Modeling of anisotropic hyperelasticity and discontinuous damage in arterial walls based on polyconvex stored energy functions

D. Balzani[a,*], J. Schröder[b], D. Gross

[a] Institute of Mechanics, Technical University of Darmstadt, Department of Mechanics (AG 4), Hochschulstr. 1, 64289 Darmstadt, Germany

[b] Institute of Mechanics, University of Duisburg-Essen, Campus Essen, Department of Civil Engineering (FB 10), Universitaetsstr. 15, 45117 Essen, Germany

Abstract

In this paper an anisotropic damage model is proposed respecting discontinuous damage effects observed in a certain range of over-expansion of arteries. The model is applied to a polyconvex stored energy function for transversely isotropic hyperelasticity, which possesses the advantage of avoiding material instabilities in the elastic range. Numerical examples are presented in order to provide an insight into the performance of the proposed model.

Keywords: Arterial walls; Soft tissues; Polyconvex energy; Anisotropic; Hyperelastic; Damage

1. Introduction

The development of optimized methods for the resetting of artery stenosis, caused by atherosclerotic plaques, demands simulation models that are able to reflect the material behavior of arterial walls. For an overview of arterial wall mechanics see Holzapfel et al. [1] and Gasser and Holzapfel [2]. In this paper the proposed damage model, formulated in the framework of internal variables, is applied to the anisotropic polyconvex model for soft tissues, introduced in Schröder and Neff [3], which is embedded in the concept of integrity bases, see Spencer [4], Boehler [5] and Betten [6]. Polyconvexity in the sense of Ball [7,8], cf. Marsden and Hughes [9] and Ciarlet [10], implies the fulfillment of the Legendre–Hadamard condition. With respect to this, a comparison of several constitutive models for soft tissues is investigated in Schröder et al. [11].

2. Continuum-mechanical foundations

Let the body of interest be denoted by $\mathcal{B} \subset \mathbb{R}^3$ for the undeformed reference configuration and $\mathcal{S} \subset \mathbb{R}^3$ for the current configuration. The deformation of the body is respected by the motion of points $\boldsymbol{X} \in \mathcal{B}$, being transformed to the actual position $\boldsymbol{x} \in \mathcal{S}$ by the deformation map $\varphi_t : \mathcal{B} \rightarrow \mathcal{S}$ at time $t \in \mathbb{R}_+$. The deformation gradient $\boldsymbol{F}$ and the deformation measure, the right Cauchy–Green deformation tensor $\boldsymbol{C}$, are defined by

$$\boldsymbol{F}(\boldsymbol{X}) := \mathrm{Grad}\varphi_t(\boldsymbol{X}) \quad \text{and} \quad \boldsymbol{C} := \boldsymbol{F}^T\boldsymbol{F}, \tag{1}$$

respectively. Focusing on hyperelasticity the existence of a stored energy function ψ is postulated, which is defined per unit reference volume. In order to satisfy the principle of material frame-indifference the constitutive equations are formulated in the right Cauchy–Green deformation tensor. Neglecting dissipative effects the second Piola–Kirchhoff stresses $\boldsymbol{S}$ and the interrelation of $\boldsymbol{S}$ and the Kirchhoff stresses $\boldsymbol{\tau}$ are given by

$$\boldsymbol{S} = 2\partial_C\psi \quad \text{and} \quad \boldsymbol{\tau} = \boldsymbol{FSF}^T \tag{2}$$

For taking into account anisotropic material behavior additional argument tensors, the so-called structural tensors, are necessary. The idea in this context is to replace an anisotropic tensor function by an isotropic one via suitable structural tensors. These tensors $\boldsymbol{M}$ are invariant under transformations, say rigid body rotations $\boldsymbol{Q}$, being elements of the (transversely isotropic) material symmetry group G_{ti} and

$$\boldsymbol{M} = \boldsymbol{Q}^T\boldsymbol{MQ} \; \forall \; \boldsymbol{Q} \in G_{ti} \subset \mathrm{SO}(3) \tag{3}$$

