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Abstract

For simulations of boundary value problems using anisotropic hyperelastic constitutive equations at moderate strains anisotropic polyconvex energies can preferably be used because the existence of minimizers is then automatically guaranteed. For this reason, we investigate the adaptability of anisotropic polyconvex energy functions for the phenomenological description of real anisotropic material responses. Here we focus on the fitting of the fourth-order tangent moduli near the reference state to some experimental data of anisotropic materials. We use anisotropic energies which can be generated for arbitrary anisotropy classes and automatically satisfy the polyconvexity condition. In this paper we consider orthotropic and monoclinic materials.

1. Introduction.

In the framework of finite elasticity the mathematical treatment of boundary value problems is based on the direct methods of variations, i.e., finding a deformation which minimizes the elastic free energy function subject to specific boundary conditions. The existence of minimizers for the variational functional is guaranteed if the functional to be minimized is sequentially weakly lower semicontinuous (s.w.l.s.) and coercive. Polyconvex functions are always s.w.l.s. and are therefore usually considered, see BALL [1]. For isotropic materials there exists a wide range of constitutive functions, e.g., the Neo-Hooke-, Ogden-, Mooney-Rivlin-type energy functions, that satisfy the polyconvexity requirement. In this context see also STEIGMANN [19], HARTMANN & NEFF [7] and MIELKE [11]. In the case of anisotropy, especially transverse isotropy and orthotropy, polyconvex energies have already been proposed in SCHRÖDER & NEFF [12, 13]. Further extensions and case studies presented in [13] are documented in SCHRÖDER, NEFF & BALZANI [14], BALZANI [3], ITSKOV & AKSEL [8] and MARKERT, EHLERS & KARAJAN [10]. A direct extension of [13] to materials with cubic symmetry is proposed in KAMBOUCHEV, FERNANDEZ & RADOVITZKY [9]. Furthermore, a general method for the construction of polyconvex energies for arbitrary anisotropy is given in SCHRÖDER, NEFF & EBBING [15]. This concept is primarily based on the introduction of an anisotropic metric tensor that reflects the symmetry properties of the underlying crystal class. An adjustment of two superimposed transversely isotropic response functions to experimental data of overstretched arterial walls is discussed in BALZANI, NEFF, SCHRÖDER & HOLZAPFEL [4]. An analysis of thin shells in consideration of anisotropic polyconvex energy densities is given in BALZANI, GRUTTMANN & SCHRÖDER [5].

In this contribution we are interested in the description of orthotropic and monoclinic materials by using anisotropic polyconvex energies. For the construction of orthotropic

and monoclinic energy densities we choose the method proposed in SCHRÖDER, NEFF & EBBING [15]. Considering this concept we automatically ensure the polyconvexity of the energy functions and satisfy the stress free reference configuration condition a priori. The main goal of this contribution is the investigation of the adaptability of these anisotropic polyconvex energy functions to experimental measurements. Thus we focus on the approximation of the anisotropic fourth-order elasticity tensors at the reference state by use of some available data from realistic anisotropic materials.

2. Mechanical and Mathematical Preliminaries.

The body of interest in the reference configuration is denoted by $\mathcal{B}_0 \subset \mathbb{R}^3$, parametrized in \mathbf{X} , and the current configuration by $\mathcal{B}_t \subset \mathbb{R}^3$, parametrized in \mathbf{x} . The nonlinear deformation map $\varphi_t : \mathcal{B}_0 \rightarrow \mathcal{B}_t$ at time $t \in \mathbb{R}_+$ maps points $\mathbf{X} \in \mathcal{B}_0$ onto points $\mathbf{x} \in \mathcal{B}_t$. The deformation gradient \mathbf{F} is defined by

$$\mathbf{F}(\mathbf{X}) := \text{Grad}\varphi_t(\mathbf{X}), \quad (2.1)$$

with the Jacobian $J(\mathbf{X}) := \det \mathbf{F}(\mathbf{X}) > 0$. For the geometrical interpretations of some polynomial invariants we often use expressions based on the mappings of the infinitesimal line $d\mathbf{X}$, area $d\mathbf{A} = \mathbf{N}dA$ and volume elements dV , respectively. These material quantities are mapped to their spatial counterparts $d\mathbf{x}$, $d\mathbf{a} = \mathbf{n}da$ and dv via

$$d\mathbf{x} = \mathbf{F}d\mathbf{X}, \quad \mathbf{n}da = \text{Cof}[\mathbf{F}]\mathbf{N}dA \quad \text{and} \quad dv = \det[\mathbf{F}]dV. \quad (2.2)$$

Equation (2.2)₂ is the well-known Nanson's formula. It should be mentioned right away that the argument $(\mathbf{F}, \text{Cof}\mathbf{F}, \det\mathbf{F})$ plays an important role in the definition of polyconvexity.

