Spatial representation of evolving anisotropy at large strains

Magnus Harrysson *, Anders Harrysson, Matti Ristinmaa

Division of Solid Mechanics, Lund University, Box 118, S-221 00 Lund, Sweden

Received 30 May 2006; received in revised form 22 September 2006; accepted 4 October 2006
Available online 11 October 2006

Abstract

A phenomenological model for evolving anisotropy at large strains is presented. The model is formulated using spatial quantities and the anisotropic properties of the material is modeled by including structural variables. Evolution of anisotropy is accounted for by introducing substructural deformation gradients which are linear maps similar to the usual deformation gradient. The evolution of the substructural deformation gradients is governed by the substructural plastic velocity gradients in a manner similar to that for the continuum. Certain topics related to the numerical implementation are discussed and a simple integration scheme for the local constitutive equations is developed. To demonstrate the capabilities of the model it is implemented into a finite element code. Two numerical examples are considered: deformation of uniform plate with circular hole and the drawing of a cup. In the two examples it is assumed that initial cubic material symmetry applies to both the elastic and plastic behavior. To be specific, a polyconvex Helmholtz free energy function together with a yield function of quadratic type is adopted.

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Keywords: Anisotropy; Spatial form; Finite strains

1. Introduction

Anisotropic materials are characterized by preferred directions representing the directional dependency of the material. The preferred directions can either be phenomenological in the sense that they may represent macroscopic properties or be directly related to the underlying physical properties, such as the fiber directions found in fiber-reinforced composites. The modeling of anisotropy is usually done by the introduction of tensor-valued quantities, that represent the preferred directions in the material. The introduction of these additional tensor quantities, here called structural tensors, within the framework of isotropic tensor functions was done in an attractive fashion by Spencer (1984) and Boehler (1987). An approach to model anisotropy was taken by Menzel and Steinmann (2001, 2003b), Ekh et al. (2003) and Johansson et al. (2005) where a fictitious configuration was utilized. This fictitious configuration contains a, in general, non-spherical energy metric...
which is connected to the metric of the intermediate configuration by a tangent map. This metric will then, in a fairly simple way, account for the description of somewhat restricted form of anisotropy.

Large inelastic deformations occur in many manufacturing processes. Since these deformations can be expected to lead to evolution of the directionally dependent properties of the material, being able to describe this phenomenon is of considerable importance. If one assumes that the directionally dependent properties are embedded into the substructure, the task becomes that of describing how the substructure evolves relative to the continuum. In one approach discussed extensively by e.g. Kratochvil (1971), Lorent (1983), Dafalias (1985, 1987, 1998) and Arravas (1992, 1994), a kinematic quantity called the plastic spin, representing the spinning of the substructure relative to the continuum is utilized. The establishment of evolution laws for the plastic spin was here derived from the representation theorem. More recently, evolution laws for the plastic spin was developed by e.g. van der Giessen (1991), Itskov and Aksel (2004) and Tsakmakis (2004) where thermodynamical considerations was taken. A second approach to describe the evolution of the substructure is to introduce evolution laws for the preferred directions directly, i.e. the structural tensors being regarded as internal variables and proper evolution laws are obtained by considering thermodynamical aspects, e.g. van der Giessen (1989), Imatani and Maugin (2002), Reese (2003) and Menzel and Steinmann (2003a).

A description of the kinematics of the substructure was investigated, in detail, by Harrysson and Ristinmaa (2006) where the evolution of the preferred directions was assumed to be guided by individual linear maps. These maps were introduced in a fashion similar to the deformation gradient, but acting on the substructure. By the introduction of the substructural deformation gradient, a quantity similar to the velocity gradient arises, but ones again acting on the substructure, in this respect cf. also van der Giessen (1989). In addition, when considering elasto-plasticity a multiplicative split of the substructural deformation gradient similar to the continuum was utilized. This allowed the continuum and the substructure to be described by evolution laws that were similar in structure. The evolution laws derived also revealed the coupling between the plastic spin and the use of evolution laws for the preferred directions. In Harrysson and Ristinmaa (2006) the theory was derived using the intermediate configuration.

In the present paper, a spatial form of elasto-plastic anisotropic material model at finite deformation, based on the framework of a multiplicative split of the deformation and the substructural deformation gradient as proposed by Harrysson and Ristinmaa (2006), is developed. This implies that to model anisotropic material behavior both Helmholtz’ free energy function and the yield function will be described using spatial quantities. It is shown that, in this spatial setting, the constitutive laws can be derived in a straightforward fashion from the thermodynamic framework. Since spatial quantities are used, the physical interpretation of the evolution laws is also more evident. In addition, the spatial formulation leads to a formulation suitable for numerical implementation.

The numerical implementation of the presented constitutive model into a finite element program is also investigated. As for a general anisotropic material the standard exponential integrator for the constitutive equations is not convenient to use, this due to the non-coaxiality of the stresses and their conjugated flow directions. Here, a fairly simple integration procedure for the local constitutive equations is developed. Moreover, to ensure quadratic convergence some issues related to the consistent tangent stiffness tensor are discussed.

Finally, two numerical examples are studied. Although the setting is of a general form, the numerical example will be restricted to investigate the behavior for single crystal aluminum showing cubic symmetry.

2. Preliminaries

First and second order tensors are denoted by bold-face Roman or Greek letters. The second order unit tensor is denoted by \( I \). The trace of a second order tensor is denoted by \( \text{tr}[\cdot] \). The deviatoric part is given by \( \text{dev}[\cdot] = [\cdot] - (1/3)\text{tr}[\cdot] I \). The inverse and the transpose of a second order tensor are denoted by \( [\cdot]^{-1} \) and \( [\cdot]^T \), respectively. The inner product is designated as \( A:B = \text{tr}[A^T B] \) and the tensor or dyadic product as \( \otimes \). The symmetric and the skew-symmetric part of a second order tensor is denoted by \( \text{sym}[\cdot] = \frac{1}{2} ([\cdot] + [\cdot]^T) \) and \( \text{skew}[\cdot] = \frac{1}{2} ([\cdot] - [\cdot]^T) \), respectively.
3. Kinematic description

Let $\Omega_0 \subset \mathbb{R}^3$ denote the region occupied by the body at time $t_0$ as the reference configuration and let the motion of the body be described by the non-linear map $\varphi : \Omega_0 \times T \rightarrow \Omega \subset \mathbb{R}^3$ where $T$ is the time interval and $\Omega$ defines the region occupied by the body at the current state. The linear mapping defined by the deformation gradient $F = \det X\varphi$ describes the local deformation of the body, where $X$ is the position vector in the reference configuration. To assure the uniqueness of the map it is assumed that $J = \det(F) > 0$. Time differentiation of the deformation gradient results in

$$\dot{F} = LF$$  \hspace{1cm} (1)$$

where $L$ is the spatial velocity gradient. This can be divided as

$$L = \text{sym}[L] + \text{skew}[L] = D + W$$  \hspace{1cm} (2)$$

where $D$ and $W$ are known as the rate of deformation tensor and the spin tensor, respectively. The deformation state of the body is described by the spatial Finger tensor, i.e.

$$b = FF^T$$  \hspace{1cm} (3)$$

When investigating anisotropic materials, quantities that represent the preferred directions, i.e. the substructure of the material, needs to be introduced. If large strains and anisotropy are taken into account, it is to be expected that evolution of the substructure will take place during deformation. To model the evolution taking place of the substructure it is assumed that

$$v^{(z)} = \Lambda^{(z)}v^{(z)}_0$$  \hspace{1cm} (4)$$

where $v^{(z)}_0$ and $v^{(z)}$ represent director vectors in the reference configuration and the current configuration, respectively. The superscript $(z)$ indicates there to be different preferred directions of the material. From (4) it is evident that each $\Lambda^{(z)}$ represents a linear map in the same sense as the deformation gradient does, but is related to the substructure instead of to the continuum.