* Corresponding author. Tel.: +49 2011 833 142; Fax: +49 2011 832680; E-mail: balzani@mechanik.tu-darmstadt.de

Computational Fluid and Solid Mechanics 2005
K.J. Bathe (Editor)

holds with SO(3) denoting the special orthogonal group. Let $\boldsymbol{a}$ be the preferred direction of the material with $\|\boldsymbol{a}\| = 1$, then a suitable structural tensor is defined as $\boldsymbol{M} := \boldsymbol{a} \otimes \boldsymbol{a}$. This leads to an isotropic tensor function fulfilling

$$\psi = \psi(\boldsymbol{C}, \boldsymbol{M}) = \psi(\boldsymbol{Q}^T\boldsymbol{C}\boldsymbol{Q}, \boldsymbol{Q}^T\boldsymbol{M}\boldsymbol{Q}) \; \forall \boldsymbol{Q} \in \mathrm{SO}(3) \quad (4)$$

Now we are able to express the functional dependence of ψ in terms of the invariants of the argument tensors ($\boldsymbol{C}$, $\boldsymbol{M}$):

$$I_1 := \mathrm{tr}\, \boldsymbol{C}, \quad I_2 := \mathrm{tr}[Cof\boldsymbol{C}], \quad I_3 := \det \boldsymbol{C},$$
$$J_4 := \mathrm{tr}[\boldsymbol{C}\boldsymbol{M}], \quad J_5 := \mathrm{tr}[\boldsymbol{C}^2\boldsymbol{M}] \quad (5)$$

These invariants form a possible polynomial basis for the stored energy, i.e. $\psi = \psi(I_1, I_2, I_3, J_4, J_5)$.

3. Polyconvex hyperelastic model for arterial walls

In order to guarantee physically reasonable material behavior several constitutive inequalities have been proposed in the literature. A quite suitable condition is the Legendre–Hadamard inequality, which investigates the existence of positive wave speeds by analyzing the acoustic tensor. If the acoustic tensor is positive definite then the material is said to be materially stable; this does not imply the existence of minimizers of the value-boundary problem arising from the Finite-Element-Method. A practicable framework, which guarantees the existence of minimizers and fulfills the Legendre–Hadamard condition, is the polyconvexity condition of Ball [7, 8]. A basis for constitutive modeling using polyconvex stored energies is given in Schröder and Neff [12], where the proof of polyconvexity is exposed for a variety of anisotropic stored energy functions.

Arterial walls are mainly stiffened by collagen fibers which are arranged helically crosswise around the artery. These fibers are embedded in an incompressible matrix material, which can be represented by the isotropic polyconvex function

$$\psi^{iso} = \alpha_1 \frac{I_1}{I_3^{1/3}} + \alpha_2 \frac{I_2}{I_3^{1/3}} - \alpha_3 \ln(I_3) + \alpha_4\left(I_3^{\alpha_5} + \frac{1}{I_3^{\alpha_5}} - 2\right) \quad (6)$$

introduced in Schröder and Neff [3]. The fact that the fibers, oriented mainly in two directions, do not differ with the direction, leads to the assumption that the material behavior remains the same for each fiber orientation. For orthotropic materials with weak interactions between the two preferred directions $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ the superposition of two transversely isotropic models with identical material parameters seems to be appropriate, see e.g. Schröder et al. [11] and Holzapfel et al. [1]. Thus, the material behavior of the fibers can be represented by the polyconvex function

$$\sum_{a=1}^{2} \psi^{ti,(a)} = \sum_{a=1}^{2} \Big[\alpha_6(J_5^{(a)} - I_1 J_4^{(a)} + I_2) + \alpha_7 \frac{J_4^{(a)\alpha_8}}{I_3^{1/3}} + \alpha_9(I_1 J_4^{(a)} - J_5^{(a)}) + \alpha_{10} J_4^{(a)\alpha_{11}}\Big] \quad (7)$$

