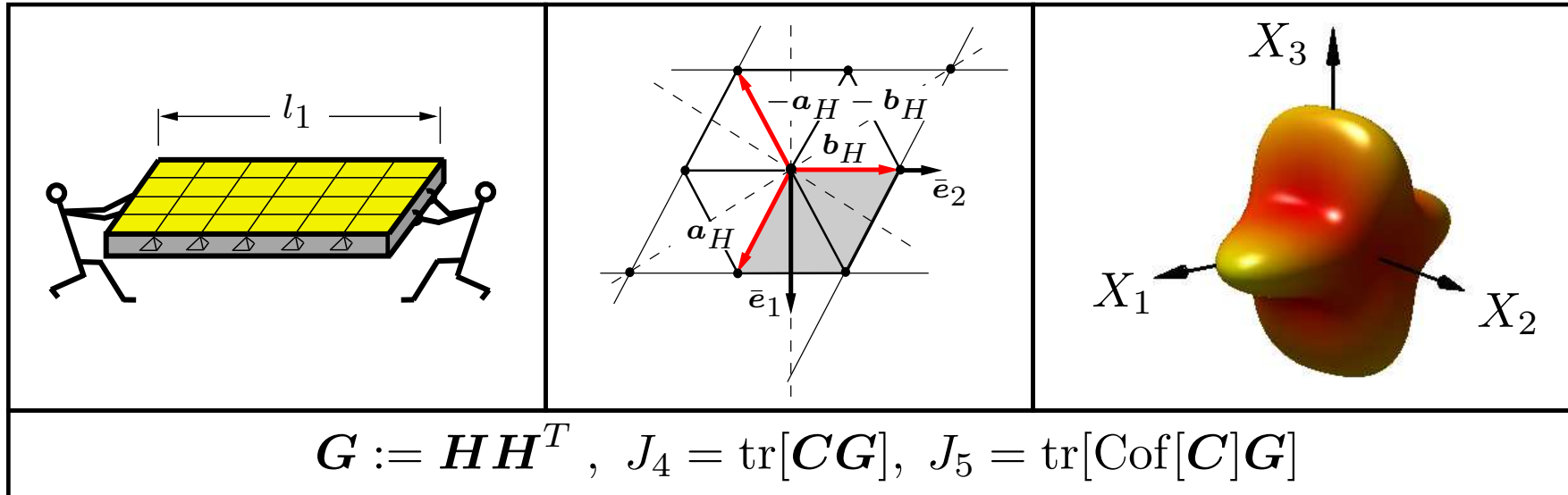


Polyconvex Models for Arbitrary Anisotropic Materials

Vera Ebbing, Jörg Schröder, Patrizio Neff

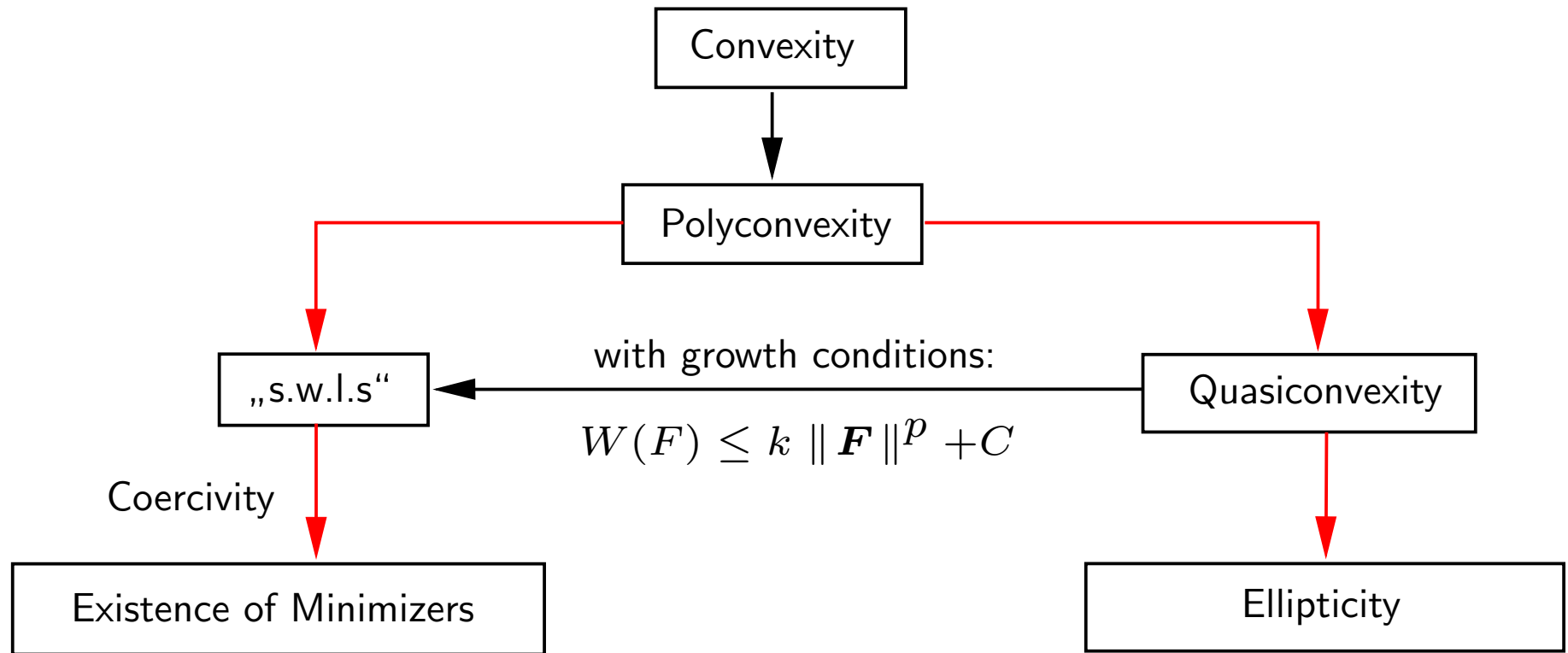


- Generalized Convexity Conditions
 - Crystallographic Motivated Structural Tensors
 - Polyconvex Functional Bases
- Polyconvex Anisotropic Free Energy Functions for More General Anisotropy Classes

DFG-Project: NE 902/2-1 SCHR 570/6-1

J. SCHRÖDER, P. NEFF & V. EBBING [2008], "Anisotropic Polyconvex Energies on the Basis of Crystallographic Motivated Structural Tensors", submitted to *JMPS*

Generalized Convexity Conditions: Implications



Quasiconv.: $W(\bar{\mathbf{F}}) \cdot \text{Vol}(\mathcal{B}) \leq \int_{\mathcal{B}} W(\bar{\mathbf{F}} + \nabla \mathbf{w}) dV \rightarrow \bar{\mathbf{F}}$ is global minimizer.