To model the inelastic behavior of the material an intermediate configuration, $\bar{\Omega}$, is introduced. This can be viewed as a stress-free configuration which is obtained by releasing the elastic deformations from the current configuration. This results in the well-known multiplicative split of the deformation gradient

$$F = F^eF^p$$  \hspace{1cm} (5)$$

cf. Kröner (1960) and Lee (1969), where $F^e$ and $F^p$ denote the elastic deformation gradient and the plastic deformation gradient, respectively. Since (5) is only defined locally the intermediate configuration, defined by $F^p$, does not generally fulfill the compatibility requirements. The mappings are assumed to fulfill $J^e = \det(F^e) > 0$ and $J^p = \det(F^p) > 0$ such that the inverses $F^{e-1}$ and $F^{p-1}$ exist. Analogous to (1) the elastic, $L^e$, and the plastic, $l^p$, velocity gradients are defined as

$$\dot{F}^e = L^eF^e$$ and $$\dot{F}^p = l^pF^p$$  \hspace{1cm} (6)$$

respectively. Taking advantage of the above relations, time differentiation of (5) and comparison with (1) yields

$$L = L^e + F^eF^{e-1}$$  \hspace{1cm} (7)$$

From the above it is evident that $L^e$ is related to the current configuration whereas $l^p$ is related to the intermediate configuration. Moreover, similar to (5), adopting a multiplicative split for the substructure, cf. Harrysson and Ristinmaa (2006), results in the decomposition

$$\Lambda^{(z)} = \beta^{(z)}\alpha^{(z)}$$  \hspace{1cm} (8)$$

Here $\beta^{(z)}$ are related to the elastic deformation and $\alpha^{(z)}$ are assumed to evolve due to the plastic deformation, cf. Fig. 1. The multiplicative structure in (8) allows for the introduction of the elastic, $\Gamma^{(z)}$, and the plastic, $\Lambda^{(z)}$, velocity gradients operating on the substructure via
Proceeding in the same fashion for the substructure as for the continuum a time differentiation of (8) and taking advantage of (9) results in

$$\dot{\Delta}^{-1} = \Gamma^{(s)} + \beta^{(s)} \Lambda^{(s)} \beta^{(s)}$$  \hspace{1cm} (10)

In conclusion, $\Gamma^{(s)}$ are related to the current configuration and $\Lambda^{(s)}$ are quantities related to the intermediate configuration.

From the definition of the intermediate configuration it is clear that it is not uniquely defined, since an arbitrary rotation still leaves it stress free. It has been shown by Harrysson and Ristinmaa (2006) that the general format for the evolution laws in the intermediate configuration are given as

$$\dot{F}^p = F^p F^p, \hspace{0.5cm} F^p = F^p + \omega$$

$$\ddot{\psi}^{(s)} = \Lambda^{(s)} \dot{\psi}^{(s)}, \hspace{0.5cm} \Lambda^{(s)} = \dot{\Lambda}^{(s)} + \omega$$  \hspace{1cm} (11)

The second order tensor $\omega$ represents an additional spin term, one given by the choice of intermediate configuration $\Omega$. The objective quantities $F^p$ and $\Lambda^{(s)}$ need to be specified by constitutive assumptions.

As discussed in Harrysson and Ristinmaa (2006), several possible choices of the intermediate configuration exist. The most obvious choice is $\omega = 0$ which results in an invariant objective intermediate configuration, observe that this is not equivalent to the well-known isoclinic configuration. For the particular situation in which the triad $\psi^{(s)}$ coincides with $v_0^{(s)}$ the isoclinic configuration of Mandel (1971) is obtained, that is by assuming $\ddot{\psi}^{(s)} = 0$. Note that since a plastic spin of the continuum, skew($L^p$), in the intermediate configuration is generally present, plastic evolution of the preferred directions relative to the continuum occurs, cf. Harrysson and Ristinmaa (2006). Observe also the choice of isoclinic intermediate configuration puts restrictions on the evolution laws that can be used for the substructure. A third possible choice of the intermediate configuration is obtained via the choice $\omega = -\text{skew}(L^p)$, leaving $\dot{L} = \text{sym}(L^p)$, resulting in the so-called spin-less intermediate configuration, cf. Boyce et al. (1988) and Dafalias (1998). Note as well that the format (11) allows for the general format of multiple plastic spins introduced by Dafalias (1998) to be retrieved, cf. Harrysson and Ristinmaa (2006).

In the present work, the objective is to find a spatial formulation corresponding to (11), i.e. a push-forward to the current configuration. Observe that the evolution of the material directions requires some additional constitutive assumption regarding the elastic map for the director vectors. This is needed in order to introduce a connection between the substructure and the continuum. If the material only undergoes elastic deformation it is from a physical point of view expected that the substructure and the continuum deforms together in a convected sense. This constitutive assumption gives that

$$\beta^{(s)} = F^s$$  \hspace{1cm} (12)

The spatial format equivalent to (11) can be found by considering the elastic Finger tensor.
\[ b^e = F^e F^{eT} \]  \hspace{1cm} (13)

Time differentiation and taking advantage of (7) provides
\[ \dot{b}^e = L b^e + b^e L^T - (L^p b^e + b^e L^{pT}) \]  \hspace{1cm} (14)

where the spatial form of \( L^p \) has been introduced as
\[ L^p = F^p F^{e-1} = F^e (L^p_g + \omega) F^{e-1} \]  \hspace{1cm} (15)

For later use it is noted that \( L^p \) can be splitted in a manner similar to (2) as
\[ L^p = D^p + W^p, \quad D^p = \text{sym}(L^p) \quad \text{and} \quad W^p = \text{skew}(L^p) \]  \hspace{1cm} (16)

where the plastic rate of deformation tensor is defined by \( D^p \) and the plastic spin of the continuum by \( W^p \). Note that the arbitrary spin, \( \omega \), will not enter (14) since
\[ F^e \omega F^{e-1} b^e + b^e F^{e-1T} \omega = 0 \]  \hspace{1cm} (17)

Thus the choice of the intermediate configuration has no influence on the evolution of \( b^e \). From (12) it also follows that
\[ \dot{v}^{(a)} = \chi^{(a)} \psi^{(a)}; \quad \psi^{(a)} = F^e \tilde{v}^{(a)} \]  \hspace{1cm} (18)

Time differentiation of (18b), as well as taking advantage of the above relation and of (9) and (7), gives that
\[ \dot{v}^{(a)} = L v^{(a)} + (\dot{\lambda}^{(a)} - L^p) v^{(a)} \]  \hspace{1cm} (19)

where, in a manner similar to (15), the spatial form of \( \lambda^{(a)} \) has been introduced as
\[ \dot{\lambda}^{(a)} = F \lambda^{(a)} F^{e-1} = F (\Lambda^{(a)} + \omega) F^{e-1} \]  \hspace{1cm} (20)

Later on structural tensors defined as \( m^{(a)} = v^{(a)} \otimes v^{(a)} \), cf. Spencer (1984) and Boehler (1987), will enter the formulation, and consequently time differentiation of the structural tensors, \( m^{(a)} \), needs to be evaluated. From the definition of \( m^{(a)} \), together with (19), it follows that
\[ \dot{m}^{(a)} = L m^{(a)} + m^{(a)} L^T + (\dot{\lambda}^{(a)} - L^p) m^{(a)} + m^{(a)} (\dot{\lambda}^{(a)} - L^p)^T \]  \hspace{1cm} (21)

A glance at (14) and either (19) or (21) reveals that \( \omega \) is not present in the spatial setting. This is also to be expected from a physical point of view, since the choice of intermediate configuration should not affect the response of the material.