see Schröder and Neff [3]. The mixed invariants $J_4^{(a)} = \boldsymbol{C} : \boldsymbol{M}_{(a)}$ and $J_5^{(a)} = \boldsymbol{C}^2 : \boldsymbol{M}_{(a)}$ are governed by the structural tensors $\boldsymbol{M}_{(a)} = \boldsymbol{a}_{(a)} \otimes \boldsymbol{a}_{(a)}$ with the preferred directions $\boldsymbol{a}_{(a)}$, $a = 1..2$, representing the fiber directions. In order to guarantee polyconvexity we have to respect $\alpha_8 \geqslant 1$ and $\alpha_{11} \geqslant 1$ and the remaining parameters have to be greater than zero. With Eqs. (6) and (7) we obtain the complete polyconvex stored energy function for arterial walls in the form

$$\psi = \psi^{iso} + \sum_{a=1}^{2} \psi^{ti,(a)} \quad (8)$$

As a simple example for the material stability of the polyconvex model a localization analysis is now performed; for details on this subject we refer to Schröder et al. [11], where the localization of several constitutive models for soft tissues is investigated. The acoustic tensor can be calculated by the formula

$$\bar{Q}(\boldsymbol{N})_{ab} = \mathrm{A}_{a\;\,b}^{\;A\;\,B} N_A N_B \quad \text{with} \quad \mathrm{A}_{a\;\,b}^{\;A\;\,B} = D_F^2 W(\boldsymbol{F}) \quad \text{and} \quad W(\boldsymbol{F}) = \psi(\boldsymbol{C}) \quad (9)$$

given in index notation. Herein $\boldsymbol{N}$ denotes the normal vector in spherical coordinates $\boldsymbol{N}(\bar{\alpha}, \bar{\beta}) = [\sin(\bar{\beta})\cos(\bar{\alpha}), \sin(\bar{\beta})\sin(\bar{\alpha}), \cos(\bar{\beta})]^T$. A sufficient condition for material stability is $q := \mathrm{sign}[\min[q_1, q_2, q_3]]\, |q_3| > 0$ with $q_1 = \bar{Q}_{11}$, $q_2 = \bar{Q}_{11}\bar{Q}_{22} - \bar{Q}_{12}\bar{Q}_{21}$ and $q_3 = \det[\bar{\mathbf{Q}}]$ for all directions of the cross-sectional area represented by $\boldsymbol{N}$, because then the acoustic tensor is positive definite. As a numerical example a cube, consisting of the Media and Adventitia of an arterial wall, is compressed up to the stretch $\lambda_1 = 0.4$ by utilizing the polyconvex model. The material parameters for the Media and Adventitia of an artery have been fitted in Schröder et al. [11] and are given in Table 1. The setup of the experiment is demonstrated in Fig. 1(a) while the values of q are plotted for each orientation of cross-sections within the test materials in Figs 1(b) and (c). We observe only positive values for q, therefore, the material is stable for the considered experiment (and for all other possible deformation states, whereas different often used models proposed in the literature fail, see Schröder et al. [11]).

Table 1
Material parameters for an artery

	α_1 [kPa]	α_2 [kPa]	α_3 [kPa]	α_4 [kPa]	α_5 [−]	α_6 [kPa]	α_7 [kPa]	α_8 [−]	α_9 [kPa]	α_{10} [kPa]	α_{11} [−]
Media	1.502	0.0015	0.328	6.019	10.223	0.310	0.0325	7.339	0.027	0.041	1.077
Adventitia	0.107	0.0002	0.132	4.278	5.940	0.066	0.0002	1.477	0.0003	0.012	5.381

