

4 Constitutive Equations

The kinematic equations introduced in Chapter 2 are essential to describe motion and deformation of a body, whereas the local balance equations of Chapter 3 are the differential equations that determine the time evolution of the wanted fields. Altogether they are not yet a closed set of equations, since they do not distinguish one material from another. In addition, constitutive laws¹ are required which should in appropriate form specify the material behavior as a function of strain and stress state. Here we make no attempt to review the huge body of constitutive theories available in continuum mechanics but restrict ourself to some essential equations; for more details see [Ber05, Hol00, MS04, Ogd97] and others. In this chapter we will summarize the general prerequisites for constitutive equations and we will introduce some elastic material models.

4.1 Elasticity

Let us consider an infinitesimal material neighborhood undergoing a deformation along a path Γ . The deformation is defined by a deformation gradient $\mathbf{F} : [t_1, t_2] \rightarrow \text{GL}^+(3, \mathbb{R})$. Then, the work of deformation associated with this path is

$$W = \int_{t_1}^{t_2} \mathbf{P}(t) \cdot \mathbf{F}(t) dt. \quad (4.1)$$

A material is said to be an **elastic material** if the work of deformation is path independent. Consequently holds

$$\int_{\Gamma'} P_{iJ} dF_{iJ} = \int_{\Gamma''} P_{iJ} dF_{iJ}$$

for all paths of deformation $\Gamma', \Gamma'' \in \text{GL}^+(3, \mathbb{R})$ defined by functions $\mathbf{F}', \mathbf{F}'' : [t_1, t_2] \rightarrow \text{GL}^+(3, \mathbb{R})$ such that $\mathbf{F}'(t_1) = \mathbf{F}''(t_1)$ and $\mathbf{F}'(t_2) = \mathbf{F}''(t_2)$. For all closed paths of deformation the work of deformation is zero.

¹which are not given by law but are assumptions basing on observation and generalization

4.1.1 Variational form

The definition of elasticity implies that for any deformation path Γ starting at a fixed reference placement and terminating at \mathbf{F} the **strain energy density** W is of the form

$$W(\mathbf{F}) = \int_{\Gamma} \mathbf{P} \, d\mathbf{F}. \quad (4.2)$$

Clearly, the elastic strain energy density is a function of the deformation only. In addition we know the gradient, i.e., the work conjugate stress tensor

$$P_{iJ}(\mathbf{F}) = \frac{\partial W}{\partial F_{iJ}}(\mathbf{F}). \quad (4.3)$$

The strain energy density acts as a potential for the stress tensor. Relation (4.3) is, therefore, the general *variational form* of elastic **constitutive laws**. Elastic materials with variational constitutive relations like (4.3) are also called **hyperelastic** materials.

In contrast to that, models with an *ad hoc* formulation of the elastic constitutive law are called **hypoelastic** materials. The hypoelastic constitutive relation is formulated in rate form, i.e., the stress rate is defined. In original hypoelastic theory [TN65], the stress rate is a function of the rate of deformation tensor (2.47) and additional contributions, e.g., the stress itself $f(d_{kl}, \sigma_{ij}, \dots)$. However, such constitutive relations (which are not elastic in the sense of the above definition) are not employed in modern constitutive theories. Instead, the name hypoelastic mostly refers to a rate formulation of the elastic law, e.g.,

$$\hat{\boldsymbol{\sigma}}(\mathbf{F}) = {}^{<4>} \mathbb{C}(\mathbf{F}) \, d(\mathbf{F}), \quad (4.4)$$

where $\hat{\boldsymbol{\sigma}}$ denotes a physical meaningful (objective) time derivative of the Cauchy stress tensor. The components of the stiffness tensor ${}^{<4>} \mathbb{C}(\mathbf{F})$ are expressions of the elastic constants which in turn depend on the actual definition of the stress rate (and thus on the deformation). Because of the properties of the rate of deformation tensor (cf. Section 2.5) hypoelastic constitutive laws do not strictly reflect the path independence of elasticity. Moreover, the derivation of objective rates of stress tensors and the corresponding stiffness tensors is not trivial, see, e.g. [Ber05].

From the theoretical point of view there is no reason to work with hypoelastic constitutive relations. However, the majority of commercial finite element programs still applies constitutive relations like (4.4). For that reason we mention this approach here. In the remaining of this text we speak about elasticity meaning the constitutive equations in its variational form (4.2–4.3).

4.1.2 Internal energy, stresses and elasticity tensor

The of a strain-energy function $W(\mathbf{F})$ of an elastic material corresponds to the Helmholtz free energy density introduced in Chapter 3. To be more precise, inserting (4.3) into the mechanical energy balance equation (3.33) gives the identity

$$U = W(\mathbf{F}) = A(\mathbf{F}), \quad (4.5)$$

which states that the internal energy density of an elastic body coincides (up to an inconsequential additive constant) with the strain energy density.

From the definition of elasticity it follows that a material is elastic if and only if for all closed paths of deformation the rate of free energy vanishes, i.e., if the deformation of the material does not entail dissipation or hysteresis. This yields to the definition of elasticity in terms of continuum thermodynamics where a material is said to be elastic if it produces *no entropy*. The second law of thermodynamics degenerates to an equation. Following a strategy known as Coleman-Noll procedure we expand the Clausius-Planck inequality (3.44) to write

$$\mathbf{P} \cdot \dot{\mathbf{F}} - \dot{A} = \left(\mathbf{P} - \frac{\partial \dot{A}}{\partial \dot{\mathbf{F}}} \right) \cdot \dot{\mathbf{F}} = 0. \quad (4.6)$$

Only if the term in brackets vanishes equation (4.6) holds for every rate of deformation. In consequence, this relates the stresses to the energy function as in the constitutive relation (4.3).