It turns out that the spatial setting of the evolution equations can be represented in the form of Lie derivatives. Accordingly, the spatial form equivalent to (11) is given by (14) and (19), i.e.
\[ \mathcal{L}_v (b^e) = -2 \text{sym}(L^p b^e) \]
\[ \mathcal{L}_v (v^{(a)}) = -(L^p - \dot{\lambda}^{(a)}) v^{(a)} \]  \hspace{1cm} (22)

and for the structural tensors
\[ \mathcal{L}_v (m^{(a)}) = -2 \text{sym}((L^p - \dot{\lambda}^{(a)}) m^{(a)}) \]  \hspace{1cm} (23)

where the definitions
\[ \mathcal{L}_v (b^e) = F \frac{\partial}{\partial t} (F^{-1} b^e F^{eT}) F^T \]
\[ \mathcal{L}_v (v^{(a)}) = F \frac{\partial}{\partial t} (F^{-1} v^{(a)}) \]  \hspace{1cm} (24)

have been used. It is interesting to observe that while performing the derivations with reference to the intermediate configuration it is important to specify a choice of the intermediate configuration. Whereas utilizing a description in the current configuration, a choice of intermediate configuration is not required.
4. Thermodynamic consideration

The second law of thermodynamics can be formulated in terms of the dissipation inequality, which for isothermal conditions can be formulated as

\[ \gamma = \tau : D - \rho_0 \dot{\psi} \geq 0 \]  

(25)

where the Kirchhoff stress tensor, \( \tau \) was introduced. Here \( \rho_0 \) represents the density in the reference configuration and \( \dot{\psi} \) is Helmholtz’ free energy per unit mass. For simplicity it will be assumed that a split of the free energy function into an elastic and a plastic part can be made, resulting in

\[ \psi = \psi^e(b^e, m^{(2)}) + \psi^p(\kappa) \]

(26)

The structural tensors \( m^{(2)} = v^{(2)} \otimes v^{(2)} \) are here introduced to describe the anisotropic behavior of the material. Moreover, \( \psi^p(\kappa) \) is the plastic potential representing isotropic hardening and \( \kappa \) is an internal variable. For simplicity, only a scalar-valued internal variable is considered. It is noted that due to the objective requirements, as \( b^e \) and \( m^{(2)} \) are objective tensors, Helmholtz’ free energy must fulfill

\[ \psi^e(b^e, m^{(2)}) = \psi^e(Qb^e Q^T, Qm^{(2)} Q^T) \quad \forall Q \in O(3) \]

(27)

To conclude, \( \psi^e \) must be described by invariants of \( b^e \) and \( m^{(2)} \) as well as the joint invariants of \( b^e \) and \( m^{(2)} \).

Taking advantage of (26), the dissipation inequality can then be written as

\[ \gamma = \tau : D - \rho_0 \frac{\partial \psi^e}{\partial b^e} : b^e - \sum \rho_0 \frac{\partial \psi^e}{\partial m^{(2)}} : m^{(2)} - K \kappa \geq 0 \]

(28)

where the conjugated force to the isotropic hardening variable \( K \) has been introduced as

\[ K = \rho_0 \frac{\partial \psi^p}{\partial \kappa} \]

(29)

Insertion of (21) and (14) in the dissipation inequality equation (28) and using the symmetric properties of \( b^e \) and \( m^{(2)} \) then yields

\[ \gamma = \left( \tau - 2\rho_0 \frac{\partial \psi^e}{\partial b^e} b^e - 2\rho_0 \sum \frac{\partial \psi^e}{\partial m^{(2)}} m^{(2)} \right) : L + \left( 2\rho_0 \frac{\partial \psi^e}{\partial b^e} b^e + 2\rho_0 \sum \frac{\partial \psi^e}{\partial m^{(2)}} m^{(2)} \right) : L^p \]

\[ - 2\rho_0 \sum \frac{\partial \psi^e}{\partial m^{(2)}} m^{(2)} : \kappa - K \kappa \geq 0 \]

(30)

From the objective requirements stated by (27) it follows that (30) can be rewritten and reduced. Time differentiation of both the left and the right side of (27) leads to

\[ \frac{\partial \psi^e}{\partial b^e} : \dot{b}^e + \sum \frac{\partial \psi^e}{\partial m^{(2)}} : \dot{m}^{(2)} = \frac{\partial \psi^e}{\partial Qb^e Q^T} : \dot{Q}b^e Q^T + \sum \frac{\partial \psi^e}{\partial Qm^{(2)} Q^T} : \dot{Q}m^{(2)} Q^T \]

(31)

Since \( Q \) is an orthogonal tensor, time differentiation yields

\[ \dot{Q} = Q\theta \]

(32)

where \( \theta \) is a skew-symmetric tensor. Inserting (32) into (31) and using the symmetric properties of \( b^e \) and \( m^{(2)} \) one can conclude that

\[ \frac{\partial \psi^e}{\partial b^e} : \dot{b}^e + \sum \frac{\partial \psi^e}{\partial m^{(2)}} : \dot{m}^{(2)} = \frac{\partial \psi^e}{\partial b^e} : \dot{b}^e + \sum \frac{\partial \psi^e}{\partial m^{(2)}} : m^{(2)} + \left( 2\frac{\partial \psi^e}{\partial b^e} b^e + 2\sum \frac{\partial \psi^e}{\partial m^{(2)}} m^{(2)} \right) : \theta \]

(33)

By investigation of this relation it is clear that the quantity within the parenthesis is symmetric. Taking advantage of this result allows the dissipation inequality to be written as
\[ \gamma = \left( \tau - 2\rho_0 \frac{\partial \psi^e}{\partial \dot{b}^e} \dot{b}^e - 2\rho_0 \sum \frac{\partial \psi^e}{\partial \dot{m}^{(x)}(x)} m^{(x)} \right) : \mathbf{D} + \left( 2\rho_0 \frac{\partial \psi^e}{\partial \dot{b}^e} \dot{b}^e + 2\rho_0 \sum \frac{\partial \psi^e}{\partial \dot{m}^{(x)}(x)} m^{(x)} \right) : \mathbf{D}^0 - 2\rho_0 \sum \frac{\partial \psi^e}{\partial \dot{m}^{(x)}(x)} m^{(x)} : \dot{\lambda}^{(x)} - K \dot{\kappa} \geq 0 \]  