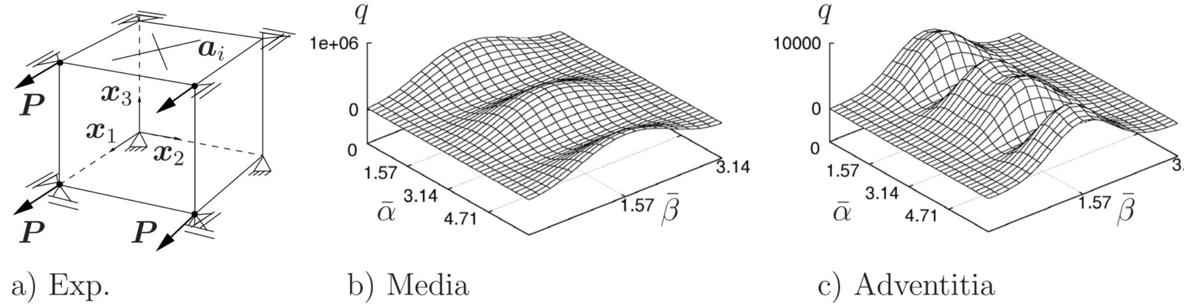

Fig. 1. (a) Setup of experiment with preferred directions $\boldsymbol{a}_{(1)} = (0.8746, 0.4848, 0.0)^T$ and $\boldsymbol{a}_{(2)} = (0.8746, -0.4848, 0.0)^T$ and q at stretch $\lambda_1 = 0.4$ gathered by the polyconvex model for the (b) Media and (c) Adventitia.

4. Anisotropic discontinuous damage model

Breakage of micro fibrils induced by fracture of collagen-crosslinks within arterial walls may be interpreted as reason for discontinuous damage effects, which are observed in experiments. This is the reason for the assumption implying that damage occurs only in fiber direction. Thus, the energy is subdivided into an undamaged isotropic part and a damaged anisotropic part, leading to

$$\psi(\boldsymbol{C},\ \boldsymbol{M}_{(\mathrm{a})},\ D_{(\mathrm{a})}) = \tilde{\psi}(\boldsymbol{C}) + \sum_{\mathrm{a}=1}^{2}\left[(1-D_{(\mathrm{a})})\hat{\psi}^0_{(\mathrm{a})}(\boldsymbol{C},\ \boldsymbol{M}_{(\mathrm{a})})\right] \tag{10}$$

where $\tilde{\psi}$, $\hat{\psi}^0_{(\mathrm{a})}$ and $D_{(a)}$ denote the isotropic energy, transversely isotropic net-energy and the damage variable for each preferred direction $\boldsymbol{a}_{(a)}$ respectively. In compliance with thermodynamic consistency the second law of thermodynamics has to be fulfilled. Starting from the Clausius–Duhem inequality for isothermal conditions $\mathcal{D} = \frac{1}{2}S : \dot{C} - \dot{\psi} \geq 0$ we receive the constitutive equation for the stresses

$$\boldsymbol{S} = 2\partial_C\psi = 2\partial_{\boldsymbol{C}}\tilde{\psi} + \sum_{\mathrm{a}=1}^{2}[\hat{\boldsymbol{S}}_{(\mathrm{a})}], \quad \text{with}$$
$$\hat{\boldsymbol{S}}_{(\mathrm{a})} = 2(1-D_{(\mathrm{a})})\partial_C\hat{\psi}^0_{(\mathrm{a})} \tag{11}$$

and the reduced dissipation inequality

$$\mathcal{D} = \sum_{a=1}^{2}\left[\hat{\psi}^{\,0}_{(a)}\dot{D}_{(a)}\right] \geq 0 \tag{12}$$