In order to obtain numerical solutions of nonlinear finite-deformation problems the linearized stress state is of central importance. Therefore we proceed expressing relation (4.3) in incremental form. This can be accomplished in a number of mathematically equivalent ways. For instance, taking differentials of (4.3) gives

$$dP_{iJ} = C_{iJkL}(\mathbf{F}) dF_{kL}, \quad (4.7)$$

where $C_{iJkL}(\mathbf{F})$ are the *Lagrangian elastic moduli*. The elastic moduli are the components of the fourth-order **elasticity tensor** $\overset{<4>}{\mathbb{C}}$ in material description

$$\overset{<4>}{\mathbb{C}} = C_{iJkL} \mathbf{e}_i \otimes \mathbf{e}_J \otimes \mathbf{e}_k \otimes \mathbf{e}_L \quad \text{with} \quad C_{iJkL}(\mathbf{F}) = \frac{\partial^2 W}{\partial F_{iJ} \partial F_{kL}}(\mathbf{F}). \quad (4.8)$$

The elasticity tensor is always symmetric in its first and second and in its third and fourth index. This symmetry is known as *minor symmetry*,

$$C_{iJkL} = C_{JikL} = C_{iJLk} = C_{JiLk}. \quad (4.9)$$

If derived from a scalar-valued energy function as presumed here by (4.8), the tensor $\langle^4\rangle\mathbb{C}$ also possesses *major symmetry*, i.e., it is symmetric in the sense

$$C_{iJkL} = C_{kLJi} \quad \Leftrightarrow \quad \langle^4\rangle\mathbb{C} = \langle^4\rangle\mathbb{C}^\top. \quad (4.10)$$

A standard exercise shows that a fourth-order tensor with major and minor symmetry has only 21 independent components.

4.2 General requirements on the strain-energy function

Throughout this text we focus for simplicity on homogeneous (or homogenized) materials. A material is said to be **homogeneous** when the distribution of the internal structure is such, that every material point has the same mechanical behavior. On the other hand, in a **heterogeneous** material the strain-energy function will additionally depend on the position of the material point in the reference placement \mathbf{X} . (A common approach to simplify that situation is to homogenize the material by “averaging” over the internal structure, see Chapter ??.)

Hence, the strain-energy density is a postulated scalar-valued function of one tensorial variable, namely the deformation gradient \mathbf{F} . For convenience we require this function to vanish in the reference placement where $\mathbf{F} = \mathbf{I}$, i.e., the reference placement is stress free. From physical observations we conclude that the strain energy increases monotonically with the deformation,

$$W(\mathbf{I}) = 0 \quad \text{and} \quad W(\mathbf{F}) \geq 0. \quad (4.11)$$

The strain energy function attains its global minimum for $\mathbf{F} = \mathbf{I}$ at the stress free state.

Moreover, let us require that an infinite amount of energy is necessary to expand a body infinitely and to compress a body to zero volume, respectively.

$$W(\mathbf{F}) \rightarrow \infty \quad \text{as} \quad \det \mathbf{F} \rightarrow \infty \quad (4.12)$$

$$W(\mathbf{F}) \rightarrow \infty \quad \text{as} \quad \det \mathbf{F} \rightarrow 0. \quad (4.13)$$

The strain-energy density $W(\mathbf{F})$ and the resulting constitutive equation must, of course, fulfil some requirements which arise from mathematical theory as well as from the physical nature of the material under consideration.

4.2.1 Polyconvexity

From a mathematical prospective the fundamental issue is to guarantee the existence of (unique) solutions for a given constitutive model. Local existence and uniqueness theorems in nonlinear elastostatics and elastodynamics are based on **ellipticity**. The ellipticity condition states that an energy function $W(\mathbf{F})$ leads to an elliptic system if and only if the well known Legendre-Hadamard condition holds,

$$\frac{\partial^2 W}{\partial \mathbf{F} \partial \mathbf{F}}(\mathbf{F}) \geq 0 \quad (4.14)$$

for all $\mathbf{F}(\mathbf{X}) \in \text{GL}^+(3, \mathbb{R})$, $\mathbf{X} \in \mathbb{R}^3$. If the inequality holds we say that W is strongly elliptic or uniform rank-1 convex.

Originally, global existence theory for elastic problems was based on **convexity** of the free energy function. A scalar function is said to be convex if, for all $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^3$, holds

$$\phi(\lambda \mathbf{x}_1 + (1 - \lambda) \mathbf{x}_2) \leq \lambda \phi(\mathbf{x}_1) + (1 - \lambda) \phi(\mathbf{x}_2) \quad \lambda \in (0, 1). \quad (4.15)$$

However, from a physical point of view that condition may be too strong. As pointed out by Ball [Bal77], convexity precludes some special but eminent physical phenomena as, e.g., buckling or wrinkling of structures. This leads to the important concept of **quasiconvexity**, introduced by Morrey in [Mor52]. On a fixed domain Ω a function W is quasiconvex if

$$\int_{\Omega} (W(\mathbf{F} + \text{grad } \mathbf{u})) dx \geq \int_{\Omega} W(\mathbf{F}) dx \quad \forall \mathbf{F} \in \text{GL}^+(3, \mathbb{R}), \mathbf{u} \in C_0^\infty. \quad (4.16)$$

Morrey showed that (under suitable growth conditions) quasiconvexity is a necessary and sufficient condition for a functional to be weakly lower semi-continuous, i.e., $W(\mathbf{F}) \geq \alpha$. Thus, quasiconvexity is closely related to the existence of minimizers of an energy function.

Unfortunately, condition (4.16) is a global one and, therefore, complicated to handle. A concept of greater practical importance is that of **polyconvexity**. Following Marsden and Hughes [MH83], we define an energy function $W(\mathbf{F})$ to be polyconvex if and only if there exists a function ϕ which is convex and has arguments \mathbf{F} , $\text{cof}(\mathbf{F})$ and $\det(\mathbf{F})$, such that

$$W(\mathbf{F}) = \phi(\mathbf{F}, \text{cof}(\mathbf{F}), \det(\mathbf{F})). \quad (4.17)$$

The polyconvexity condition has an additive nature, i.e., if the functions ϕ_i are all convex in their respective arguments then the function $W(\mathbf{F}) = \phi_1(\mathbf{F}) + \phi_2(\text{cof}(\mathbf{F})) + \phi_3(\det \mathbf{F})$

is polyconvex. This property turns out to be very useful to establish constitutive models because it permits to construct energy functions out of simpler ones.

Finally, as shown in [MH83], the following implication chain relates all introduced concepts

$$\text{convexity} \Rightarrow \text{polyconvexity} \Rightarrow \text{quasiconvexity} \Rightarrow \text{rank-1-convexity (ellipticity)} .$$

For homogenous and isotropic elastic materials we commonly require the strain energy function to be a convex potential. However, non-convex energy functions are encountered in many applications such as phase transitions in shape memory alloys [Bha03, RC05], in phase field theory (see Section ??) and, in particular, in dissipative materials under finite deformations. Non-convex potentials govern the microstructural development of a priori heterogeneous materials (such as textured materials or single crystals, [CJM02, JM02, ME99]) as well as deformation phase decompositions in initially homogeneous materials.