(34)

Since the dissipation inequality should hold for arbitrary values of \( \mathbf{D} \), the following definition of the Kirchhoff stress tensor is assumed

\[ \tau = 2\rho_0 \frac{\partial \psi^e}{\partial \dot{b}^e} \dot{b}^e + 2\rho_0 \sum \frac{\partial \psi^e}{\partial \dot{m}^{(x)}(x)} m^{(x)} \]  

(35)

Note that (35) is not unique, i.e. other possibilities to satisfy (34) exist. The same format for the Kirchhoff stress tensor was found in Menzel and Steinmann (2003a), although using a different approach. Use of (35) in (33) yields the reduced form of the dissipation inequality

\[ \gamma = \tau : \mathbf{D}^0 - \sum \dot{r}^{(x)} : \dot{\lambda}^{(x)} - K \dot{\kappa} \geq 0 \]  

(36)

where the structural force \( \dot{r}^{(x)} \) conjugated to the plastic structural velocity gradient has been introduced as

\[ \dot{r}^{(x)} = 2\rho_0 \frac{\partial \psi^e}{\partial \dot{m}^{(x)}(x)} m^{(x)} \]  

(37)

To derive the evolution laws, it is noted that the dissipation inequality can be written as

\[ \gamma = \gamma_{\text{mech}} + \gamma_{\text{sub}} \geq 0 \]  

(38)

where \( \gamma_{\text{mech}} \) and \( \gamma_{\text{sub}} \) are defined as

\[ \gamma_{\text{mech}} = \tau : \mathbf{D}^0 - K \dot{\kappa}; \quad \gamma_{\text{sub}} = - \sum \dot{r}^{(x)} : \dot{\lambda}^{(x)} \]  

(39)

A conservative approach to fulfill (38) is to assume that \( \gamma_{\text{mech}} \geq 0 \) and \( \gamma_{\text{sub}} \geq 0 \) independently. From the definition above it is evident that \( \gamma_{\text{mech}} \) is related to the evolution of the continuum of the body whereas \( \gamma_{\text{sub}} \) is related to the evolution of the substructure.

Consider first the evolution laws related to \( \gamma_{\text{mech}} \). To be able to detect when plastic deformation has occurred an elastic domain is introduced as

\[ \mathcal{E} = \{ (\tau, m^{(z)}, K) \mid f(\tau, m^{(z)}, K) \leq 0 \} \]  

(40)

The yield function, \( f \), is assumed to be a convex function of the variables \( \tau \) and \( K \).

One way of ensuring that the dissipation inequality is fulfilled is to assume the existence of a convex function \( g(\tau, m^{(z)}, K) \) with the properties \( g(\tau, m^{(z)}, K) = g(0, m^{(z)}, 0) \geq 0 \). The part \( \gamma_{\text{mech}} \) of the dissipation inequality can then be fulfilled if

\[ \mathbf{D}^0 = \lambda \frac{\partial g}{\partial \tau}, \quad \dot{\kappa} = -\lambda \frac{\partial g}{\partial K} \]  

(41)

where \( \lambda \) is the non-negative plastic multiplier. Associated plasticity theory is obtained by putting \( f = g \), which also conforms with the theory for maximum plastic dissipation. Using the same arguments as for \( g \) allows one to introduce a potential function related to the substructure as \( g_r = g_r(\dot{r}^{(z)} \dot{z}) \). The second part \( \gamma_{\text{sub}} \) of the dissipation inequality is then fulfilled for

\[ \dot{\lambda}^{(z)} = -\lambda \frac{\partial g_r}{\partial \dot{r}^{(z)}} \]  

(42)

The use of convex potential functions is one way to obtain thermodynamic consistent evolution equations. A more general approach is to postulate the evolution law for the internal variables and show that this specific choice fulfills the dissipation inequality (36), i.e. postulate the following format

\[ \dot{\lambda}^{(z)} = -\lambda \mathbf{P}^{(z)}(\tau, m^{(z)}, K, a) \]  

(43)
where $\mathbf{a}$ denotes additional quantities. This approach will be utilized in the sequel.

Furthermore, to derive an analytical expression for the plastic multiplier, $\dot{\lambda}$, use is made of the consistence condition i.e. $f = 0$. Here the yield function is assumed to be a function of the Kirchhoff stress tensor, the structural tensors and the hardening variable. For a simple notation to be obtained, it is assumed that the Kirchhoff stress tensor is a function of the elastic Finger deformation tensor and the structural tensors yielding $f(\tau(\mathbf{b}^e, \mathbf{m}^{(s)}), \mathbf{m}^{(s)}, K) = \hat{f}(\mathbf{b}^e, \mathbf{m}^{(s)}, K)$. The consistency condition then give

$$\dot{\hat{f}} = \frac{\partial \hat{f}}{\partial \mathbf{b}^e} : \dot{\mathbf{b}}^e + \sum \frac{\partial \hat{f}}{\partial \mathbf{m}^{(s)}} : \dot{\mathbf{m}}^{(s)} + \frac{\partial \hat{f}}{\partial K} \dot{K} = 0$$

By using the definitions for $\dot{\mathbf{b}}^e$ and $\dot{\mathbf{m}}^{(s)}$ together with the relations for $\mathbf{D}^e$, $\dot{\mathbf{x}}^{(s)}$ and $\dot{\kappa}$ one obtains the expression for the plastic multiplier.

$$\dot{\lambda} = \frac{2}{H} \left( \frac{\partial \hat{f}}{\partial \mathbf{b}^e} : \dot{\mathbf{b}}^e + \sum \frac{\partial \hat{f}}{\partial \mathbf{m}^{(s)}} : \dot{\mathbf{m}}^{(s)} \right) : \mathbf{D}$$  \hspace{1cm} (45)

where the term within parenthesis is symmetric using the same arguments as in (27) and (33). The parameter $H$ is further given by

$$H = 2 \frac{\partial \hat{f}}{\partial \mathbf{b}^e} : \frac{\partial \mathbf{g}}{\partial \mathbf{e}} + 2 \sum \frac{\partial \hat{f}}{\partial \mathbf{m}^{(s)}} : \left( \frac{\partial \mathbf{g}}{\partial \mathbf{e}} + \mathbf{P} \right) + \frac{\partial \hat{f}}{\partial K} \mathbf{D}^e : \frac{\partial \mathbf{g}}{\partial \kappa}$$

where the notation $\mathbf{D}^e = \rho_0 \frac{\partial \mathbf{e}^e}{\partial \kappa}$ have been used. Expressions for (45) and (46) in $f$ can be obtained by using the chain rule.

5. Specific model

The specific material model considered obeys cubic material symmetry. Moreover it will be assumed that the director vectors representing the preferred direction in the intermediate configuration remain orthogonal and of unit length during plastic deformation.