We assume the existence of a scalar-valued dissipation potential $\varphi_{(a)} = \hat{\varphi}_{(a)}\,(\dot{D}_{(a)})$, which is convex in the flux variable $\dot{D}_{(a)}$. By partial differentiation the work-conjugated variable results in $\hat{\psi}^0_{(a)} = \partial_{\dot{D}_{(a)}}\varphi_{(a)}$. Legendre–Fenchel transformation leads to the dual dissipation potential $\varphi^*(\hat{\psi}^0_{(a)}) = \sup_{\dot{D}_{(a)}}(\hat{\psi}^0_{(a)}\dot{D}_{(a)} - \varphi(\dot{D}_{(a)}))$ and the dual work-conjugated variable $\dot{D}_{(a)} = \partial_{\hat{\psi}^0_{(a)}}\varphi^*$, in this context see Lemaitre and Chaboche [13]. Integration of the damage variable yields $D_{(a)}$ as a function of $\hat{\psi}^0_{(a)}$. With Eq. (12) we are able to construct a function for the damage, which is given by

$$D_{(a)}(\hat{\psi}^0_{(a)}) = \gamma_1(1 - e^{(-\beta_{(a)}/\gamma_2)}) \tag{13}$$

The discontinuity in damage evolution enforces a special definition of the internal variable, beholding the maximum value of the transversely isotropic net-energy reached up to actual time. The explicit formulation of the internal variable is defined as

$$\beta_{(a)} = \sup_{0\leq \mathrm{s}\leq \mathrm{t}}\left[\hat{\psi}^{\,0}_{(a),\,s} - \hat{\psi}^{\,0}_{(a),\,0}\right] \tag{14}$$

A damage criterion is necessary in order to possess an activating condition for the damage evolution. This criterion is defined by

$$\phi_{(a)} := \beta_{(a)} - \left(\hat{\psi}^0_{(a)} - \hat{\psi}^0_{(a),0}\right) > 0 \tag{15}$$

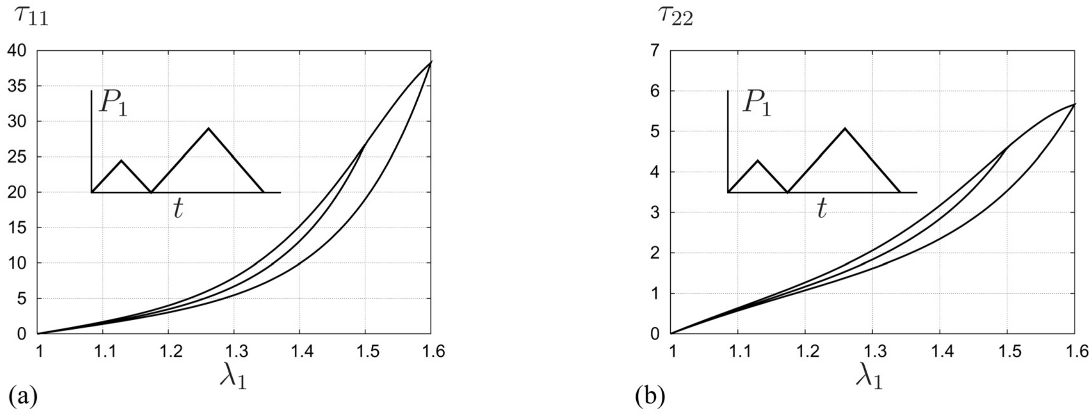

Fig. 2. (a) Kirchhoff stresses τ_{11} and (b) τ_{22} versus stretch λ_1 in a cycled tension test (see experiment in Figure 1(a)) of the Media of an artery.

inducing evolution of damage merely if the criterion is fulfilled. $\hat{\psi}^0_{(a),0}$ denotes the transversely isotropic net-energy for the reference configuration ($\boldsymbol{F} = \boldsymbol{1}$). With the linearization of the damage variable

$$\Delta D_{(a)} = \frac{\partial D_{(a)}}{\partial \beta_{(a)}} \Delta \beta_{(a)} = \frac{\partial D_{(a)}}{\partial \beta_{(a)}} \frac{1}{(1 - D_{(a)})} \hat{\boldsymbol{S}} : \Delta \boldsymbol{E} \qquad (16)$$