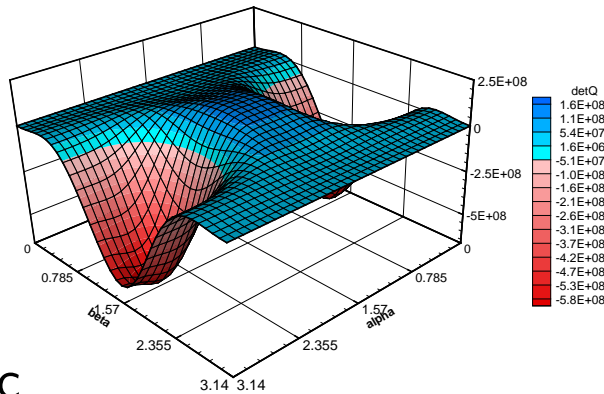
Ellipticity: Positive definite acoustic tensor \rightarrow Real wave speeds.



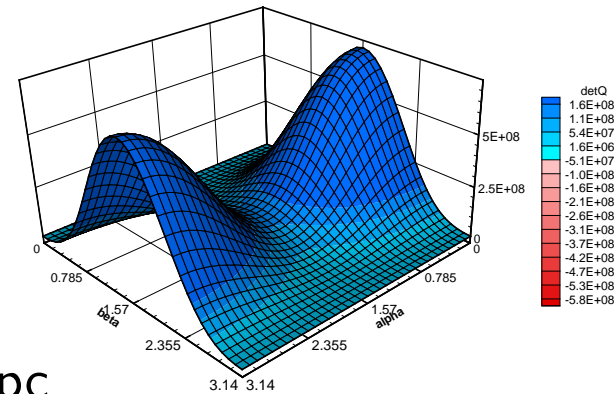
Polyconvexity Condition

Polyconvexity \Rightarrow Quasiconvexity \Rightarrow Ellipticity

Localization analysis for constrained compression test



not pc



pc

Polyconvexity, BALL [1977]

The elastic free energy $W(\mathbf{F})$ is polyconvex if and only if there exists a function $P : \mathbb{M}^{3 \times 3} \times \mathbb{M}^{3 \times 3} \times \mathbb{R} \mapsto \mathbb{R}$ (in general non unique) such that

$$W(\mathbf{F}) = P(\mathbf{F}, \text{Cof} \mathbf{F}, \det \mathbf{F})$$

and the function $\mathbb{R}^{19} \mapsto \mathbb{R}$, $(X, Y, Z) \mapsto P(X, Y, Z)$ is convex.

Common Polyconvex Energy Functions

- **Isotropy**: Polyconvex models, e.g. OGDEN-type models ($\alpha_1, \alpha_2, \delta_1 \geq 0$)

$$\psi^{iso} = \alpha_1 I_1 + \alpha_2 I_2 + \delta_1 I_3^2 - (2\alpha_1 + 4\alpha_2 + 2\delta_1) \ln \sqrt{I_3},$$

formulated in principal invariants $I_1 = \text{tr}\mathbf{C}$, $I_2 = \text{tr}[\text{Cof}\mathbf{C}]$ and $I_3 = \det\mathbf{C}$.

BALL [2002], Some open problems in elasticity, **Problem 2:**

“Are there ways of verifying polyconvexity and quasiconvexity for a useful class of anisotropic stored-energy functions?”

- **Anisotropy: Transversely isotropic** ($a=1$) and **orthotropic** ($a = 3$) polyconvex energy functions first derived in SCHRÖDER & NEFF [2001,2003] formulated in

$$\text{tr}[\mathbf{C}\mathbf{M}^i], \text{tr}[\text{Cof}[\mathbf{C}]\mathbf{M}^i], \text{tr}[\mathbf{C}(\mathbf{1} - \mathbf{M}^i)], \text{tr}[\text{Cof}[\mathbf{C}](\mathbf{1} - \mathbf{M}^i)], \quad i = 1, \dots, a$$

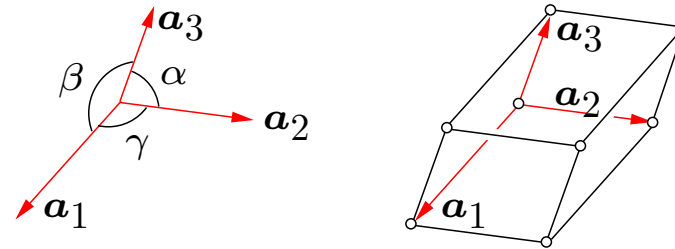
- **Further extensions** and case studies are documented in: STEIGMANN [2003], SNB [2004], ITSKOV & AKSEL [2004], MARKERT, EHLERS & KARAJAN [2005], BALZANI [2006], BNSH [2006], EHRET & ITSKOV [2007].

Are there ways of verifying polyconvexity for the further ten classes of anisotropic stored-energy functions?