The elastic part of Helmholtz’ free energy function is assumed to be divided into an isotropic and an anisotropic part

$$\psi^e = \psi^e_{\text{iso}} + \psi^e_{\text{aniso}}$$

The isotropic part is taken as

$$\rho_0 \psi^e_{\text{iso}} = \frac{K_b}{2} \left[ \frac{\mathbf{I}_2^e - 1}{2} - \ln \mathbf{F}^e \right] + \frac{1}{2} \mu (\text{tr} \mathbf{b}^e - 3)$$

The material parameters $K_b$ and $\mu$ represents, for isotropy, the initial bulk modulus and the shear modulus, respectively. Furthermore, $\mathbf{b}^e = (\mathbf{F})^{-2/3} \mathbf{b}^e$ is the isochoric part of elastic Finger deformation tensor. The isotropic part of Helmholtz’ free energy, given by (48), is known to be polyconvex in the sense of Ball (1977b,a), cf. also Ciarlet (1988) and Schröder and Neff (2003). Polyconvexity guaranties the existence of at least one minimizer to the elastic energy. When constructing the anisotropic part of the free energy function some further investigation is needed. A set of transversely and orthotropic strain energy functions that are polyconvex was derived by Schröder and Neff (2003) and further elaborated by Itskov and Aksel (2004). However, here we adopt the work of Steigmann (2003) who showed that the following invariants

$$I_4 = (\mathbf{C}^e : \mathbf{M}^{(1)})^{1/2}, \quad I_5 = (\mathbf{C}^e : \mathbf{M}^{(2)})^{1/2}, \quad I_6 = (\mathbf{C}^e : \mathbf{M}^{(3)})^{1/2}$$

are convex with respect to $\mathbf{F}^e$. Here, $\mathbf{M}^{(s)} = \mathbf{\psi}^{(s)} \otimes \mathbf{\psi}^{(s)}$ represents the structural variables in the intermediate configuration and $\mathbf{C}^e = \mathbf{F}^e \mathbf{C} \mathbf{F}^e$ is the elastic Cauchy–Green deformation tensor. From the above definitions and (18b) one obtains the spatial forms of the invariants as

$$I_4 = \text{tr}(\mathbf{m}^{(1)})^{1/2}, \quad I_5 = \text{tr}(\mathbf{m}^{(2)})^{1/2}, \quad I_6 = \text{tr}(\mathbf{m}^{(3)})^{1/2}$$
Taking advantage of the above invariants the following form of an anisotropic free energy function suitable for cubic materials is proposed as

\[ \rho_0 \psi_{\text{aniso}} = a(I_4 + I_5 + I_6 - \ln(J^r)) - 3 \] (51)

Here \( a \) is a non-negative material parameter. As all invariants involved in (51) are convex it is concluded that Helmholtz’ free energy function is polyconvex. From this specific form of elastic free energy and the definition (35) the Kirchhoff stress tensor is given by

\[ \tau = \frac{K_b}{2}(J^r - 1)I + \mu \text{dev}(h^e) + a(m^{(1)} + \bar{m}^{(2)} + \bar{m}^{(3)} - I) \] (52)

where

\[ m^{(s)} = \frac{m^{(s)}}{\text{tr}(m^{(s)})^{1/2}} \] (53)

It is noted that (52) will result in a stress free reference state, i.e. when \( F^e = I \), if the director vectors are orthogonal in the intermediate configuration. The calibration of the elastic material constants is obtained from the initial stiffness, defined as

\[ \mathcal{L}_0^e = \frac{\partial \tau}{\partial F^e} F^{eT} |_{F^e = I} = 2 \left[ \frac{\partial \tau}{\partial b^e} b^e + \sum \frac{\partial \tau}{\partial m^{(s)}} m^{(s)} \right] |_{F^e = I} \] (54)

Related calculations are made in Appendix B where the consistent tangent stiffness is derived. For the initial stiffness it is noted that the material is stress free, i.e. \( \tau = 0 \). Straightforward derivation then provides

\[ \mathcal{L}_0^e = \left( K_b - \frac{2}{3} \mu \right) I \otimes I + 2 \mu \mathcal{L} \otimes \mathcal{L} + 2a \sum \left[ I \otimes m^{(s)} - \frac{m^{(s)} \otimes m^{(s)}}{2 \text{tr}(m^{(s)})^{1/2}} \right] \] (55)

where \( \mathcal{A} \otimes \mathcal{B} = 1/2 (\mathcal{A} \otimes \mathcal{B} + \mathcal{B} \otimes \mathcal{A}) \), see Appendix B. To calibrate the three elastic material constants, the global Cartesian base vectors are aligned along \( v^{(s)} \). Adopting Voigt notation, the matrix representation of (55) is given by

\[ [\mathcal{L}_0^e] = \begin{bmatrix}
\mathcal{L}_{11}^e & \mathcal{L}_{12}^e & \mathcal{L}_{12}^e \\
\mathcal{L}_{11}^e & \mathcal{L}_{12}^e & \mathcal{L}_{12}^e \\
\mathcal{L}_{11}^e & \mathcal{L}_{12}^e & \mathcal{L}_{44}^e \\
\text{sym} & \mathcal{L}_{44}^e & \mathcal{L}_{44}^e
\end{bmatrix} \] (56)

where

\[ \mathcal{L}_{11}^e = K_b + \frac{4}{3} \mu + a, \quad \mathcal{L}_{12}^e = K_b - \frac{2}{3} \mu, \quad \mathcal{L}_{44}^e = \mu + a \] (57)

As evident (56) represents initial cubic symmetry, where \( \mathcal{L}_{11}^e, \mathcal{L}_{12}^e \), and \( \mathcal{L}_{44}^e \) can be found from experimental tests. It will be assumed that the hardening of the material can be described by an exponential form and the plastic part of the free energy function is, therefore, assumed to take the form of

\[ \rho_0 \psi^p = R_\infty (\kappa + e_0 e^{-\xi/\mu}) \] (58)

The hardening function is obtained from (29) as

\[ K = \rho_0 \frac{\partial \psi^p}{\partial \kappa} = R_\infty (1 - e^{-\xi/\mu}) \] (59)

where \( R_\infty \) and \( e_0 \) are material constants.

Considering anisotropic formats for the yield function, highly advanced models exists, such as the models of Barlat and Lian (1989), Barlat et al. (1991) and Karafillis and Boyce (1993). For the purpose considered
here it suffices to use the most simple yield surface as possible. Following Darrieulat et al. (1992) a yield function for cubic symmetry is given by

\[ f = Aj + (1 - A) \sum_{x=1}^{3} (i^{(x)})^2 - \frac{2}{3} \sigma^2, \quad \sigma = \sigma_{yy} + K \]  

where the stress invariants are introduced as

\[ j = \text{dev}(\tau) : \text{dev}(\tau), \quad i^{(x)} = \text{dev}(\tau) : m^{(x)} \]  

Here \( A \) is a material parameter controlling the shape of the yield surface. It was shown by Montheillet et al. (1985) that (60) is a quadratic approximation of the Bishop and Hill (1951) polyhedron for an fcc crystal. The evolution laws related to the continuum is found by assuming associated plasticity in (41).