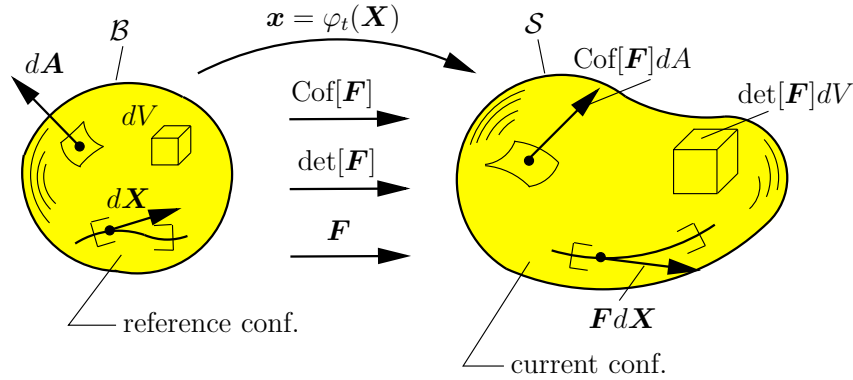


Figure 1: Reference- and actual configuration of the considered body.

For finite elasticity we assume the existence of a free energy function $W(\mathbf{F})$ for the solution of boundary value problems. The underlying boundary value problem is governed by minimizing the potential of the whole system with respect to φ , i.e.,

$$\begin{aligned} \Pi(\varphi) &= \int_{\mathcal{B}} W(\mathbf{F}) dV - \int_{\mathcal{B}} \rho_0 \bar{\mathbf{b}} \cdot \varphi dV - \int_{\partial\mathcal{B}} \bar{\mathbf{t}} \cdot \varphi dA \rightarrow \text{stat.}, \\ \text{with } \varphi &= \bar{\varphi} \text{ on } \partial\mathcal{B}_\varphi. \end{aligned} \quad (2.3)$$

The scalar value ρ_0 denotes the referential density, the vector $\bar{\mathbf{b}}$ is the given body force and the vector $\bar{\mathbf{t}}$ designates the surface tractions. In order to meet the objectivity condition (principle of material frame indifference) a priori, we use the well-known reduced constitutive equations in terms of the right Cauchy–Green tensor $\mathbf{C} := \mathbf{F}^T \mathbf{F}$ and set $\psi(\mathbf{C}) = W(\mathbf{F})$. Since we focus on the formulation of anisotropic hyperelastic energies we have to take into account the principle of material symmetry. For this we have to ensure the invariance of $W(\mathbf{F})$ with respect to the symmetry transformations $W(\mathbf{F}\mathbf{Q})$ for all $\mathbf{Q} \in \mathcal{G} \subset O(3)$, where \mathcal{G} represents the so-called material symmetry group. Thus the reduced constitutive equations must satisfy

$$\psi(\mathbf{C}) = \psi(\mathbf{Q}\mathbf{C}\mathbf{Q}^T) \quad \forall \quad \mathbf{Q} \in \mathcal{G}, \quad (2.4)$$

which is the principle of material symmetry expressed in terms of ψ .