Anisotropic Elasticity

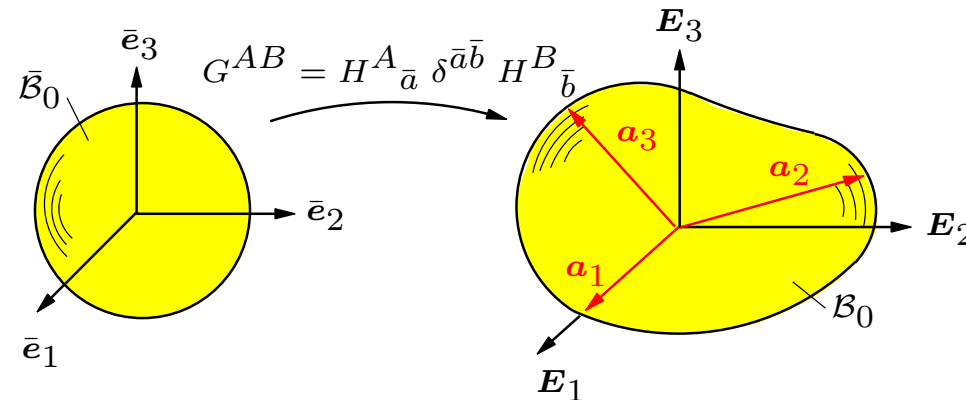
12 anisotropy classes / 32 crystal classes / 7 crystal systems



with $a = \|\mathbf{a}_1\|$, $b = \|\mathbf{a}_2\|$, $c = \|\mathbf{a}_3\|$

No.	crystal system	edge lengths	axial angle
1	triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$
2	monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90^\circ; \gamma \neq 90^\circ$
3	trigonal	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$
4	hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ; \gamma = 120^\circ$
5	rhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
6	tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
7	cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$

General Anisotropy in Polyconvex Framework



Main idea: Introduction of an **anisotropic metric tensor G** :

- G is a **second-order, symmetric** and **positive definite** structural tensor .
- G is the **push-forward** of a cartesian metric of a fictitious reference configuration $\bar{\mathcal{B}}_0$ onto the real reference configuration \mathcal{B}_0 :

$$\rightarrow G = HH^T \quad \rightarrow G = QGQ^T \quad \forall Q \in \mathcal{G} \subset O(3).$$

\implies Principle of Material Symmetry is automatically satisfied :

$$C \cdot G = QCQ^T \cdot G = C \cdot Q^T GQ \quad \forall Q \in \mathcal{G} \subset O(3).$$

Literature: ZHENG & SPENCER [1993], ZHENG [1994], XIAO [1996],
APEL [2004], XIAO, BRUHNS & MEYER [2007]

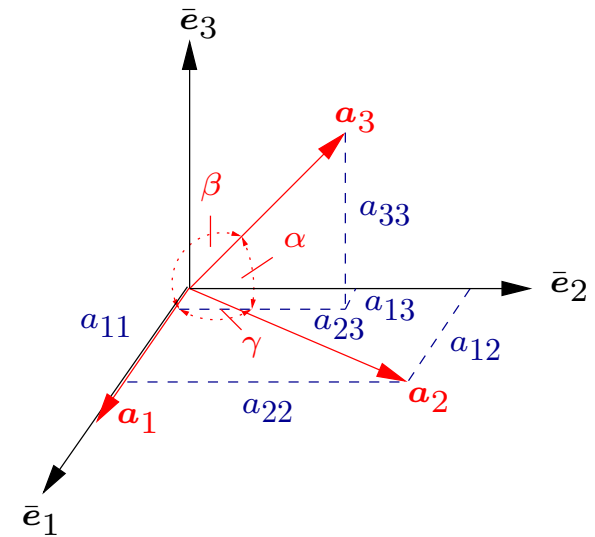
Metric Tensors for the Seven Crystal Systems

Linear Mapping of the cartesian base vectors onto crystallographic motivated base vectors:

$$\mathbf{H} : \bar{\mathbf{e}}_i \mapsto \mathbf{a}_i \rightarrow \mathbf{H} = [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3] \quad \text{with} \quad \mathbf{a}_i = \mathbf{H} \bar{\mathbf{e}}_i$$

Special choice: $\mathbf{a}_1 \parallel \bar{\mathbf{e}}_1$, $\mathbf{a}_2 \perp \bar{\mathbf{e}}_3$:

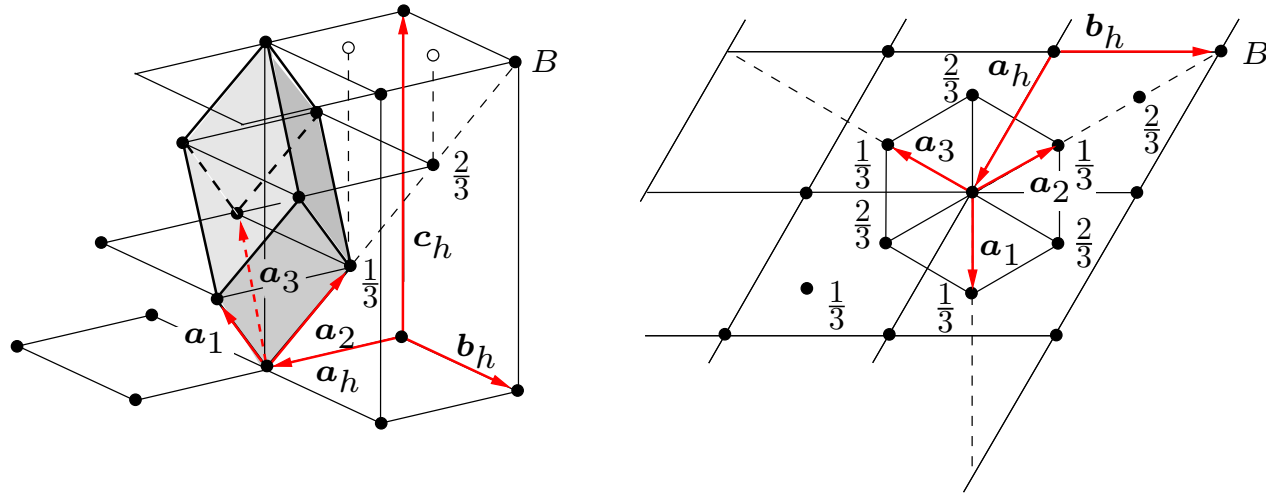
$$\mathbf{H} = \begin{bmatrix} a & b \cos \gamma & c \cos \beta \\ 0 & b \sin \gamma & c (\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\ 0 & 0 & c [1 + 2 \cos \alpha \cos \beta \cos \gamma - (\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma)]^{1/2} / \sin \gamma \end{bmatrix}$$