Regarding the evolution of the substructure, it is assumed that the plastic velocity gradients for the substructure \( \dot{\lambda}^{(x)} \) are identical for all preferred directions. Following Harrysson and Ristinmaa (2006), it is also assumed that

\[ \dot{\lambda} = -\frac{\eta}{2} (b^e \tau e^{-1} - \tau) \]  

where \( \eta \) is a material parameter. Here the superscript \((z)\) has been dropped. Note further that (62) can be interpreted as the substructure will evolve until the Kirchhoff stress and the elastic Finger deformation tensor becomes co-axial. It is also recognized that by performing a pull-back to the intermediate configuration one obtains

\[ \Lambda = F^{-1} \dot{\lambda} F = -\frac{\eta}{2} (\Sigma - \Sigma^T) \]  

where \( \Sigma = F^e \tau e^{-T} \) is the Mandel stress tensor. \( \Lambda \) is obviously a skew-symmetric quantity which implies that the preferred directions \( \lambda^{(x)} \) in the intermediate configuration remain orthogonal and of unit length when exposed to plastic deformation, see also Harrysson and Ristinmaa (2006). To show that \( \gamma_{\text{sub}} \geq 0 \) is fulfilled certain minor algebraic manipulations are needed. First, adding and subtracting the term \( \frac{\partial \psi}{\partial \dot{\lambda}} b^e : \dot{\lambda} \) from (39b) gives

\[ \gamma_{\text{sub}} = -\left( \frac{\partial \psi}{\partial \dot{\lambda}} b^e + \sum r^{(x)} \right) : \dot{\lambda} + \frac{\partial \psi}{\partial b^e} b^e : \dot{\lambda} = -\tau : \dot{\lambda} + \frac{\partial \psi}{\partial b^e} b^e : \dot{\lambda} \]  

where the definition of the Kirchhoff stress has been used. By insertion of (62) it is straightforward to show that the last term in (64) is equal to zero. The remaining term requires further investigation. By use of the definition of \( b^e \) and the identity \( F^e F^{-1} = I \) one obtains

\[ \gamma_{\text{sub}} = \frac{\lambda \eta}{2} [\Sigma : \Sigma - \Sigma : \Sigma^T] \]  

which can be rewritten as the quadratic form

\[ \gamma_{\text{sub}} = \lambda \eta [\Sigma - \Sigma^T] : [\Sigma - \Sigma^T] \geq 0 \]  

Thus \( \gamma_{\text{sub}} \geq 0 \) is fulfilled as long as \( \eta > 0 \).

6. Numerical examples

To demonstrate the capabilities of the model, simulations were performed by using the finite element code ABAQUS/Standard where the proposed constitutive model was implemented using the user material function “umat”. The numerical handling of the model, i.e. the integration of the constitutive relations and the development of a consistent tangent stiffness, is presented in Appendices A and B. In all simulations the 8-node linear hybrid brick element C3D8H was used. The material parameters used in the simulations are found by considering data for single crystal aluminum. From Simmons and Wang (1971) the initial elastic stiffness
parameters are found as $L_{11} = 108 \text{ GPa}$, $L_{12} = 62 \text{ GPa}$ and $L_{44} = 28 \text{ GPa}$. Taking advantage of (57) it then follows that

$$K_b = 74 \text{ GPa}, \quad \mu = 18 \text{ GPa}, \quad a = 10 \text{ GPa}$$

The initial yield stress and the hardening parameters are calibrated by curve fitting to the experimental data for aluminum along the [100] crystallographic orientation reported by Fortunier et al. (1987). This resulted in

$$\sigma_{y0} = 10 \text{ MPa}, \quad A = 0.409, \quad R_\infty = 27.7 \text{ MPa}, \quad \epsilon_0 = 0.01$$

Furthermore, the value of $A$ was suggested by Darrieulat et al. (1992) for a fcc crystal structure. The preferred directions $v_0^{(1)}$, $v_0^{(2)}$, and $v_0^{(3)}$ are here taken as the crystallographic directions $[100]$, $[010]$ and $[001]$, respectively. Evidently, crystal plasticity could be used in this example, however, our intention is to evaluate the proposed theory.

### 6.1. Deformation of uniform plate with circular hole

In this first simple example the performance of the model is studied for a uniform plate with a circular hole. A sketch of the geometry is shown in Fig. 2. The geometry is modeled using 1920 elements. The plate is subjected to a deformation controlled load which increases to a maximum value of 12.5 mm. One end of the specimen is totally clamped. This example was also considered by Menzel and Steinmann (2003a) for an orthotropic material model.

Two different initial orientations of the preferred directions of the material were simulated, one where the substructure has an $\alpha = 30^\circ$ off-axis orientation and in the other the initial orientation of the substructure is aligned to the global $e_a$, i.e. $\alpha = 0^\circ$, cf. Fig. 2.

For the off-axis orientation, four different values of the material parameter $\eta$ in (62) were used. This to investigate how the change of the substructure will affect the global deformation. The deformation shape for the reference simulation, i.e. $\alpha = 0^\circ$, is displayed in Fig. 3 which reveals that the deformation becomes very localized. For $\alpha = 30^\circ$ the deformed geometry for different values of the material parameter $\eta$ can be seen in Fig. 4. From Fig. 4 it is noted that the initial off-axis orientation of the substructure plays a crucial role as a non-symmetric deformation shape is obtained. Furthermore, it is noted that the value of the material constant

![Fig. 2. Dimensions and boundary conditions of the analyzed structure (mm). Uniform thickness, $t = 3$ mm is assumed.](image)

![Fig. 3. Uniform plate with hole with substructure aligned to the deformation axis, i.e. $\alpha = 0^\circ$. (a,b) Show deformed mesh and (c,d) shows contour plot of $\kappa$ for deformed shape for deformations $u = 6.25$ and 12.5 mm, respectively.](image)
$g$ will have an effect on deformation shape. For a high value of $g$ the deformation of the hole will become more localized, similar to the reference simulation. The evolution of the preferred directions was also studied for a material point, marked $A$ in Fig. 2, during the deformation process. This point is located halfway through the thickness of the strip. The angle $a$ between the director vector $v^{(1)}$ in the current configuration and $e_1$ is displayed in Fig. 5. It can be seen that the value of the parameter $g$ has a significant impact on the evolution of the preferred directions, explaining the different global deformation shapes for the different values of $g$ in Fig. 4.

![Fig. 4. Uniform plate with hole with $\alpha = 30^\circ$ off-axis orientation. Contour plot of $\kappa$ and deformed shape for deformations $u = 6.25$ and 12.5 mm. (a,b) $\eta = 0$ [1/MPa]. (c,d) $\eta = 3000$ [1/MPa]. (e,f) $\eta = 10,000$ [1/MPa]. (g,h) $\eta = 20,000$ [1/MPa].](image)

![Fig. 5. Evolution of angle $\alpha$ between $v^{(1)}$ and $e_1$ for different values of $\eta$. Solid line represent $\eta = 0$ [1/MPa], dashed line represent $\eta = 3000$ [1/MPa], dash dotted line represent $\eta = 10,000$ [1/MPa] and solid line with squares represent $\eta = 20,000$ [1/MPa]. Initial value $\alpha = 30^\circ$.](image)
6.2. Drawing of a cup

This example is taken from a manufacturing process concerning the drawing of a cup. Similar studies have been conducted by e.g. Becker et al. (1993). When a cylindrical cup is drawn from a circular blank, the rim of the cup is usually undulating with various of high points and low points, called ears and troughs, respectively. This undulating effect is not expected from an ideal isotropic material, hence earing is related to the preferred orientation of the crystals in the original sheet. Furthermore, the final shape of the ears and troughs are influenced by some texture evolution. From experiments, it is found that material with cubic symmetry properties where the [001] crystallographic direction is normal to the sheet show four ears and troughs, see Tucker (1961). Here it is investigated if the model presented can retrieve this earing shape of the cup.