3. Orthotropic and Monoclinic Polyconvex Energy Functions.

For the construction of orthotropic and monoclinic energy functions we use a method introduced by SCHRÖDER, NEFF & EBBING [15]. The proposed concept for the construction of polyconvex energy functions for arbitrary anisotropy classes is based on the introduction of an anisotropic metric tensor \mathbf{G} that incorporates the symmetry properties of the associated crystal class. In order to meet the principle of material symmetry (2.4), the anisotropic energy functions considered in terms of the right Cauchy–Green tensor and the metric tensor \mathbf{G} have to satisfy

$$\mathbf{C} \cdot \mathbf{G} = \mathbf{Q}\mathbf{C}\mathbf{Q}^T \cdot \mathbf{G} = \mathbf{C} \cdot \mathbf{Q}^T \mathbf{G} \mathbf{Q} \quad \forall \mathbf{Q} \in \mathcal{G} \subset O(3). \quad (3.1)$$

Thus the invariance requirement for the metric tensor

$$\mathbf{G} = \mathbf{Q}\mathbf{G}\mathbf{Q}^T \quad \forall \mathbf{Q} \in \mathcal{G} \subset O(3) \quad (3.2)$$

must be ensured. Formulations of orthotropic energies are governed by the orthotropic metric tensor \mathbf{G}^o appearing in the diagonal form

$$\mathbf{G}^o = \text{diag}(a, b, c) \quad \text{with} \quad a, b, c > 0. \quad (3.3)$$

\mathbf{G}^o is invariant with respect to transformations of the underlying material symmetry group:

$$\mathcal{G}^o = \{\mathbf{1}, -\mathbf{1}, \mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3\}. \quad (3.4)$$

The transformations $\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3$ are reflections with respect to the X_2 – X_3 –, X_1 – X_3 – and X_1 – X_2 –plane defined by the matrices

$$\mathbf{R}_1 = \text{diag}(-1, 1, 1), \quad \mathbf{R}_2 = (1, -1, 1), \quad \mathbf{R}_3 = \text{diag}(1, 1, -1), \quad (3.5)$$

respectively. In order to formulate monoclinic energies the monoclinic metric tensor have to be taken into account. The monoclinic metric tensor \mathbf{G}^m is of the general type

$$\mathbf{G}^m = \begin{bmatrix} a & d & 0 \\ d & b & 0 \\ 0 & 0 & c \end{bmatrix} \quad \text{with} \quad a, c > 0, \quad ab > d^2. \quad (3.6)$$

Here the invariance requirement with respect to transformations of the material symmetry group \mathcal{G}^m is also ensured, i.e.,

$$\mathbf{G} = \mathbf{Q}\mathbf{G}^m\mathbf{Q}^T \quad \forall \mathbf{Q} \in \mathcal{G}^m \subset \text{O}(3). \quad (3.7)$$

In detail the monoclinic material symmetry group is given by

$$\mathcal{G}^m = \{\mathbf{1}, -\mathbf{1}, \mathbf{D}_3, \mathbf{R}_3\}, \quad (3.8)$$

where the element \mathbf{D}_3 denotes a rotation through π about the X_3 -axis, i.e.,

$$\mathbf{D}_3 = \text{diag}(-1, -1, 1). \quad (3.9)$$

The orthotropic and monoclinic free energy functions, respectively, are assumed to be of the additive type

$$\psi = \psi^{iso}(I_1, I_2, I_3) + \psi^{aniso}(I_3, J_{4j}, J_{5j}), \quad (3.10)$$

with the principle isotropic invariants

$$I_1 = \text{tr}\mathbf{C} = \mathbf{1} \cdot \mathbf{C}, \quad I_2 = \text{tr}[\text{Cof}\mathbf{C}] = \mathbf{1} \cdot \text{Cof}\mathbf{C}, \quad I_3 = \det\mathbf{C} \quad (3.11)$$

and the anisotropic invariants

$$J_{4j} = \text{tr}[\mathbf{C}\mathbf{G}_j], \quad J_{5j} = \text{tr}[\text{Cof}[\mathbf{C}]\mathbf{G}_j], \quad (3.12)$$

governed by m -different metrics \mathbf{G}_j . Furthermore, these generic individual anisotropic invariants are polyconvex, see SCHRÖDER, NEFF & EBBING [15]. As isotropic part a polyconvex compressible Mooney-Rivlin model is considered, i.e.,

$$\psi^{iso} = \alpha_1 I_1 + \alpha_2 I_2 + \delta_1 I_3 - (2\alpha_1 + 4\alpha_2 + 2\delta_1)\ln(\sqrt{I_3}), \quad \text{with } \alpha_1, \alpha_2, \delta_1 \geq 0, \quad (3.13)$$