E.g. Monoclinic Metric Tensor ($a \neq b \neq c, \alpha = \beta = 90^\circ, \gamma \neq 90^\circ$):

$$\mathbf{G}^m = \mathbf{H}^m \mathbf{H}^{mT} = \begin{bmatrix} a^2 + b^2 \cos^2 \gamma & b^2 \cos \gamma \sin \gamma & 0 \\ b^2 \cos \gamma \sin \gamma & b^2 \sin^2 \gamma & 0 \\ 0 & 0 & c^2 \end{bmatrix} \rightarrow \mathbf{G}^m = \begin{bmatrix} \tilde{a} & \tilde{d} & 0 \\ \tilde{d} & \tilde{b} & 0 \\ 0 & 0 & \tilde{c} \end{bmatrix}$$

Crystallographic Motivated Trigonal Metric Tensor



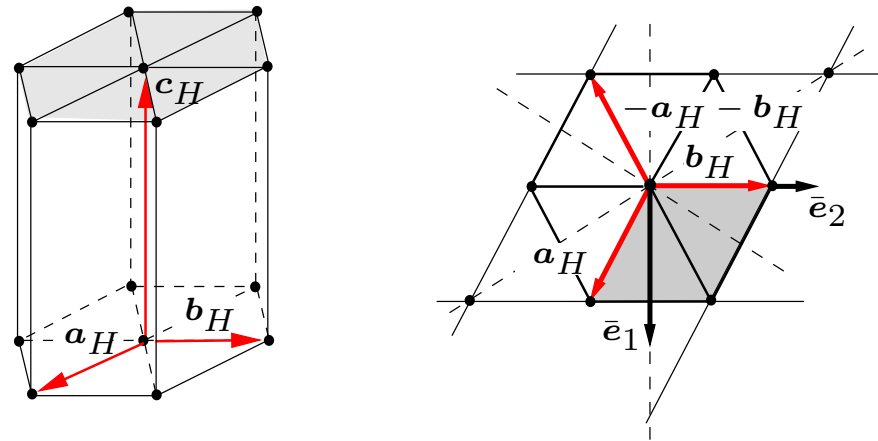
Considering **rhombohedral base vectors** in **hexagonal centered cell**

$$\mathbf{a}_1 = \frac{1}{3}(2\mathbf{a}_h + \mathbf{b}_h + \mathbf{c}_h), \quad \mathbf{a}_2 = \frac{1}{3}(-\mathbf{a}_h + \mathbf{b}_h + \mathbf{c}_h), \quad \mathbf{a}_3 = \frac{1}{3}(-\mathbf{a}_h - 2\mathbf{b}_h + \mathbf{c}_h),$$

with threefold axis $\mathbf{c}_h = (\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3) \parallel \mathbf{e}_3$, leads to trigonal metric tensor

$$\mathbf{G}^{ht} = \mathbf{H}^{ht} \mathbf{H}^{htT} = \text{diag}(a^2, a^2, c^2) \rightarrow \mathbf{G}^{ht} = \mathbf{Q} \mathbf{G}^{ht} \mathbf{Q}^T \quad \forall \mathbf{Q} \in \mathcal{G}^{ht}$$

Crystallographic Motivated Hexagonal Metric Tensor



BRAVAIS [1866]: Inherent sixfold symmetry of **primitive hexagonal cell** is captured by **three hexagonal base vectors** in the $\bar{e}_1 - \bar{e}_2$ -plane

$$a_H, \quad b_H, \quad (-a_H - b_H).$$

This symmetry indicates that $\bar{e}_1 - \bar{e}_2$ -plane acts as **isotropy plane**, LOVE [1907]. Therefore the fictitious deformation has to be of the type

$$H^h = \text{diag}(a, a, c) \rightarrow G^h = \text{diag}(a^2, a^2, c^2) \rightarrow G^h = QG^h Q^T \quad \forall Q \in \mathcal{G}^h$$

Proof of Polyconvexity of $\text{tr}[\mathbf{C}\mathbf{G}]$ and $\text{tr}[\text{Cof}[\mathbf{C}]\mathbf{G}]$

Generic **polyconvex** anisotropic functions

$$[\text{tr}(\mathbf{F}^T \mathbf{F} \mathbf{G})]^k \quad \text{and} \quad [\text{tr}(\text{Cof}(\mathbf{F}^T) \text{Cof}(\mathbf{F}) \mathbf{G})]^k$$

with $k \geq 1$ and $\mathbf{G} \in \mathbb{P}_{\text{sym}}$.

Proof of Convexity. With identity $[\text{tr}(\mathbf{F}^T \mathbf{F} \mathbf{G})]^k = \|\mathbf{F}\mathbf{H}\|^{2k} = \langle \mathbf{F}\mathbf{H}, \mathbf{F}\mathbf{H} \rangle^k$ we obtain

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

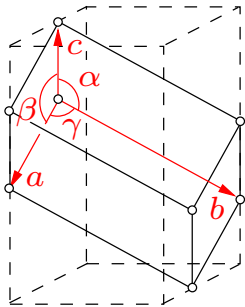
Detailed proofs are given in SCHRÖDER, NEFF & EBBING [2008].