Material instability phenomena can be interpreted as deformation microstructures, they are also associated with non-convex potentials. Such microstructures may be resolved by relaxation techniques based on a convexification of the (incremental) potential, whereby the relaxed problem then allows for a well-posed numerical analysis. For a concise mathematical background of the subject see [Dac89, Mül96], mathematical treatments in the continuum mechanical context can be found in [BCHH05, CKA02, Car05] and applications to special problems of metal plasticity and biological tissues are reported, e.g., in [C.03, CM03, KFR05] and [BSGN05, BNSH05, SN03], respectively.

4.2.2 Objectivity and material frame indifference

It is obvious to claim that the deformation and consequently the strain energy density of a material point must not depend on the position of the observer who records the motion. In other words, two observers located at different positions in space should see at one instance an identical response of the material point. This requirement is called **observer invariance** or **objectivity**. If a physical quantity depends on the position of the observer than a change of observer, or, in mathematical terms, an action of a Euclidean group, induces a transformation of motion φ into $\hat{\varphi}$. The second observer records the motion as being shifted by a vector $\mathbf{c}(t)$ and rotated by a finite rotation $\mathbf{Q} \in \text{SO}(3)$, i.e.,

$$\begin{aligned} \mathbf{x} &= \varphi(\mathbf{X}, t) \\ \Rightarrow \quad \mathbf{Q}(t) \varphi(\mathbf{X}, t) + \mathbf{c}(t) &= \hat{\varphi}(\mathbf{X}, t) = \mathbf{Q}(t) \mathbf{x} + \mathbf{c}(t), \end{aligned} \tag{4.18}$$

where we assume the initial placement to be observer independent.

Closely related to observer invariance is the expectation that the energy of a deformed elastic body remains unchanged when a rigid-body motion is superposed on an existing deformation. This requirement leads to the **principle of material-frame indifference**. Material-frame indifference is a somewhat questionable requirement because in some — rare — cases it might be physical meaningful that material properties change with, e.g., superposed fast rotations. The validity of this principle, its physical interpretation and the fundamental differences of the principles of objectivity and of material-frame indifference are subject of extensive discussions in theoretical literature, see, e.g., [BS99, BS01, Mus98]. We consider here only traditional, acceleration-independent solid materials. In this case both, the agreement among observers about the perceived material response, i.e., objectivity, and the invariance of material response to superposed rigid body motions, i.e., material-frame indifference, coincide de facto. For more theoretical details we refer to the cited literature.

With (4.18) we can now derive the action of an Euclidean group on other kinematic quantities, primarily on the deformation gradient $\mathbf{F}(\mathbf{X}, t)$,

$$\hat{\mathbf{F}} = \frac{\partial \hat{\varphi}}{\partial \mathbf{X}} = \frac{\partial \hat{\varphi}}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \mathbf{Q}\mathbf{F}. \quad (4.19)$$

With the polar decomposition (2.23) and (2.27) follows immediately

$$\hat{\mathbf{U}} = \mathbf{U} \quad (4.20)$$

$$\hat{\mathbf{R}} = \mathbf{Q}\mathbf{R} \quad (4.21)$$

$$\hat{\mathbf{V}} = \mathbf{Q}\mathbf{V}\mathbf{Q}^\top. \quad (4.22)$$

By presuming the strain-energy density being solely a function of the deformation gradient, invariance upon translation is ensured. This leads to the following definition: An elastic material is said to be **objective** (and material frame indifferent) if its strain-energy density is invariant upon rotations. It holds for $\mathbf{Q} \in \text{SO}(3)$

$$W(\mathbf{Q}\mathbf{F}) = W(\mathbf{F}) \quad (4.23)$$

for all $\mathbf{F} \in \text{GL}^+(3, \mathbb{R})$. A strain-energy density function is objective if and only if it can be expressed as a function of the right Cauchy-Green tensor $\mathbf{C} = \mathbf{F}^\top \mathbf{F} = \mathbf{U}^2$, equation (2.36). It is clear from (4.19) and (4.20) that a function of the form $W(\mathbf{U}^2) = W(\mathbf{C})$ is objective. To prove the necessity condition, assume, conversely, that $W(\mathbf{F})$ is objective. Let $\mathbf{F} = \mathbf{R}\mathbf{U}$ be the polar decomposition of \mathbf{F} and $\mathbf{Q} \equiv \mathbf{R}^{-1}$. Then, by definition (4.23) is

$$\begin{aligned} W(\mathbf{F}) &= W(\mathbf{R}^{-1}\mathbf{F}) \\ &= W(\mathbf{U}) = W(\mathbf{C}). \end{aligned} \quad (4.24)$$

By minor abuse of notation we write subsequently $W(\mathbf{F})$ and $\mathbf{P}(\mathbf{F})$ etc., meaning the corresponding function of argument $\mathbf{F}^\top \mathbf{F} = \mathbf{C}$.

Transformation rules for the stresses and the elastic moduli follow. Let $W(\mathbf{F})$ be objective and imagine perturbing it by an infinitesimal deformation $d\mathbf{F}$. Then definition (4.23) demands

$$W(\mathbf{Q}(\mathbf{F} + d\mathbf{F})) = W(\mathbf{F} + d\mathbf{F}). \quad (4.25)$$

Expand this expression to employ the definition of the stresses (4.3).

$$W(\mathbf{Q}\mathbf{F}) + \frac{\partial W}{\partial F_{iJ}}(\mathbf{Q}\mathbf{F}) Q_{ij} dF_{jJ} = W(\mathbf{F}) + \frac{\partial W}{\partial F_{iJ}}(\mathbf{F}) dF_{iJ}$$

By virtue of (4.23) and with (4.3) this identity reduces to

$$P_{iJ}(\mathbf{Q}\mathbf{F}) Q_{ij} dF_{jJ} = P_{jJ}(\mathbf{F}) dF_{iJ}. \quad (4.26)$$

Because $d\mathbf{F}$ is arbitrary we conclude that

$$Q_{ij} P_{iJ}(\mathbf{Q}\mathbf{F}) = P_{jJ}(\mathbf{F}), \quad (4.27)$$

or, taking \mathbf{Q} to the right-hand side of this equation

$$\mathbf{P}(\mathbf{Q}\mathbf{F}) = \mathbf{Q}\mathbf{P}(\mathbf{F}) \quad \forall \mathbf{Q} \in \text{SO}(3). \quad (4.28)$$

To establish the transformation rule for the elastic moduli we start with equation (4.28) and imagine perturbing it by an infinitesimal deformation $d\mathbf{F}$. By objectivity of the stress tensor holds

$$P_{iJ}(\mathbf{Q}(\mathbf{F} + d\mathbf{F})) = Q_{ij} P_{jJ}(\mathbf{F} + d\mathbf{F}). \quad (4.29)$$