we obtain the linearized stresses in the form $\triangle \boldsymbol{S} = \mathbb{C}^{eD} : \triangle \boldsymbol{E}$ with the tangent moduli

$$\mathbb{C}^{eD} = \tilde{\mathbb{C}}^e + \sum_{a=1}^{2} \left(\hat{\mathbb{C}}^e_{(a)} + \mathbb{C}^D_{(a)} \right), \quad \text{with} \quad \tilde{\mathbb{C}}^e = 4 \frac{\partial^2 \tilde{\psi}}{\partial \boldsymbol{C} \partial \boldsymbol{C}},$$

$$\hat{\mathbb{C}}^e_{(a)} = (1 - D_{(a)})\, 4 \frac{\partial^2 \hat{\psi}^0_{(a)}}{\partial \boldsymbol{C} \partial \boldsymbol{C}} \qquad (17)$$

and

$$\mathbb{C}^D_{(a)} = \begin{cases} -\frac{\partial D_{(a)}}{\partial \beta_{(a)}} \frac{1}{(1 - D_{(a)})^2} \hat{\boldsymbol{S}}_{(a)} \otimes \hat{\boldsymbol{S}}_{(a)} & , \text{ if } \phi^{trial}_{(a)} \leq 0 \\ = 0 & , \text{ if } \phi^{trial}_{(a)} > 0 \end{cases} \qquad (18)$$

and the trial value $\phi^{\mathrm{trial}}_{(\mathrm{a})} = \beta_{(\mathrm{a})}(\mathrm{t_n}) - [\hat{\psi}^0_{(\mathrm{a})}(\mathrm{t_{n+1}}) - \hat{\psi}^0_{(\mathrm{a}),0}(\mathrm{t_o})]$ of the damage criterion.

5. Numerical examples

In this section the material parameters of Table 1 and $\gamma_1 = 0.9$, $\gamma_2 = 0.3$ kPa for the Media and $\gamma_1 = 0.7$, $\gamma_2 = 0.3$ kPa for the Adventitia are utilized. In the first numerical example a test cube of the Media of an artery is exposed to the experiment shown in Fig. 1(a) and loaded cyclically. The material response is illustrated in Fig. 2, in which the discontinuous damage effect can be observed.

The second example considers the inhomogeneous deformation in the cross-section of an atherosclerotic artery. The system is illustrated in Fig. 3 and solved via the Finite-Element-Method using quadratic triangle elements. The atherosclerotic plaque is modeled by an isotropic Neo-Hooke material and consists of calcification (treated as nearly rigid), an extracellular lipid pool ($E = 5.0$ kPa, $v = 0.499$) and the plaque itself ($E = 100.0$ kPa, $v = 0.499$). In Fig. 3(b) the distribution of damage $D_{(1)}$ is plotted for the deformed configuration. It should be noted that the utilized material parameters are relatively arbitrarily chosen.

6. Conclusion

In this paper an anisotropic discontinuous damage model has been proposed, which was able to reflect qualitatively experimental observations made in arterial walls. The discontinuous damage effect was biomechanically motivated by the breakage of collagen cross-links, thus, damage was assumed to act only on the stored energy describing the fibers. The weak interaction between the two fiber directions has been considered by the superposition of two transversely isotropic models. Furthermore, material stability has been respected by applying a polyconvex stored energy function, which has been shown in a brief localization analysis. At the end some numerical examples demonstrated the performance of the proposed model.

