \frac{1}{(g_j)^{\beta_{rj}}} J_{5j}^{\beta_{rj}+1})\boldsymbol{C}^{-1} \\ & + \frac{1}{(g_j)^{\alpha_{rj}}} J_{4j}^{\alpha_{rj}} \boldsymbol{G}_j - \frac{1}{(g_j)^{\beta_{rj}}} J_{5j}^{\beta_{rj}} I_3 \boldsymbol{C}^{-1}\boldsymbol{G}_j\boldsymbol{C}^{-1} \Bigg], \end{aligned}$$

with $\boldsymbol{S}(\boldsymbol{C}=\boldsymbol{1}) = \boldsymbol{0}$.

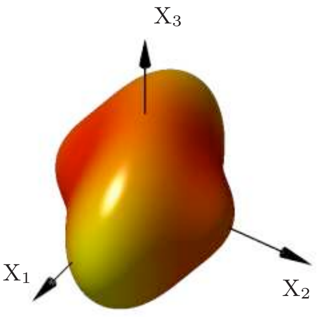
Anisotropic Moduli–Fitting to Referential Data

Minimizing of error function

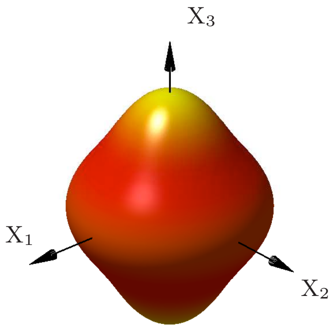
$$e = \frac{\parallel \mathbb{C}^{(V)comp} - \mathbb{C}^{(V)exp} \parallel}{\parallel \mathbb{C}^{(V)exp} \parallel},$$

with $\mathbb{C}^{(V)comp} = 4\partial_{\boldsymbol{CC}}\psi^{aniso}$ in Voigt notation.

Characteristic Surfaces of Young's Moduli:



Aegirite: $n = m = 3$:
$e = 1,65\%$



Rhenium: $n = m = 3$:
$e = 7,87 \cdot 10^{-7}\%$

References

[1] Ball, J.M. [1977], "Convexity Conditions and Existence Theorems in Non–Linear Elasticity", *Arch. Rat. Mech. Anal.*, 63, 337–403
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[4] Schröder, J. & Neff, P. [2003], "Invariant Formulation of Hyperelastic Transverse Isotropy Based on Polyconvex Free Energy Functions", *Int. J. Solid. Struct.*, 40, 401–445
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Prof. Dr.-Ing. Jörg Schröder, Dipl.-Ing. Vera Ebbing
Universität Duisburg-Essen, Institute of Mechanics

Dr. rer. nat. habil. Patrizio Neff
Technische Universität Darmstadt, Dept. of Mathematics