Expanding this expression gives

$$P_{iJ}(\mathbf{Q}\mathbf{F}) + \frac{\partial^2 W}{\partial F_{iJ} \partial F_{kL}}(\mathbf{Q}\mathbf{F}) Q_{kl} dF_{lL} = Q_{ij} P_{jJ}(\mathbf{F}) + Q_{ij} \frac{\partial^2 W}{\partial F_{jJ} \partial F_{kL}}(\mathbf{F}) dF_{kL}.$$

By the presumed objectivity of stress tensor and by the definition of the tangent moduli (4.8) this identity reduces to

$$C_{iJkL}(\mathbf{Q}\mathbf{F}) Q_{kl} dF_{lL} = Q_{ij} C_{jJkL}(\mathbf{F}) dF_{kL}. \quad (4.30)$$

Again, $d\mathbf{F}$ is arbitrary, and we conclude for the tangential moduli

$$C_{iJkL}(\mathbf{Q}\mathbf{F}) = Q_{ij} Q_{kl} C_{jJlL}(\mathbf{F}). \quad (4.31)$$

4.2.3 Material symmetry

Further constraints to the form of the strain-energy density function arise from material symmetry. If the material response in some preferred directions is identical, the strain-energy function is expected to reflect that property. A finite rotation $\mathbf{Q} \in \text{SO}(3)$ is said to be a material **symmetry transformation** of a solid elastic material if for all $\mathbf{F} \in \text{GL}^+(3, \mathbb{R})$ holds

$$W(\mathbf{F}\mathbf{Q}) = W(\mathbf{F}). \quad (4.32)$$

In general, not all finite rotations $\mathbf{Q} \in \text{SO}(3)$ are symmetry transformations. Nonetheless the set of all symmetry transformations of a material defines a subgroup $S \subset \text{SO}(3)$. To prove this consider a rotation $\mathbf{Q}_1 \in S$. Then, by (4.32),

$$W(\mathbf{F}\mathbf{Q}_1^{-1}) = W((\mathbf{F}\mathbf{Q}_1^{-1})\mathbf{Q}_1) = W(\mathbf{F}), \quad (4.33)$$

and, hence, $\mathbf{Q}_1^{-1} \in S$. Now let $\mathbf{Q}_1, \mathbf{Q}_2 \in S$. By the same argument is

$$W(\mathbf{F}(\mathbf{Q}_1\mathbf{Q}_2)) = W((\mathbf{F}\mathbf{Q}_1)\mathbf{Q}_2) = W(\mathbf{F}\mathbf{Q}_1) = W(\mathbf{F}), \quad (4.34)$$

and, $\mathbf{Q}_1\mathbf{Q}_2 \in S$. Consequently, S defines a group.

To deduce the **transformation rules** for the stresses and the elastic modulus we apply the same procedure as above. Let $\mathbf{Q} \in S$ be an arbitrary finite rotation, $\mathbf{F} \in \text{GL}^+(3, \mathbb{R})$ be a local deformation, and imagine perturbing it by an arbitrary infinitesimal deformation $d\mathbf{F}$. Then symmetry demands that

$$W((\mathbf{F} + d\mathbf{F})\mathbf{Q}) = W(\mathbf{F} + d\mathbf{F}). \quad (4.35)$$

Expand this expression to employ relation (4.3)

$$W(\mathbf{F}\mathbf{Q}) + \frac{\partial W}{\partial F_{iJ}}(\mathbf{F}\mathbf{Q})dF_{jI}Q_{IJ} = W(\mathbf{F}) + \frac{\partial W}{\partial F_{iJ}}(\mathbf{F})dF_{iJ}.$$

By symmetry of the material we get

$$P_{iJ}(\mathbf{F}\mathbf{Q})dF_{jJ}Q_{IJ} = P_{iJ}(\mathbf{F})dF_{iJ}, \quad (4.36)$$

and, because $d\mathbf{F}$ is arbitrary,

$$P_{iI}(\mathbf{F}\mathbf{Q})Q_{JI} = P_{iJ}(\mathbf{F}). \quad (4.37)$$

Equivalently we may write

$$\mathbf{P}(\mathbf{F}\mathbf{Q}) = \mathbf{P}(\mathbf{F})\mathbf{Q}. \quad (4.38)$$

Further, from the material symmetry of the stress tensor follows that

$$P_{iJ}((\mathbf{F} + d\mathbf{F})\mathbf{Q}) = P_{jI}(\mathbf{F} + d\mathbf{F})Q_{IJ}. \quad (4.39)$$

Expanding this expression, applying (4.38) and the definition of the elastic moduli (4.8) gives

$$\begin{aligned} P_{iJ}(\mathbf{F}\mathbf{Q}) + \frac{\partial^2 W}{\partial F_{iJ} \partial F_{kL}}(\mathbf{F}\mathbf{Q}) dF_{kK} Q_{KL} &= P_{iI}(\mathbf{F})Q_{IJ} + \frac{\partial^2 W}{\partial F_{iI} \partial F_{kL}}(\mathbf{F}) dF_{kL} Q_{IJ} \\ C_{iJkL}(\mathbf{F}\mathbf{Q}) dF_{kK} Q_{KL} &= C_{iIkL}(\mathbf{F}) dF_{kL} Q_{IJ}, \end{aligned} \quad (4.40)$$

and, we conclude

$$C_{iJkL}(\mathbf{F}\mathbf{Q})Q_{LK} = C_{iIkL}(\mathbf{F})Q_{IJ} \quad (4.41)$$

$$\Leftrightarrow C_{iJkL}(\mathbf{F}\mathbf{Q}) = C_{iIkK}(\mathbf{F})Q_{IJ}Q_{KL}. \quad (4.42)$$

For the strain-energy function of materials with symmetry exists representation theorems. These theorems (which state that a scalar function of any number of tensor invariants under a symmetry group can be expressed as a function of a finite number of scalar invariants, none of which is expressible as a function of the remaining ones) are fundamental for the definition of the strain-energy function.

4.3 Isotropy

A special but very important class of materials are isotropic materials. From the physical point of view isotropic materials are materials without any preferred direction. In terms of material symmetry an elastic material is said to be isotropic if its symmetry group $S \equiv \text{SO}(3)$. It is said to be anisotropic otherwise.