Polyconvex Functional Bases \mathcal{P}

– Evaluation of Polyconvex Invariants $C \cdot G$ and $\text{Cof}C \cdot G$ –

Triclinic system: 2nd-order SST



$$G^a = \begin{bmatrix} \tilde{a} & \tilde{d} & \tilde{e} \\ \tilde{d} & \tilde{b} & \tilde{f} \\ \tilde{e} & \tilde{f} & \tilde{c} \end{bmatrix}$$

Ordering with respect to individual entries of G yields

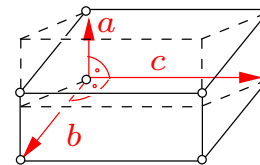
$$\mathcal{P}^a := \{ C_{11}, C_{22}, C_{33}, C_{12}, C_{13}, C_{23} \}.$$

Classical Basis:

$$\mathcal{I}^a := \{ C_{11}, C_{22}, C_{33}, C_{12}, C_{13}, C_{23} \}.$$

→ complete description

Monoclinic system: 2nd-order SST



$$G^m = \begin{bmatrix} \tilde{a} & \tilde{d} & 0 \\ \tilde{d} & \tilde{b} & 0 \\ 0 & 0 & \tilde{c} \end{bmatrix}$$

$$\mathcal{P}^m := \{ C_{11}, C_{22}, C_{33}, C_{12}, \text{Cof}C_{11} = C_{22}C_{33} - C_{23}^2, \text{Cof}C_{22} = C_{11}C_{33} - C_{13}^2, \text{Cof}C_{33} = C_{11}C_{22} - C_{12}^2, \text{Cof}C_{12} = C_{13}C_{23} - C_{12}C_{33} \}.$$

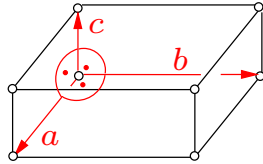
Classical Basis:

$$\mathcal{I}^m := \{ C_{11}, C_{22}, C_{33}, C_{12}, C_{13}^2, C_{23}^2, C_{13}C_{23} \}.$$

→ complete description

Polyconvex Functional Bases \mathcal{P}

Rhombic system: 2nd-order SST

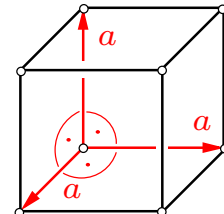


$$\mathbf{G}^o = \begin{bmatrix} \tilde{a} & 0 & 0 \\ 0 & \tilde{b} & 0 \\ 0 & 0 & \tilde{c} \end{bmatrix}$$

$$\mathcal{P}^o := \{ C_{11}, C_{22}, C_{33}, C_{22}C_{33} - C_{23}^2, C_{11}C_{33} - C_{13}^2, C_{11}C_{22} - C_{12}^2 \}.$$

→ complete description

Cubic system: 4th-order SST

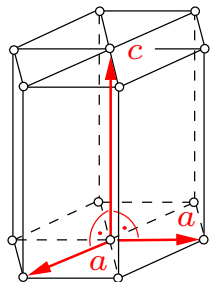


$$\mathbf{G}^c = \begin{bmatrix} \tilde{a} & 0 & 0 \\ 0 & \tilde{a} & 0 \\ 0 & 0 & \tilde{a} \end{bmatrix}$$

$$\mathcal{P}^c := \{ I_1, I_2 \}.$$

→ incomplete description

Hexagonal system: 6th-order SST

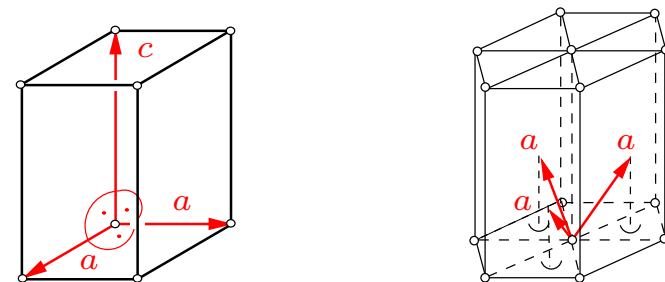


$$\mathbf{G}^h = \begin{bmatrix} \tilde{a} & 0 & 0 \\ 0 & \tilde{a} & 0 \\ 0 & 0 & \tilde{c} \end{bmatrix}$$

$$\mathcal{P}^h := \{ C_{11} + C_{22}, C_{33}, C_{22}C_{33} + C_{11}C_{33} - (C_{23}^2 + C_{13}^2), C_{11}C_{22} - C_{12}^2 \}.$$

→ complete description

Tetragonal, Trigonal system: 4th-order SSTs



$$\mathbf{G}^t = \mathbf{G}^{ht} = \mathbf{G}^h$$

$$\mathcal{P}^t = \mathcal{P}^{ht} = \mathcal{P}^h$$

→ incomplete description



Generic Polyconvex Anisotropic Energy Functions

Additive decomposition of the free energy in isotropic and anisotropic terms, i.e.,

$$\psi = \psi^{iso}(I_1, I_2, I_3) + \psi^{aniso}(I_3, J_{4j}, J_{5j}),$$

with $J_{4j} = \text{tr}[\mathbf{C}\mathbf{G}_j]$, $J_{5j} = \text{tr}[\text{Cof}[\mathbf{C}]\mathbf{G}_j]$ and the j -th metric tensor \mathbf{G}_j .

For the isotropic part ψ^{iso} we choose a compressible MOONEY-RIVLIN model, i.e.,

$$\psi^{iso} = \alpha_1 I_1 + \alpha_2 I_2 + \delta_1 I_3 - \delta_2 \ln(\sqrt{I_3}), \quad \forall \alpha_1, \alpha_2, \delta_1, \delta_2 \geq 0.$$

Suitable polyconvex anisotropic energies in terms of $f_{3rj}, f_{4rj}, f_{5rj}, f_{6rj}, f_{7rj}$

$$\begin{aligned} \psi_1^{aniso} &= \sum_{r=1}^n \sum_{j=1}^m [f_{3rj}(I_3) + f_{4rj}(J_{4j}) + f_{5rj}(J_{5j})], \\ \psi_2^{aniso} &= \sum_{r=1}^n \sum_{j=1}^m [f_{3rj}(I_3) + f_{6rj}(I_3, J_{4j}) + f_{7rj}(I_3, J_{5j})], \\ \psi_3^{aniso} &= \sum_{r=1}^n \sum_{j=1}^m [f_{3rj}(I_3) + f_{4rj}(J_{4j}) + f_{5rj}(J_{5j}) \\ &\quad + f_{6rj}(I_3, J_{4j}) + f_{7rj}(I_3, J_{5j})]. \end{aligned}$$

Further details: SCHRÖDER, NEFF & EBBING [2008].