The experimental setup is sketched in Fig. 6 where axisymmetry with respect to the punch direction is understood. During the drawing process, the punch is pressed down into the female die to form a cup. To hold the sheet, a blank holder is used. In this simulation setup, it is assumed that the sheet holder is fixated in a position leaving the distance to the female die equal to the initial thickness of the sheet. Furthermore, Coulomb friction with \( \mu = 0.01 \) was assumed between the tools and the sheet. This setup was also used by Apel (2004). The tools, i.e. the punch, the female die and the blank holder are modeled as rigid bodies and the sheet is modeled using 6880 elements.

![Fig. 6. Sketch of experimental setup. Lengths in millimeter. Thickness of sheet is 0.81 mm.](image)

![Fig. 7. Final stage of simulations for different values of the \( \eta \) parameter. (a) \( \eta = 0 \) [1/MPa], (b) \( \eta = 3000 \) [1/MPa], (c) \( \eta = 10,000 \) [1/MPa] and (d) \( \eta = 20,000 \) [1/MPa].](image)
To test the implementation the model was reduced to isotropic material symmetry. For this case the cup was completely symmetric and no ears were developed as expected.

As a general observation one can see that the characteristic geometry of four ears was obtained, see Fig. 7. These results were also found be e.g. Becker et al. (1993) but here crystal plasticity was used. To investigate the influence of the structural evolution, different values of the $\eta$ parameters were used in the simulations. In Fig. 7 the final stage of the simulation for four different values of the $\eta$ parameters can be seen. As can be seen in Figs. 7 and 8, the shape of the ear and troughs are more pronounced as $\eta$ takes a low value and become less pronounced as this value increases. This is due to the more rapid reorientation of the preferred directions as this material parameter takes a larger value. The profiles of the ears obtained at the end of the simulations are shown in Fig. 8 where the simulations are compared to the experimental data from Tucker (1961). The simulations show good agreement to the experimental data.

7. Conclusions

A large strain elasto-plastic model for anisotropic material in a spatial setting was presented in this paper. The kinematic assumption of linear maps, similar to the deformation gradient, describing the evolution of the substructure, as discussed in Harrysson and Ristinmaa (2006), was utilized. It was shown that the multiplicative structure of the deformation gradient for the continuum and the substructure allows for the elastic Finger tensor and the preferred directions, defined in the current configuration, to conveniently be described by Lie derivatives. These Lie derivatives will then be related to the plastic velocity gradient and the corresponding substructural velocity gradients for the substructure. Moreover, it was assumed that the elastic part of Helmholtz’ free energy function was completely described by the elastic Finger tensor and the preferred directions. This in turn allowed for admissible forms of the plastic velocity gradient and the substructural velocity gradients to be established.

As a prototype model for anisotropy, cubic symmetry was considered for the elastic as well as plastic behavior. In the model a polyconvex form of Helmholtz’ free energy function and a simple quadratic yield function, both displaying cubic symmetry, were utilized. The model was implemented into a finite element code, where a simple integration method preserving plastic incompressibility for the constitutive equations, based on the Lie derivatives was utilized. Furthermore, the algorithmic tangential stiffness was established to ensure satisfying convergence rate.

Two numerical examples was examined. In the first example, it was found that the initial direction of the preferred directions are crucial for the final stage of deformation. Furthermore, the effects of varying the value of the $\eta$ factor was examined. Here it was found that the value of $\eta$ had an affect in the deformation shape. The evolution of the preferred directions was also examined for different values of $\eta$ and for a high value the preferred direction $\nu^{(1)}$ tend to align to the axis of deformation. In the second example, involving the drawing of a
cup, it was found that this approach allows, when a simple yield function possessing cubic symmetry is used, to reproduce the earing shapes found from experiments for a single crystal material with the [001] crystallographic direction normal to the metal sheet. Good agreement to experimental data was found. The effect of varying the value of the $\eta$ parameter were also investigated. It was found that a larger value of this parameter results in less pronounced earing shape of the final cup.

Appendix A. Integration of constitutive model

In order to make use of path dependent material models in a finite element context, a numerical approach for integration of the constitutive laws has to be chosen. In the presented study, use is made of the implicit backward Euler integration scheme.

A standard strategy for handling elasto-plastic problems is to first perform a check of whether plastic deformation has occurred during the time step. This is done by assuming that the time step taken is completely elastic. The trial quantities that are used for this check are defined as

$$\begin{align*}
b^{\text{e}}_{\text{trial}} &= f b^{\text{e}}_n \, f^T \\
v^{(x)}_{\text{trial}} &= f v^{(x)}_n \\
\kappa_{\text{trial}} &= \kappa_n
\end{align*}$$  \hspace{1cm} (A.1)

Here the relative deformation gradient $f = \mathbf{F} \mathbf{F}^{-1}$ has been introduced where the subscript $n$ refers to the last state of equilibrium. These trial quantities are then inserted into the yield function and a trial value is obtained $f_{\text{trial}}$. If the returned value is a feasible number, i.e. $f_{\text{trial}} \leq 0$, the assumption of a completely elastic time step was correct, in which case the quantities at the end of the time step takes on the values of the trial quantities.

However, if the trial value from the yield function is non-feasible number, $f_{\text{trial}} > 0$, the assumption was incorrect and the constitutive equations (41) and (42) need to be integrated. Adopting the exponential algorithm for the integration of the evolution laws will result in the important property, that when a pressure insensitive yield criterion is adopted the algorithm preserves the plastic volume, i.e. $J^p = 1$. In the case of elastic isotropy combined with isotropic hardening plasticity, taking advantage of the co-axiality of the quantities involved the exponential algorithm results in a very attractive integration scheme, cf. Weber and Anand (1990) and Simo (1998). However, when anisotropy is present the favorable properties that follow from co-axiality are lacking. Utilization of the exponential algorithm is then no longer straight-forward since explicit derivatives of the non-symmetric exponential tensor functions must be obtained, cf. Ortiz et al. (2001) and Wallin and Ristinmaa (2005). An alternative route is obtained by directly applying the backward Euler scheme to (A.3). For the case of isotropy this was conducted by Simo (1988) and Simo and Miehe (1992), yet on should be cautious in adopting such an approach since plastic incompressibility is generally not preserved. Usually, a post-integration correction is adopted to enforce plastic incompressibility in the above approach.