For isotropic materials the strain-energy function can be represented as a function of the invariants of the right Cauchy-Green tensor

$$W(\mathbf{C}) = W(I_1^C, I_2^C, I_3^C) \quad (4.43)$$

with (see also Appendix ??)

$$\begin{aligned} I_1^C &= \text{tr}(\mathbf{C}) \\ I_2^C &= \frac{1}{2}(\text{tr}(\mathbf{C}^2) - \text{tr}(\mathbf{C})^2) \\ I_3^C &= \det(\mathbf{C}). \end{aligned} \quad (4.44)$$

Note that this representation follows from the strain-energy function being invariant upon rotations and, thus, equation (4.43) may equivalently be written in terms of the invariants of the left Cauchy-Green tensor $W(\mathbf{b}) = W(I_1^b, I_2^b, I_3^b)$ or its related strain measures.

With similar arguments the strain-energy function of an isotropic material can be expressed as a function of the eigenvalues of the right Cauchy-Green tensor.

$$W(\mathbf{C}) = W(\lambda_1^2, \lambda_2^2, \lambda_3^2) \quad (4.45)$$

Here we made use of the fact that the eigenvalues of tensor \mathbf{C} , λ_α^2 , $\alpha = 1, 2, 3$, are the squares of the eigenvalues of tensor \mathbf{U} , λ_α . Moreover, in isotropic materials the principal directions of stress tensor and work conjugate deformation tensor coincide.

In order to express the constitutive relation in terms of strain invariants we exploit the fact, that the stress-strain relation is given by an isotropic tensor function,

$$\mathbf{Q}W(\mathbf{C})\mathbf{Q}^\top = W(\mathbf{Q}\mathbf{C}\mathbf{Q}^\top), \quad (4.46)$$

which can easily be derived from equations (4.22), (4.28) and (4.38) and is not restricted to isotropic materials. An isotropic tensor function $W(\mathbf{C})$ can explicitly be represented as

$$\frac{\partial W(\mathbf{C})}{\partial \mathbf{C}} = \alpha_1 \mathbf{I} + \alpha_2 \mathbf{C} + \alpha_3 \mathbf{C}^2, \quad (4.47)$$

where the α_i , are scalar coefficients (so-called response coefficients), which may be evaluated for each material law in terms of tensor \mathbf{C} , $\alpha_i = \alpha_i(I_1^b, I_2^b, I_3^b)$. Equation (4.47) is known as **Richter representation** or first representation theorem for isotropic tensor functions. By some algebra (see, e.g., [Gur81, Mal69]) it can alternatively be formulated as

$$\frac{\partial W(\mathbf{C})}{\partial \mathbf{C}} = \hat{\alpha}_0 \mathbf{I} + \hat{\alpha}_1 \mathbf{C} + \hat{\alpha}_2 \mathbf{C}^{-1}, \quad (4.48)$$

which is known as the **alternative Richter representation** or second representation theorem for isotropic tensor functions. The fundamental message of these theorems is that the stress response on the straining of an isotropic material is uniquely determined by only three parameters.

4.4 Elastic material models

The stress-strain relation of an elastic material follows by equation (4.3) from a strain-energy potential, which, of course, should map the physical properties for every specific

material under consideration. Consequently there exists a huge number of strain-energy functions and corresponding constitutive theories. The aim of this section is to summarize some well established and frequently employed models for reference.

4.4.1 Linear elastic materials

In linear elasticity the constitutive relation is given by **Hook's law**. The linearized or incremental strain tensor $\boldsymbol{\epsilon}$ (2.42) and the corresponding stresses $\boldsymbol{\sigma}$ are related via the linear equation

$$\boldsymbol{\sigma} = \text{<sup>4>} \mathbb{C} \boldsymbol{\epsilon}. \quad (4.49)$$

The elasticity tensor $\text{<sup>4>} \mathbb{C}$ is a function of Young's modulus E and Poisson number ν or of the Lamè constants μ and λ , respectively. For isotropic material the moduli are related by:

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \quad \mu = \frac{E}{2(1+\nu)}. \quad (4.50)$$

The material parameters are presumed to depend on temperature but not on the deformation. Then, the corresponding (isothermal) strain-energy density may be written as

$$W(\boldsymbol{\epsilon}) = \frac{\lambda}{2} (\text{tr} \boldsymbol{\epsilon})^2 + \mu \text{tr} \boldsymbol{\epsilon}^2, \quad (4.51)$$

where $\text{tr}(\cdot)$ denotes the trace of a tensor. The stress-strain relation (4.49) gets with (4.3) the well known form

$$\boldsymbol{\sigma} = \lambda \text{tr} \boldsymbol{\epsilon} \mathbf{I} + 2\mu \boldsymbol{\epsilon}. \quad (4.52)$$

With bulk modulus κ ,

$$\kappa = \frac{E}{3(1-2\nu)} = \lambda + \frac{2}{3} \mu, \quad (4.53)$$

equation (4.51) can alternatively be formulated as

$$W(\boldsymbol{\epsilon}) = \frac{1}{2} \kappa (\text{tr} \boldsymbol{\epsilon})^2 + \mu \|\boldsymbol{\epsilon}\|^2. \quad (4.54)$$

Here $\|\cdot\|$ defines the deviatoric norm of a strain tensor by $\sqrt{\frac{2}{3} \text{dev}(\cdot) \cdot \text{dev}(\cdot)}$, see Appendix.

For later reference we formulate here a temperature dependent version of the elastic strain-energy density

$$W^e(\boldsymbol{\epsilon}, T) = \frac{\kappa}{2} (\text{tr} \boldsymbol{\epsilon} - 3\alpha(T - T_0))^2 + \varrho_0 c_v T \left(1 - \log \frac{T}{T_0}\right) + \mu \|\boldsymbol{\epsilon}\|^2, \quad (4.55)$$

where α is the thermal expansion coefficient, T_0 is a reference absolute temperature, ϱ_0 is the mass density per unit undeformed volume, and c_v is the specific heat per unit mass at constant volume (which is assumed to remain constant). The first term in (4.54) and (4.55) represents the volumetric part of the elastic energy density and implies the equation of state of the material. The corresponding pressure follows as

$$p(\boldsymbol{\epsilon}, T) = \kappa (\text{tr} \boldsymbol{\epsilon} - 3\alpha(T - T_0)). \quad (4.56)$$