and as anisotropic part we choose the energy function

$$\psi^{aniso} = \sum_{r=1}^n \sum_{j=1}^m \xi_{rj} \left[\frac{1}{\alpha_{rj} + 1} \frac{1}{(g_j)^{\alpha_{rj}}} (J_{4j})^{\alpha_{rj}+1} + \frac{1}{\beta_{rj} + 1} \frac{1}{(g_j)^{\beta_{rj}}} (J_{5j})^{\beta_{rj}+1} + \frac{g_j}{\gamma_{rj}} (I_3)^{-\gamma_{rj}} \right], \quad (3.14)$$

where the trace of the metric tensor \mathbf{G}_j is denoted by $g_j := \text{tr}\mathbf{G}_j$. The polyconvexity of ψ^{aniso} is guaranteed if the conditions

$$\alpha_{rj}, \beta_{rj}, \xi_{rj} \geq 0 \quad \text{and} \quad \gamma_{rj} \geq -\frac{1}{2} \quad (3.15)$$

hold. In order to ensure the existence of global energy minimizers the polyconvexity condition together with a local coercivity condition is needed, see BALL [2]. Since ψ^{aniso} like ψ^{iso} is coercive itself we are able to neglect the isotropic part. The proof of coercivity of ψ^{aniso} and further details are also presented in [15]. The second Piola-Kirchhoff stresses are given by the well-known relation $\mathbf{S} = 2\partial_{\mathbf{C}}\psi = 2\partial_{\mathbf{C}}\psi^{iso} + 2\partial_{\mathbf{C}}\psi^{aniso} = \mathbf{S}^{iso} + \mathbf{S}^{aniso}$, with the isotropic stress tensor

$$\mathbf{S}^{iso} = 2 \left[(\alpha_1 + \alpha_2 I_1) \mathbf{1} - \alpha_2 \mathbf{C} - (\alpha_1 + 2\alpha_2) I_3 \mathbf{C}^{-1} \right] \quad (3.16)$$

and the associated anisotropic stresses \mathbf{S}^{aniso} given by

$$\mathbf{S}^{aniso} = \sum_{r=1}^n \sum_{j=1}^m 2\xi_{rj} \left[(-g_j I_3^{-\gamma_{rj}} + \frac{1}{(g_j)^{\beta_{rj}}} J_{5j}^{\beta_{rj}+1}) \mathbf{C}^{-1} + \frac{1}{(g_j)^{\alpha_{rj}}} J_{4j}^{\alpha_{rj}} \mathbf{G}_j - \frac{1}{(g_j)^{\beta_{rj}}} J_{5j}^{\beta_{rj}} I_3 \mathbf{C}^{-1} \mathbf{G}_j \mathbf{C}^{-1} \right]. \quad (3.17)$$

Furthermore, the stress-free reference configuration condition $\mathbf{S}(\mathbf{C} = \mathbf{1}) = \mathbf{0}$ is automatically satisfied for the isotropic and anisotropic stress terms, i.e., we obtain $\mathbf{S}^{iso}(\mathbf{C} = \mathbf{1}) = \mathbf{0}$ and $\mathbf{S}^{aniso}(\mathbf{C} = \mathbf{1}) = \mathbf{0}$. Hence a decoupling between the purely isotropic and anisotropic material parameters is ensured.

4. Fitting of Fourth-Order Elasticity Tensors.

In order to approximate the phenomenological response of real orthotropic and monoclinic materials with the above-mentioned anisotropic polyconvex function (3.10) we fit the linearized fourth-order elasticity tensor near the reference state \mathbf{C}_0 , with

$$\mathbf{C}_0 := 4\partial_{\mathbf{C}} \mathbf{C} \psi^{aniso} \Big|_{\mathbf{C}=\mathbf{1}}, \quad (4.1)$$

to some experimental measurements. The linearized tangent moduli \mathbf{C}_0 at the reference state is identical to the classical representation of the elasticity tensor in the small strain regime. This fact results from the linearization of the stress response functions at a natural state, i.e.,

$$Lin[\mathbf{S}] = \mathbf{C}_0 : Lin[\mathbf{E}] \quad \text{with} \quad \mathbf{C}_0 := 2 \frac{\partial \mathbf{S}}{\partial \mathbf{C}} \Big|_{\mathbf{C}=\mathbf{1}} \quad \text{and} \quad \mathbf{S}|_{\mathbf{C}=\mathbf{1}} = \mathbf{0} \quad (4.2)$$

and the Green-Lagrange strain tensor

$$\mathbf{E} := \frac{1}{2}(\mathbf{C} - \mathbf{1}), \quad (4.3)$$

which reduces to the linear relation $\boldsymbol{\sigma} = \mathbf{C}_0 : \boldsymbol{\varepsilon}$, because the term $Lin[\mathbf{S}]$ can be identified with the linear stress tensor $\boldsymbol{\sigma}$ and the term $Lin[\mathbf{E}]$ with the linear strain tensor $\boldsymbol{\varepsilon}$ in the case of small strains.