Generic Polyconvex Anisotropic Functions

Some specific functions which **automatically** satisfy the condition $\mathcal{S}|_{C=1} = 0$

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

with $\xi_{rj}, \alpha_{rj}, \beta_{rj} \geq 0,$
 $\gamma_{rj} \geq -1/2.$
 \rightarrow **coercive**

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

with $\xi_{rj}, \alpha_{rj}, \beta_{rj} \geq 0.$

$$\psi_{III}^{aniso} = \sum_{r=1}^n \sum_{j=1}^m \left[\frac{J_{4j}^{\alpha_{rj}}}{I_3^{1/3}} + \frac{J_{5j}^{\alpha_{rj}}}{I_3^{1/3}} + \frac{g_j^{\alpha_{rj}}}{\beta_{rj}} I_3^{-\beta_{rj}} \right],$$

with $\alpha_{rj} = 5/3,$
 $\beta_{rj} \geq -1/2.$

$$\psi_{IV}^{aniso} = \sum_{r=1}^n \sum_{j=1}^m \left[\frac{J_{4j}^{\alpha_{rj}}}{I_3^{1/3}} + \frac{J_{5j}^{\alpha_{rj}}}{I_3^{1/3}} - g_j^{\alpha_{rj}} \beta_{rj} \ln(I_3) \right],$$

with $\alpha_{rj} \geq 1,$
 $\beta_{rj} = \alpha_{rj} - 2/3.$

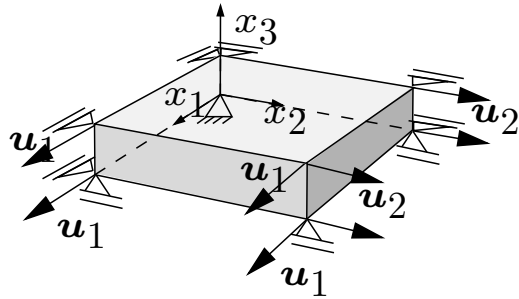
A priori stress free reference configuration: ITSKOV & AKSEL [2004].

Proof of coercivity: SCHRÖDER, NEFF & EBBING [2008].



A First Applications to Transverse Isotropy

Biaxial Homogeneous Tension Test



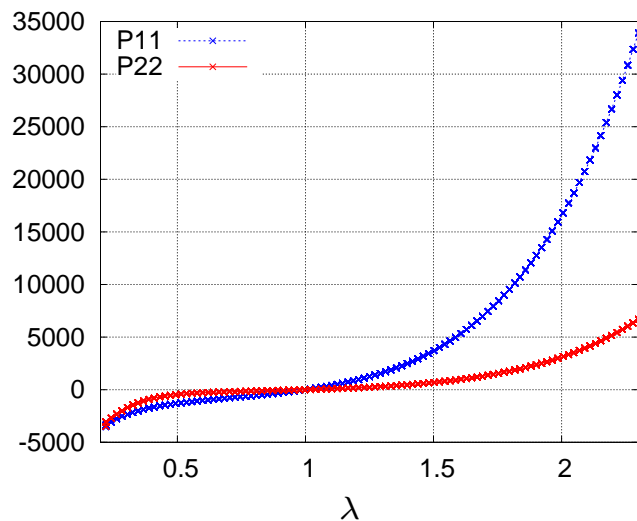
Unimodular metric tensor:

$$\mathbf{G}^{ti} = \text{diag}\left(\gamma, \frac{1}{\sqrt{\gamma}}, \frac{1}{\sqrt{\gamma}}\right)$$

Additive construction of energy function $\psi = \psi^{iso} + \psi^{ti}$, with

$$\psi^{iso} = \alpha_1 I_1 + \alpha_2 I_2 + \delta_1 I_3 - \delta_2 \ln \sqrt{I_3}$$

$$\psi^{ti} = \eta_1 (J_4^{\alpha_4} + \beta_1 J_5^{\alpha_5})$$



$$J_4 = \text{tr}[\mathbf{C}\mathbf{G}^{ti}], \quad J_5 = \text{tr}[\text{Cof}[\mathbf{C}]\mathbf{G}^{ti}]$$

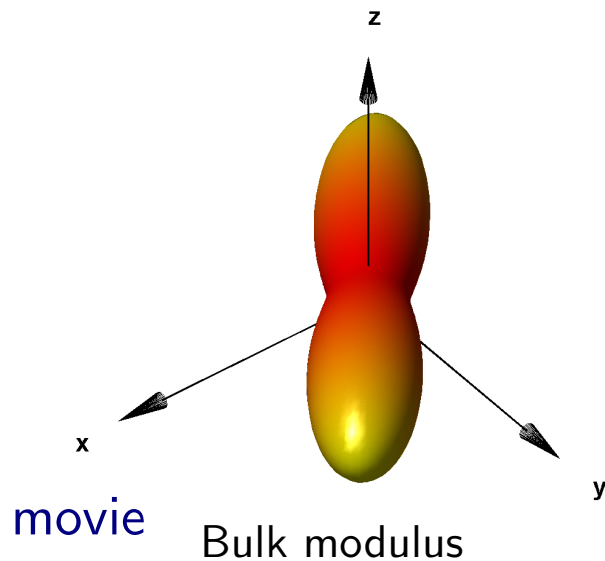
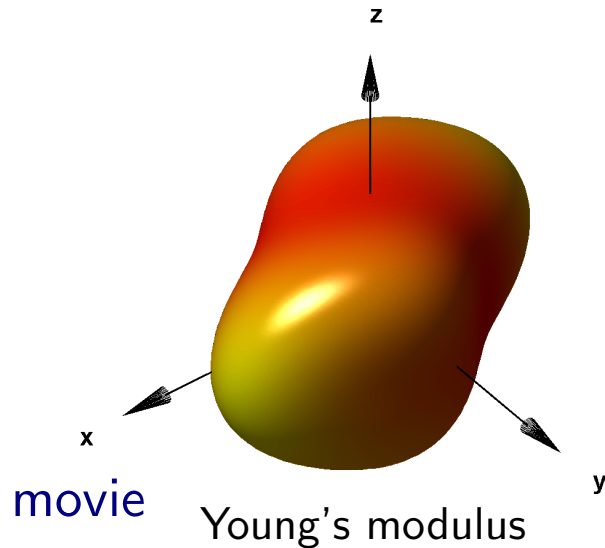
$$\gamma = 4.0, \quad \alpha_1 = 2.0, \quad \alpha_2 = 0.0,$$