As a matter of course, the linear elastic constitutive theory has major limitations. It can only be used to model small deformations, because it is based on the linearized deformation measure (2.42) and, even if the strains are small, it can only model a linear stress-strain behavior. For many practical purposes these restrictions are of no concern. Most engineering materials show elastic behavior for modest strains and the stresses are observed to be proportional to the strains in this range. In this text, however, we focus on large deformations. The easiest way to extend the linear elastic material behavior to finite kinematics is by simply replacing the infinitesimal strain $\boldsymbol{\epsilon}$ in (4.51) by the Green-Lagrange strain tensor \mathbf{E} . The result is known as the **Saint-Venant Kirchhoff** material

$$W(\mathbf{E}) = \frac{\lambda}{2} (\text{tr}(\mathbf{E}))^2 + \mu \text{tr} \mathbf{E}^2 \quad (4.57)$$

where λ and μ are again the Lamè constants (4.50). With

$$\mathbf{S} = \frac{\partial W}{\partial \mathbf{E}} = 2 \frac{\partial W}{\partial \mathbf{C}} \quad (4.58)$$

follows the stress-strain relation for the second Piola-Kirchhoff stress tensor \mathbf{S} ,

$$\mathbf{S} = \lambda \mathbf{I} \text{tr} \mathbf{E} + 2\mu \mathbf{E}. \quad (4.59)$$

Unfortunately, the energy function (4.57) fails to be polyconvex. In particular, (4.57) does not give a reasonable limit in compression because as $\det \mathbf{F} \rightarrow 0$, i.e., $\mathbf{E} \rightarrow -\frac{1}{2}\mathbf{I}$, the stresses vanishes. Consequently, from the theoretical point of view, this constitutive relation should be avoided. (Nonetheless the Saint-Venant Kirchhoff model is very common, especially for metals where the range of elastic strains is relatively small.)

4.4.2 Rubbery and biological materials

More sophisticated elastic models are required for organic materials. Some of them exhibit a nonlinear stress-strain behavior even at modest strains. More importantly,

there is a wide range of polymers and also biological tissues which are elastic up to huge strains. These materials show complex (and very different) nonlinear stress-strain behaviors. Specific strain energy-functions are designed to account for these phenomena.

The typical example for a material undergoing large strains is natural rubber. Many polymers also show (above a critical temperature) a *rubbery* behavior – the response is elastic without much rate or history dependence. Polymers with a heavily cross-linked molecular structure (elastomers) are the most likely to behave like ideal rubber, but also soft biological tissue shows rubbery behavior. Besides being elastic, the following feature is typical of rubbery materials: the material strongly resists volume changes. The bulk modulus (4.53) is comparable to that of metals. On the other hand, rubbery material is very compliant in shear, the shear modulus μ is of orders of magnitudes smaller than the shear resistance of most metals. This observation motivates the modelling of rubbery materials as being incompressible, i.e., the volume remains constant during deformation, $\det \mathbf{F} = 1$.

To assure **incompressibility** of an elastic material the strain-energy function is postulated to be of the form

$$W^{isochor} = W(\mathbf{C}) + p (\det \mathbf{F} - 1) \quad (4.60)$$

where p plays the role of a Lagrangian multiplier. By equation (4.3) follows for the first Piola-Kirchhoff stress tensor the relation

$$\mathbf{P} = p \mathbf{F}^{-\top} + \frac{\partial W}{\partial \mathbf{F}} \quad (4.61)$$

and for the second Piola-Kirchhoff stresses and the Cauchy stresses

$$\mathbf{S} = p \mathbf{F}^{-1} \mathbf{F}^{-\top} + \mathbf{F}^{-1} \frac{\partial W}{\partial \mathbf{F}} = p \mathbf{C}^{-1} + 2 \frac{\partial W}{\partial \mathbf{C}} \quad (4.62)$$

$$\boldsymbol{\sigma} = p \mathbf{I} + \frac{\partial W}{\partial \mathbf{F}} \mathbf{F}^{\top} = p \mathbf{I} + \mathbf{F} \left(\frac{\partial W}{\partial \mathbf{F}} \right)^{\top}. \quad (4.63)$$

These relations illustrate that pressure p can not be determined from the materials response but only from additional equilibrium equations and boundary conditions.

To account later for both, volume preserving as well as volumetric deformations, we decompose the deformation gradient according to relation (2.22) into an isochoric (or deviatoric) part $\mathbf{F}^{isochor}$ and a volume related part $\mathbf{F}^{vol} = \sqrt[3]{\det(\mathbf{F})} \mathbf{I}$,

$$\mathbf{F} = \mathbf{F}^{isochor} \mathbf{F}^{vol} = J^{\frac{1}{3}} \mathbf{F}^{isochor}. \quad (4.64)$$

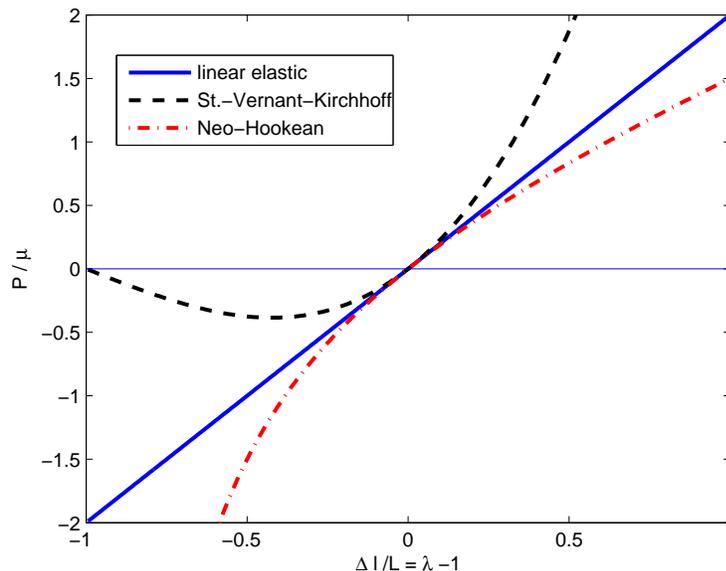


Figure 4.1: Stress-strain relations in uniaxial tension.

Let us now summarize the classical strain-energy functions for incompressible material $W(\mathbf{F}^{isochor})$ but omit the superscript *isochor* for simplicity. As before, I_i^C denotes the i -th principle invariant of the (isochoric part of) tensor \mathbf{C} , equation (4.44).

The simplest model is the **Neo-Hookean** solid,

$$W(\mathbf{C}) = \frac{\mu}{2}(I_1^C - 3). \quad (4.65)$$

First used by Treloar [Tre44], the parameter μ was originally determined from an elementary statistical mechanics treatments predicting that $\mu = \frac{N}{2}kT$, where N is the number of polymer chains per unit volume, k is the Boltzmann constant and T is the temperature. Today this model is widely used with shear modulus μ determined by experiments. The stress-strain relation follows from (4.61- 4.63).