For the approximations we use experimental data on elasticities presented in SIMMONS & WANG [18]. In detail, the fitting of moduli is done by the minimization of the error function

$$e = \frac{\| \mathbf{C}^{(V)comp} - \mathbf{C}^{(V)exp} \|}{\| \mathbf{C}^{(V)exp} \|}, \quad (4.4)$$

where $\mathbf{C}^{(V)comp} \in \mathbf{R}^{6 \times 6}$ denotes the computed tangent moduli \mathbf{C}_0 in Voigt notation. Furthermore, $\mathbf{C}^{(V)exp} \in \mathbf{R}^{6 \times 6}$ designates the associated coefficient scheme of experimental values. The used norm of the matrix schemes is defined by

$$\| \mathbf{C}^{(V)} \| = \sqrt{\sum_{i=1}^6 \sum_{j=1}^6 (\mathbf{C}_{ij}^{(V)})^2}. \quad (4.5)$$

The material parameter adjustments have been performed by the evolution strategy proposed by SCHWEFEL [16]. In order to get a better imagination of the underlying anisotropic material behavior we plot the characteristic surfaces of Young's moduli and Bulk moduli, respectively, of the adjusted materials because these plots give an impression of the anisotropy ratios. For more details see SHUVALOV [17] and BOEHLKE & BRÜGGEMANN [6].

4.1. Orthotropic Moduli.

As an example of the fitting described above, we approximate the orthorhombic material Ammonium Sulfate with the proposed model, see (3.10). Here we set $n = m = 3$ in (3.14) and take into account the orthotropic metric tensors

$$\mathbf{G}_j^o = \begin{bmatrix} a_j & 0 & 0 \\ 0 & b_j & 0 \\ 0 & 0 & c_j \end{bmatrix} \quad \text{with } a_j, b_j, c_j > 0. \quad (4.6)$$

The experimentally determined elasticities of Ammonium Sulfate are taken from SIMMONS & WANG [18] and depicted together with the computed elasticity moduli in Figure 2. Furthermore, the characteristic surfaces of Young's moduli and Bulk moduli, respectively, are also presented in Figure 3. After the optimization the non-vanishing isotropic material parameters are obtained by

$$\alpha_1 = 1.349, \quad \delta_1 = 0.226, \quad \delta_2 = 3.151, \quad (4.7)$$

and the set of the remaining anisotropic material parameters are given in Table 1.

Table 1: Material parameter set for Ammonium Sulfate

r	j	α_{rj}	β_{rj}	γ_{rj}	ξ_{rj}
1	1	1.448	1.907	-0.500	0.224
1	2	0.000	2.083	-0.312	0.663
1	3	0.428	1.288	-0.941	0.149
2	3	2.357	0.000	-0.406	0.275
3	2	0.000	2.035	-0.090	0.352
3	3	0.000	1.900	-0.500	0.700

The anisotropic metric tensors appear in the forms

$$\begin{aligned} \mathbf{G}_1^o &= \text{diag}(0.827, 0.517, 0.0000001), & \mathbf{G}_2^o &= \text{diag}(0.0000001, 0.252, 0.587), \\ \mathbf{G}_3^o &= \text{diag}(0.270, 0.957, 1.222). \end{aligned} \quad (4.8)$$

and the relative error e is 3.46%.