$$\delta_1 = 10.0, \quad \delta_2 = 786, \quad \eta_1 = 1.0, \quad \beta_1 = 7.5,$$

$$\alpha_4 = 2.0, \quad \alpha_5 = 3.0 \quad [\text{MPa}]$$

Fitting of Monoclinic Moduli $\mathbb{C} = 4\partial_{CC}^2\psi$: Augite

Characteristic surfaces



Elasticities in [GPa], SIMMONS [1971]:

$$\mathbb{C}^{(V)exp} = \begin{bmatrix} 217.8 & 72.4 & 33.9 & 24.6 & 0 & 0 \\ & 181.6 & 73.4 & 19.9 & 0 & 0 \\ & & 150.7 & 16.6 & 0 & 0 \\ & & & 51.1 & 0 & 0 \\ & sym. & & & 55.8 & 4.3 \\ & & & & & 69.7 \end{bmatrix}$$

Error for $\psi = \psi_I^{aniso}$ and $n = m = 3$:

$$e = \frac{\|\mathbb{C}^{(V)comp} - \mathbb{C}^{(V)exp}\|}{\|\mathbb{C}^{(V)exp}\|} \approx 3.48[\%]$$

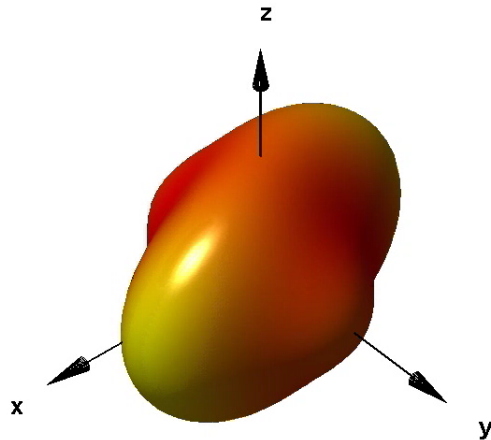
Metric Tensors:

$$\mathbf{G}_1^{ti} = \text{diag}(0.419, 0.419, 1.953),$$

$$\mathbf{G}_2^m = \begin{bmatrix} 1.503 & -0.513 & 0 \\ -0.513 & 0.934 & 0 \\ 0 & 0 & 1.572 \end{bmatrix}, \quad \mathbf{G}_3^m = \begin{bmatrix} 2.719 & 0.496 & 0 \\ 0.496 & 0.547 & 0 \\ 0 & 0 & 1.008 \end{bmatrix}$$