In Figure 4.1 the stress-strain relations in uniaxial tension are displayed. The red dash-dotted line shows the Neo-Hookean model (4.65) whereas the black dashed line results from the Saint-Venant Kirchhoff model (4.59). In the undeformed placement the tangent on both curves is the straight line of the Hookean law (4.52). The limited validity of the Saint-Venant Kirchhoff model (4.59) is clearly visible. If $\Delta l/L < -0.4226$ an instability occurs, thence for rising compression a reduced stress is observed. Clearly, the model makes sense only for small compressive strains. (The critical strain value does not

depend on the material data.). On the other hand, the Neo-Hookean model captures the physics for the full range of straining. From experiments we know that for rubbery materials under moderate straining up to 30 - 70 % the Neo-Hookean model usually fits the material behavior with sufficient accuracy.

To model rubber at high strains the one-parametric Neo-Hookean model (4.65) is meanwhile replaced by a more sophisticated development of **Ogden** [R.W72, R.W82]. Instead of using strain invariants this model expresses the strain energy density in terms of principal stretches λ_α , $\alpha = 1, 2, 3$,

$$W = \sum_{p=1}^N \frac{\mu_p}{\alpha_p} (\lambda_1^{\alpha_p} + \lambda_2^{\alpha_p} + \lambda_3^{\alpha_p} - 3), \quad (4.66)$$

where N , μ_p and α_p are material constants. In general, the shear modulus results from

$$2\mu = \sum_{p=1}^N \mu_p \alpha_p. \quad (4.67)$$

The three principal values of the Cauchy stresses can be computed from (4.66) as

$$\sigma_\alpha = p + \lambda_\alpha \frac{\partial W}{\partial \lambda_\alpha} \quad \alpha = 1, 2, 3 \text{ (no summation)}, \quad (4.68)$$

and the principal first and second Piola-Kirchhoff stresses follow by

$$P_\alpha = \lambda_\alpha^{-1} \sigma_\alpha \quad \text{and} \quad S_\alpha = \lambda_\alpha^{-2} \sigma_\alpha. \quad (4.69)$$

With $N = 3$ and values summarized in Table 4.1 the Ogden material reaches an almost perfect agreement to the experimental data of Treloar. Therefore and because it is computational simple, equation (4.66) is *the* reference material law for natural rubber.

Neo-Hookean	$\alpha_1 = 2.0$	$\mu = 4.225 \cdot 10^5 \text{ N/m}^2$
Ogden	$\alpha_1 = 1.3$	$\mu_1 = 6.3 \cdot 10^5 \text{ N/m}^2$
	$\alpha_2 = 5.0$	$\mu_2 = 0.012 \cdot 10^5 \text{ N/m}^2$
	$\alpha_3 = -2.0$	$\mu_3 = -0.1 \cdot 10^5 \text{ N/m}^2$
Mooney-Rivlin	$\alpha_1 = 2.0$	$\mu_1 = 3.6969 \cdot 10^5 \text{ N/m}^2$
	$\alpha_2 = -2.0$	$\mu_2 = -0.5281 \cdot 10^5 \text{ N/m}^2$
Arruda-Boyce	$\lambda_{lock} = 3$	$\mu_0 = 3.380 \cdot 10^5 \text{ N/m}^2$
Blatz-Ko	$\nu = 0.45$	$\mu = 4.225 \cdot 10^5 \text{ N/m}^2$
St.Vernant-Kirchhoff	$\nu = 0.45$	$\mu = 4.225 \cdot 10^5 \text{ N/m}^2$

Table 4.1.: Material parameters.

For particular values of material constants, the Ogden model (4.66) will reduce to either the Neo-Hookean solid ($N = 1$, $\alpha = 2$) or the Mooney-Rivlin material. The **Mooney-Rivlin** material can be derived from (4.66) with $N = 2$ and $\alpha_1 = 2$, $\alpha_2 = -2$, or, in other form

$$W(\mathbf{C}) = \frac{\mu_1}{2}(I_1^C - 3) - \frac{\mu_2}{2}(I_2^C - 3), \quad (4.70)$$

together with equation (4.67). The Mooney-Rivlin material was originally also developed for rubber but is today often applied to model (incompressible) biological tissue, e.g. in [Mil00, Mil01, NBPT02].

In polymers or industrial rubbers the shear modulus μ usually depends on the deformation. Earlier as natural rubber these materials exhibit a rising resistance against straining. A physically inspired model for carbon filled rubber is the **Arruda-Boyce** model. It is also sometimes called the **8-chain model** because it was derived by idealizing a polymer as 8 elastic chains inside a box [AC93]. This constitutive law has a strain energy density given by

$$W(\mathbf{C}) = \mu_0 \sum_{p=1}^N \frac{c_p}{\lambda_{lock}^{2p-2}} ((I_1^C)^p - 3^p). \quad (4.71)$$

Here, μ_0 is the (initial) shear modulus, c_p are constants following from statistical theory, λ_{lock} and N are material constants of the underlying chain model, namely the limiting chain extensibility and the number of rigid links, (see [Hol00] for illuminating explanations). Evaluating the first three terms of expression (4.71) gives

$$W(\mathbf{C}) = \mu_0 \left(\frac{1}{2}(I_1^C - 3) + \frac{1}{20\lambda_{lock}^2} ((I_1^C)^2 - 9) + \frac{11}{1050\lambda_{lock}^4} ((I_1^C)^3 - 27) \right). \quad (4.72)$$

In the example below the limiting chain extensibility is set to $\lambda_{lock} = 3$ and the initial shear modulus is 80% of the Neo-Hookean shear modulus. The special feature of this model is a high strain resistance at strains $> 300\%$ (controlled by the choice of parameters). In other words, the model has the ability to reflect the dependence of the resulting shear modulus on the deformation.

Porous (or foamed) elastomers cannot be regarded as incompressible anymore. Blatz and Ko [BK62] proposed, basing on theoretical arguments and experimental data for polyurethane rubbers, a strain-energy density of the form

$$W(\mathbf{C}) = \frac{\mu}{2}(I_1^C - 3) - \frac{\mu}{2\beta}((I_3^C)^{-\beta} - 1), \quad (4.73)$$

where β is computed from shear modulus μ and Poisson number ν as $\beta = \frac{\nu}{1-2\nu}$. In the incompressible limit is $I_3^C = 1$ and equation (4.73) reduces to the Neo-Hookean

solid. Here the model is introduced because it is — either as Blatz-Ko model or as Neo-Hookean extended to the compressible range — applied for (porous) biological tissue, see e.g. [Fun93, Far99].