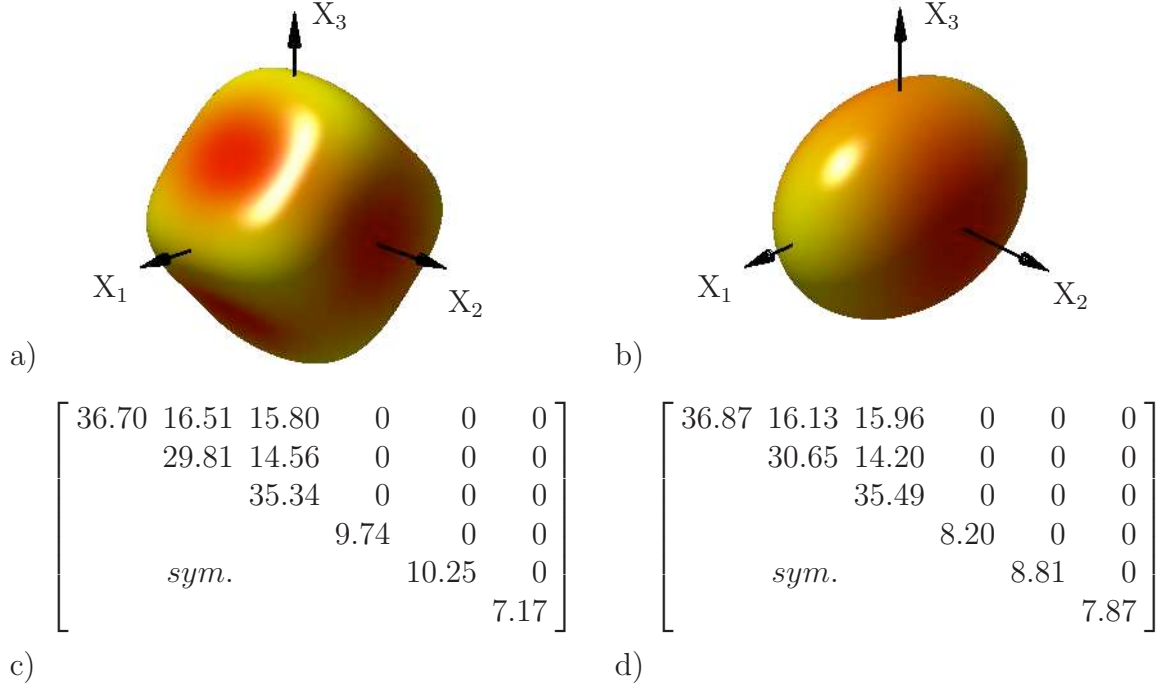


Figure 2: Orthorhombic material. Characteristic surface of: a) Young's moduli, b) Bulk moduli; c) $\mathbf{C}^{(V)exp}$ [GPa], d) $\mathbf{C}^{(V)comp}$ [GPa].

4.2. Monoclinic Moduli.

Next, we are interested in the description of the monoclinic material Feldspar (Labradorite) obtained by using a monoclinic polyconvex energy function. Here, the approximation is performed by only considering the anisotropic term ψ^{aniso} given in (3.14) together with the monoclinic metric tensors of the type

$$\mathbf{G}_j^m = \begin{bmatrix} a_j & d_j & 0 \\ d_j & b_j & 0 \\ 0 & 0 & c_j \end{bmatrix} \quad \text{with } a_j, c_j > 0, d_j^2 < a_j b_j. \quad (4.9)$$

The elasticity moduli for the monoclinic material as well as the characteristic surfaces of Young's moduli and Bulk moduli, respectively, are depicted in Figure 3a-c, experimental data on the elasticity moduli are taken from SIMMONS & WANG [18].

Table 2: Material parameter set for Feldspar (Labradorite)

r	j	α_{rj}	β_{rj}	γ_{rj}	ξ_{rj}
2	1	8.022	0.000	-0.346	2.318
3	1	5.841	0.000	-0.484	3.233
3	2	3.829	0.000	-0.085	0.152

Using $n = 3, m = 3$ and setting the first metric tensor $\mathbf{G}_1 = \text{diag}(1, 1, 1)$, the minimization of the error function yields a relative error of 5.28%. In detail, we obtain two monoclinic