Fitting of Anisotropic Moduli

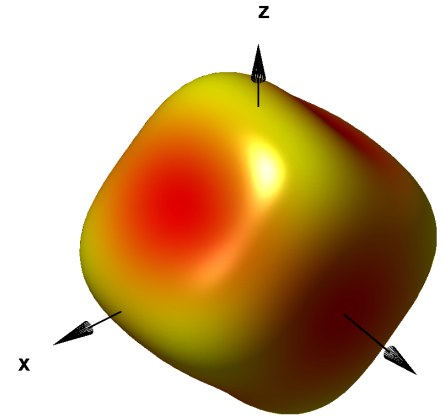
Monoclinic Materials



movie

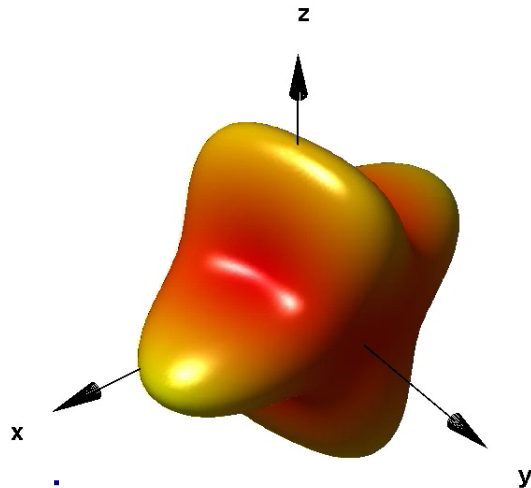
Aegirite: $e = 1.65\%$

Rhombic Materials



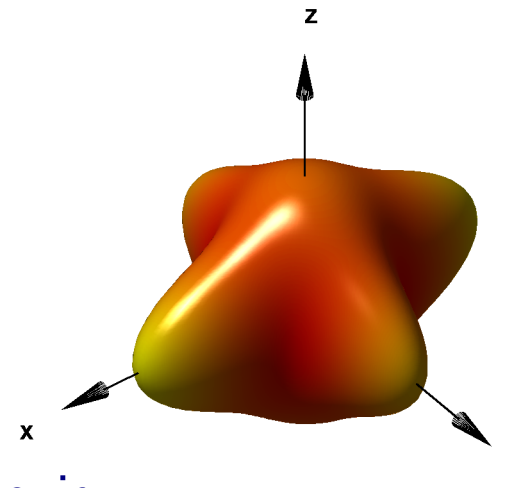
movie

Ammonium Sulfate: $e = 3.46\%$



movie

Feldspar(Labradorite): $e = 5.28\%$

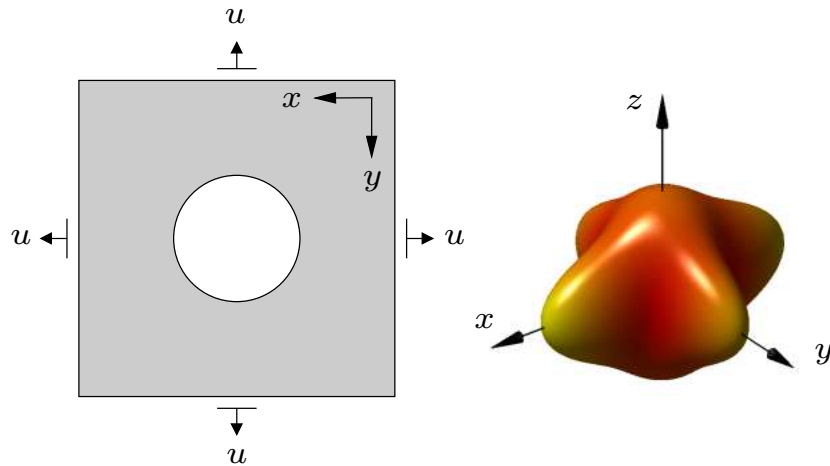


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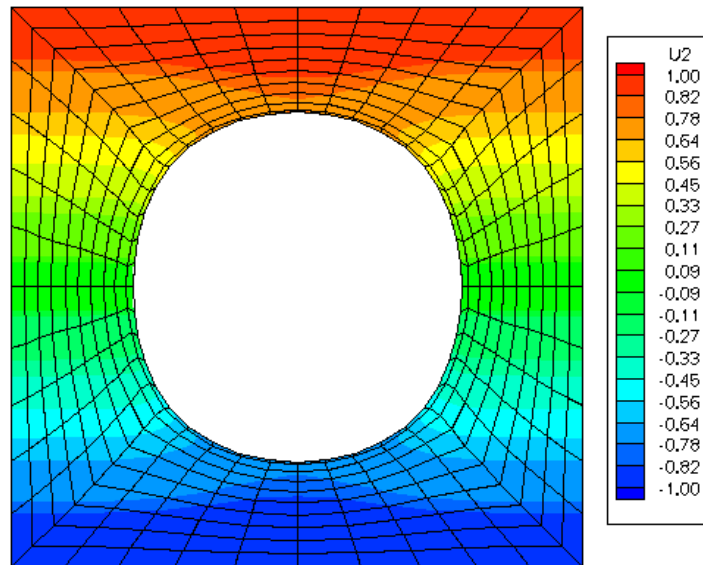
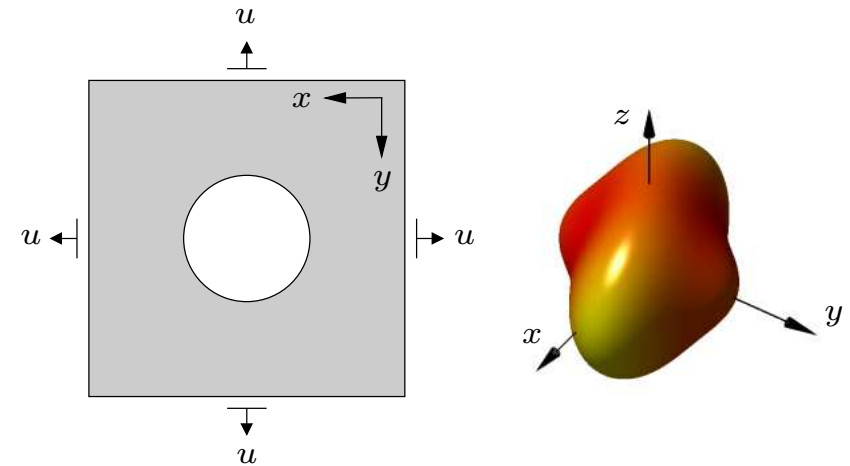
Acenaphthene: $e = 2.28\%$

Biaxial Tension Test of Perforated Plate with Centered Hole

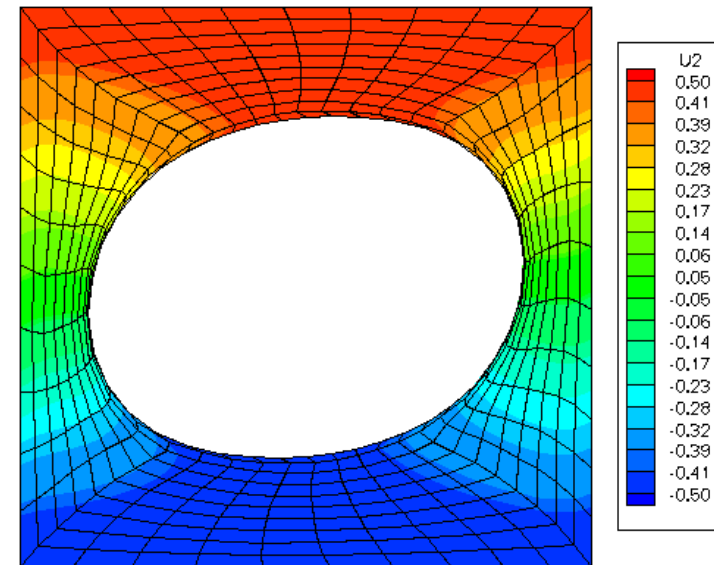
Rhombic Acenaphthene



Monoclinic Aegirite



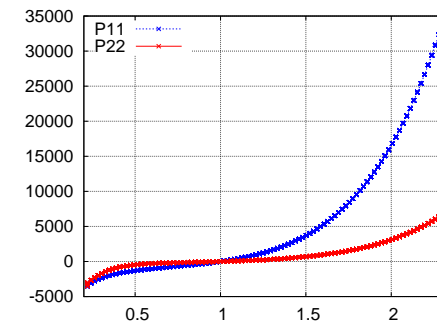
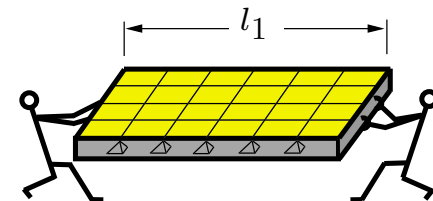
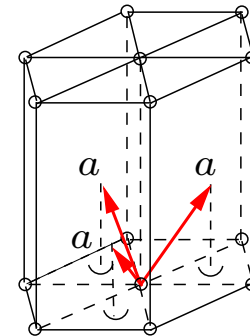
movie



movie

Polyconvex Models for Arbitrary Anisotropic Materials

- Triclinic, monoclinic, rhombic, hexagonal as well as transversely isotropic symmetries can be “*completely described*” by generic invariant functions in terms of **single, second-order, positive definite anisotropic metric tensors**.
- These invariant functions **automatically fulfill** the **polyconvexity condition**.
- The requirement of a **stress-free reference configuration** is also **automatically satisfied**.



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