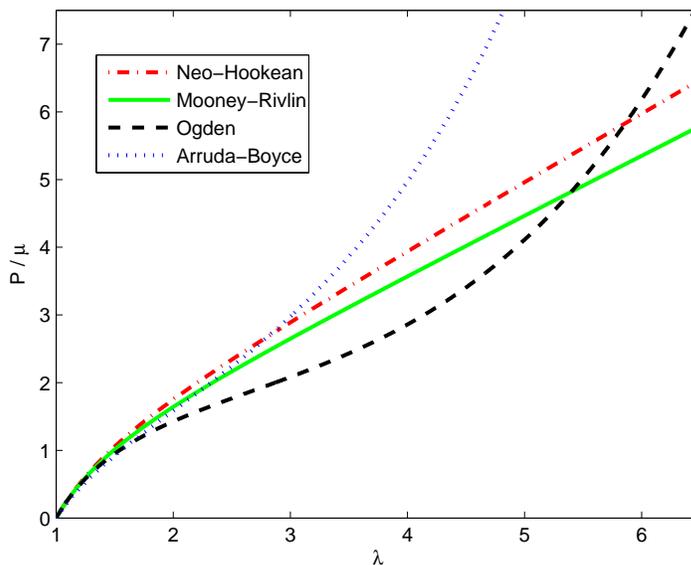


Figure 4.2: Constitutive relations for rubbery materials in uniaxial tension.

Exemplarily, let us now consider an **incompressible material under uniaxial tension** (cf. Chapter 2.6). In particular, let the stretch ratio $\lambda = l/l_0$ be given. Then we find after differentiation according to (4.68) the principal stresses

$$\sigma_\alpha = p + \sum_{p=1}^N \mu_p \lambda_p^{\alpha_p} \quad (4.74)$$

with values from Table 4.1 for Neo-Hookean, Mooney-Rivlin and Ogden material. Pressure p is determined from incompressibility and boundary condition $\sigma_2 = \sigma_3 = 0$. With (4.69) the constitutive equation reduces to a single equation of the form

$$P = \sum_{p=1}^N (\mu_p \lambda_p^{\alpha_p - 1} - \mu_p \lambda_p^{-\frac{1}{2}\alpha_p - 1}). \quad (4.75)$$

For the Arruda-Boyce model (4.71) we get by differentiation

$$P = \mu_0 \left(1 + \frac{1}{5\lambda_{lock}^2} \left(\lambda^2 + \frac{2}{\lambda} \right) + \frac{11}{175\lambda_{lock}^4} \left(\lambda^2 + \frac{2}{\lambda} \right)^2 \right) (\lambda_1 - \lambda_1^{-2}). \quad (4.76)$$

The Blatz and Ko model coincides in the incompressible case with the Neo-Hookean solid. Figure 4.2 shows the corresponding stress-strain curves for rubbery materials with material data from Table 4.1.

Above we introduced the classical strain-energy functions for incompressible materials. These isochoric functions may be extended to the **compressible range**, $J = \det \mathbf{F} \neq 1$, by replacing the kinematic constraint in (4.60) with a volumetric strain-energy function.

$$W(\mathbf{F}) = W(\mathbf{F}^{isochor}) + W(\mathbf{F}^{vol}) \quad (4.77)$$

The additive decomposition of the strain-energy density (4.77) is postulated for convenience; other formulations are possible but not necessarily superior. The easiest way to construct a volumetric addition of the strain energy density $W^{vol} \equiv W(\mathbf{F}^{vol}) = W(J)$ is by assuming a linear constitutive relation, and, consequently,

$$W^{vol}(J) = \frac{\kappa}{2}(J^2 - 1) = \frac{\kappa}{2}((I_3^C) - 1), \quad (4.78)$$

with bulk modulus κ according to (4.53). Unfortunately, such a simple extension (which is often applied, e.g., in commercial finite-element codes [Inc05]) fails to be polyconvex. In the limit $J \rightarrow 0$ the constitutive relation derived from (4.78) gives non-physical results (compare with the comments to the Saint-Venant-Kirchhoff material, Figure 4.1).

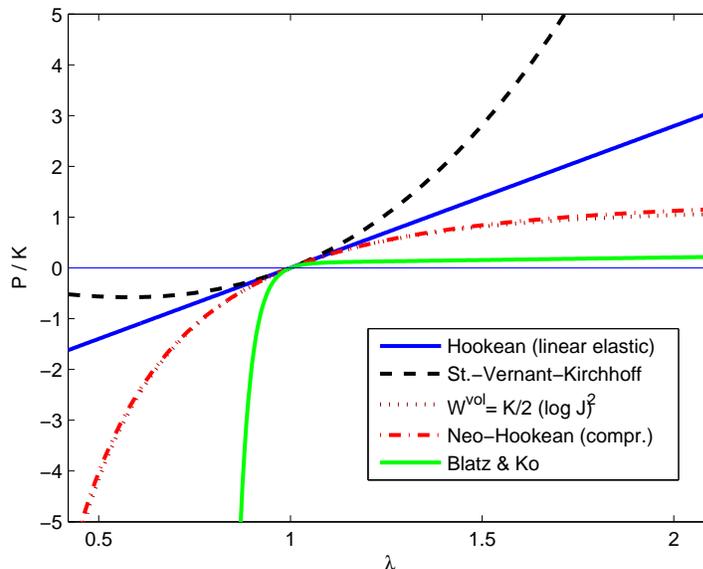


Figure 4.3: Volumetric constitutive models in pressure and hydrostatic tension.

A standard method to avoid this drawback is to introduce an (additional) logarithmic term of the Jacobian of deformation, e.g., $\kappa/2(\log J)^2$. The term vanishes for small strains, $J \approx 1$, but guarantees a realistic limit of $W^{vol} \rightarrow \infty$ for $J \rightarrow 0$.

Here we adopt for the volumetric strain-energy function a well known analytical expression of Simo and Miehe [SM92],

$$W^{vol}(J) = \frac{\kappa}{4}(J^2 - 1 - 2 \log J), \quad (4.79)$$

which was applied for biological tissue, e.g. by Pandolfi et al. [PM06]. Equation (4.79) together with (4.65) prescribe a standard form of the Neo-Hookean material extended to the compressible range. A detailed derivation of stress tensors and elastic tangent moduli can be found in [Hol00].

In Figure 4.3 the material parameter of Table 4.1 are applied to compare volumetric constitutive relations. For a hydrostatic pressure and tension test the principal first Piola-Kirchhoff stress divided by the bulk modulus κ is plotted versus the volumetric straining. For small compressions and expansions the curves are close to the linear elastic tangent but in the large strain range the different models diverge significantly.

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