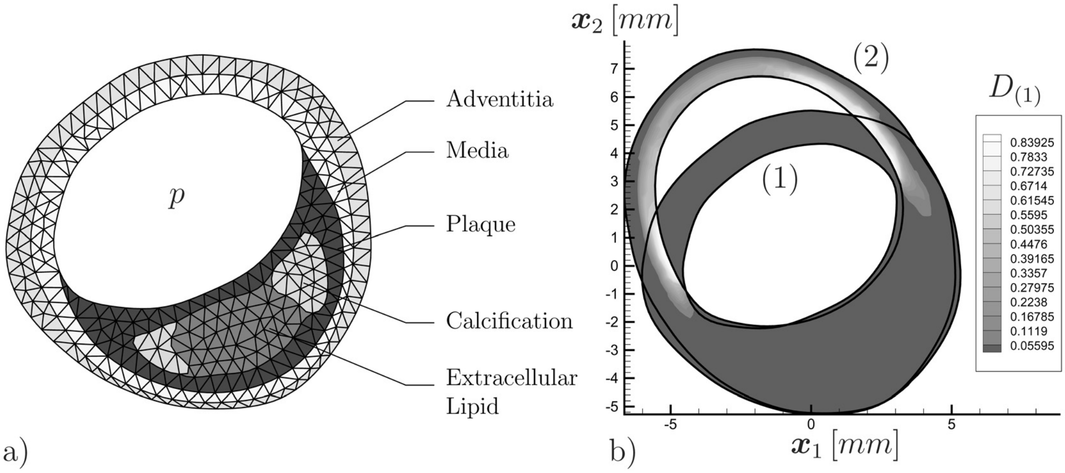

Fig. 3. (a) Mesh of the considered artery with hydrostatic pressure p in the inside and (b) undeformed (1) and deformed (2) artery with distribution of $D_{(1)}$ when $p = 1.00$ kPa.

References

[1] Holzapfel GA, Gasser TC, Ogden RW. A new constitutive framework for arterial wall mechanics and a comparative study of material models. J Elasticity 2000;61:1–48.

[2] Gasser TC, Holzapfel GA. A rate-independent elasto-plastic constitutive model for (biological) fiber-reinforced composites at finite strains: continuum basis, algorithmic formulation and finite element implementation. Comput Mech 2002;29(4–5):340–360.

[3] Schröder J, Neff P. On the construction of polyconvex transversely isotropic free energy functions. In: C Miehe, editor, Proc of the IUTAM symposium on computational mechanics of solid materials at large strains. Dordrecht: Kluwer, 2003, pp. 171–180.

[4] Spencer AJM. Theory of invariants. In: AC Eringen, editor, Continuum Physics, Vol 1. New York: Academic Press, 1971, pp. 239–353.

[5] Boehler JP. Introduction to the invariant formulation of anisotropic constitutive equations. In: JP Boehler, editor, Applications of Tensor Functions in Solid Mechanics. CISM course no. 292. Wien, New York: Springer, 1987, pp. 13–30.

[6] Betten J. Formulation of anisotropic constitutive equations. In: JP Boehler, editor, Applications of Tensor Functions in Solid Mechanics. CISM course no. 292. Wien, New York: Springer, 1987.

[7] Ball JM. Convexity conditions and existence theorems in non-linear elasticity. Arch Rational Mech Anal. Heidelberg: Springer, 1977;63:337–403.

[8] Ball JM. Constitutive inequalities and existence theorems in nonlinear elastostatics. In: Symposium on Non-well Posed Problems and Logarithmic Convexity. Lecture notes in math. London: Pitman, 1977, pp. 187–1241.

[9] Marsden JE, Hughes JR. Mathematical foundations of elasticity. New York: Dover Publications, 1983.

[10] Ciarlet PG. Mathematical elasticity, Vol 1: three dimensional elasticity. North-Holland: Elsevier Science Publishers B.V., 1988.

[11] Schröder J, Neff P, Balzani D. A variational approach for materially stable anisotropic hyperelasticity. Int J Solids Struct 2004, in press.

[12] Schröder J, Neff P. Invariant formulation of hyperelastic transverse isotropy based on polyconvex free energy functions. Int J Solids Struct 2003;40:401–445.

[13] Lemaitre J, Chaboche JL. Mechanics of solid materials. Cambridge: Cambridge University Press, 1990.