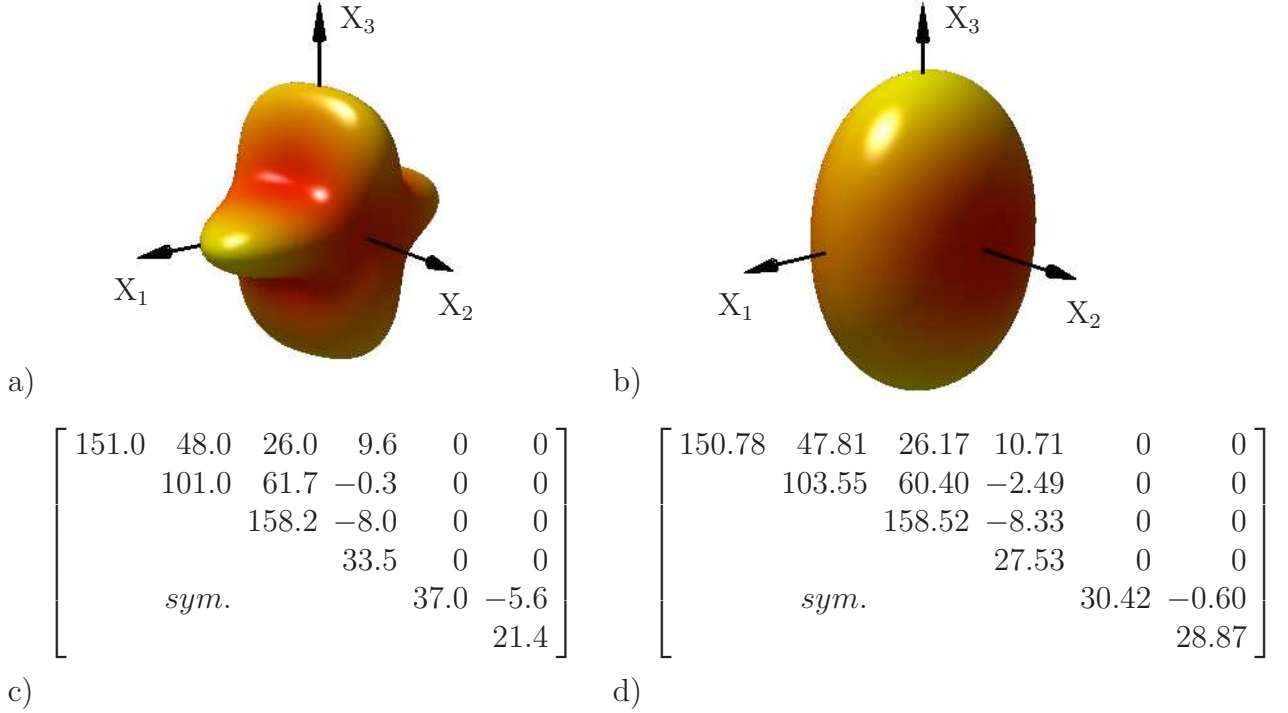


Figure 3: Monoclinic material. Characteristic surface of: a) Young's moduli, b) Bulk moduli; c) $\mathbb{C}^{(V)exp}$ [GPa], d) $\mathbb{C}^{(V)comp}$ [GPa].

metric tensors of the form

$$\mathbf{G}_1^m = \begin{bmatrix} 2.400 & 0.263 & 0 \\ 0.263 & 1.087 & 0 \\ 0 & 0 & 0.747 \end{bmatrix}, \quad \mathbf{G}_2^m = \begin{bmatrix} 0.061 & -0.268 & 0 \\ -0.268 & 1.187 & 0 \\ 0 & 0 & 2.049 \end{bmatrix} \quad (4.10)$$

and the set of non-vanishing anisotropic material parameters is presented in Table 2. The final fitted monoclinic tangent moduli are given in Figure 3d.

5. Conclusion.

In this paper we have investigated the approximation of fourth-order monoclinic and orthotropic elasticity tensors to experimental measurements by using polyconvex monoclinic and orthotropic energy functions. The construction of these energy functions is based on a new concept proposed in SCHRÖDER, NEFF & EBBING [15]. This generic concept automatically ensures the polyconvexity and the anisotropy of the energy functions. Furthermore, the stress-free reference configuration condition is automatically satisfied. The results of the adaptability of these energies show that they are also well-suitable for the description of realistic orthotropic and monoclinic material behavior.

Consequently, simulations of boundary value problems including anisotropic elastic material behavior at moderate strains can be done by using polyconvex anisotropic energy functions. It should be noted that in this case the existence of minimizers of the underlying variational functional is guaranteed and an appropriate description of real anisotropic material responses is also made possible.

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