To obtain an integration scheme for which plastic incompressibility is preserved and being as simple as possible the integration is here performed by using an implicit backward Euler integration scheme so constructed that plastic incompressibility is retained. As starting point to fulfill this constraint a split of the elastic Finger deformation tensor into a volumetric and an isochoric part is utilized. Using the definition of the Finger elastic deformation tensor together with the definition of the Lie derivative (22a), one obtains

$$\mathcal{L}_{\pi}(\mathbf{b}^{\text{e}}) = -2\text{sym}(\mathbf{L}^p \mathbf{b}^{\text{e}}) - \frac{2}{3} \frac{J^e}{J^s} \mathbf{b}^{\text{e}}$$  \hspace{1cm} (A.2)

Taking advantage of the definition given in (24a), it follows that

$$\frac{d}{dt}(\mathbf{C}^{n-1}) = -2\mathbf{F}^{-1} \text{sym}(\mathbf{L}^p \mathbf{b}^{\text{e}}) \mathbf{F}^{-T} - \frac{2}{3} \frac{J^e}{J^s} \mathbf{F}^{-1} \mathbf{b}^{\text{e}} \mathbf{F}^{-T}$$  \hspace{1cm} (A.3)

where $\mathbf{C}^n = \mathbf{F}^{-1} \mathbf{b}^{\text{e}} \mathbf{F}^{-T}$. Applying the backward Euler rule to (A.3) yields the following relation

$$\mathbf{C}^{n-1} - \mathbf{C}_n^{n-1} = -2\Delta t \mathbf{F}^{-1} \text{sym}(\mathbf{L}^p \mathbf{b}^{\text{e}}) \mathbf{F}^{-T} - \frac{2}{3} \ln \left(\frac{J^e}{J^s}\right) \mathbf{F}^{-1} \mathbf{b}^{\text{e}} \mathbf{F}^{-T}$$  \hspace{1cm} (A.4)
where the quantities are evaluated at current state if not stated otherwise. In (A.4) the last term was integrated by assuming \( F^{-1} b^c F^{-T} \) to be constant. This equation can be rearranged such that

\[
\left(1 + \frac{2}{3} \ln \left( J^e \right) \right) b^c = \bar{b}^c_{\text{trial}} - 2\Delta t \text{sym}(L^p b^c)
\]

(A.5)

Here the quantity \( \bar{b}^c_{\text{trial}} \) is introduced as

\[
\bar{b}^c_{\text{trial}} = f b^c f^T
\]

(A.6)

It is noted that this is generally not an isochoric quantity. Due to the approximations introduced when applying the backward Euler scheme to (A.3) it is not expected that the solution of (A.5) will result in \( b^c \) being an isochoric quantity. The remedy is to replace the scalar function in front of \( b^c \) with the additional variable, i.e.

\[
q b^c = \bar{b}^c_{\text{trial}} - 2\Delta t \text{sym}(L^p b^c)
\]

(A.7)

It turns out that \( q \) can be used for scaling the result, such that \( b^c \) becomes isochoric. The additional relation introduced to enforce this property is given by

\[
\det(\bar{b}^c) - 1 = 0
\]

(A.8)

The integration of the structural director vector is treated in a more straightforward fashion. Starting from the Lie derivative of the structural director vector it follows that

\[
\mathcal{L}(v^{(a)}) = F \frac{\partial \bar{\lambda}}{\partial t} (F^{-1} v^{(a)}) = -(L^p - \lambda^{(a)}) v^{(a)}
\]

(A.9)

Following the same steps as before results in

\[
v^{(a)} = v^{(a)}_{\text{trial}} - \Delta t (L^p - \lambda^{(a)}) v^{(a)}
\]

(A.10)

where the trial quantity \( v^{(a)}_{\text{trial}} \) is defined according to

\[
v^{(a)}_{\text{trial}} = f^{(a)}(\bar{\lambda})
\]

(A.11)

Using a backward Euler integration scheme for the evolution equation for the isotropic hardening parameter one obtains directly

\[
\kappa = \kappa_n + \Delta t \frac{\partial g}{\partial K}
\]

(A.12)

Using (A.7), (A.10) and (A.12), along with the constraint of requiring the yield function to be zero at the end of the time step the following local residual functions can be defined

\[
R^{(c)} = \bar{b}^c_{\text{trial}} - 2\Delta t \text{sym}[N b^c] - q b^c = 0
\]

\[
R^{(a)} = v^{(a)}_{\text{trial}} - \Delta \lambda (N - P^{(a)}) v^{(a)} - v^{(a)} = 0
\]

\[
R^f = f(\bar{\lambda}, m^{(a)}), \kappa = 0
\]

\[
R^\kappa = \kappa_n + \Delta \lambda N - \kappa = 0
\]

\[
R^q = \det(\bar{b}^c) - 1 = 0
\]

(A.13)

Here the evolution laws for the plastic velocity gradient for the continuum and for the substructure and the direction of the isotropic hardening has been replaced schematically by \( L^p = \lambda N, \lambda^{(a)} = \lambda P^{(a)} \) and \( \frac{\partial K}{\partial K} = N \) as well as \( \Delta \lambda = \Delta \bar{\lambda} \).

To solve the equation system given in (A.13), a Newton–Raphson method is used according to

\[
\mathbf{Y}^{n+1} = \mathbf{Y}^{n} - \left[ \frac{\partial \mathcal{R}}{\partial \mathbf{Y}} \right]^{-1} \mathcal{R}^{n}
\]

(A.14)

where
\[ \mathbf{R} = [\mathbf{R}^{e,i} \mathbf{R}^{(s)} \mathbf{R}^e \mathbf{R}_k \mathbf{R}^e] \] \[ \mathbf{Y} = [b^{e,i} \mathbf{v}^{(s)} \Delta \lambda \kappa \mu]^T \]

The derivatives in the Jacobian is straightforward to derive, and in the model utilized below explicit expressions have been used.

Appendix B. Consistent tangent moduli

To ensure quadratic convergence rate for the global equilibrium equations the algorithmic tangential stiffness (ATS) has to be used. To obtain the spatial form for the algorithmic tangential stiffness tensor, use is made of the material configuration and of a push-forward such as

\[ \mathcal{L}^{ATS} = 2(F \otimes F : \frac{\partial \mathbf{S}}{\partial \mathbf{C}} : (F^T \otimes F)^T) \] (B.1)

where the notation \((A \otimes B)_{ijkl} = A_{ij}B_{kl}\) is employed. Moreover, \(\mathbf{S} = F^{-1} \tau F^{-T}\) is the second Piola–Kirchhoff stress tensor. Although not written out explicitly minor symmetry of \(\mathcal{L}^{ATS}\) is used in the expressions. Note that all quantities are evaluated at the current iteration step. Taking advantage of

\[ \frac{\partial \mathbf{S}}{\partial \mathbf{F}} F^T = \frac{\partial \mathbf{S}}{\partial \mathbf{C}} : (F^T \otimes F)^T \] (B.2)

and the definition for the second Piola–Kirchhoff stress tensor results in

\[ \mathcal{L}^{ATS} = -I \otimes \tau - I \otimes \tau + \frac{\partial \mathbf{F}}{\partial \mathbf{F}} F^T \] (B.3)

where the notation \((A \otimes B)_{ijkl} = A_{ij}B_{kl}\) has been introduced. It turns out that the above format together with (A.14) allows for the ATS to be established in a straightforward manner. Assuming that the Kirchhoff stress tensor depends upon the Jacobian of the elastic deformation gradient, the isochoric part of Finger deformation tensor and the director vectors, i.e. \(\tau = \tau(J^e, b^{e,i}, \mathbf{v}^{(s)})\) yields the relation

\[ \frac{\partial \tau}{\partial \mathbf{F}} F^T = \frac{\partial \tau}{\partial J^e} \frac{\partial J^e}{\partial \mathbf{F}} F^T + \frac{\partial \tau}{\partial b^{e,i}} \frac{\partial b^{e,i}}{\partial \mathbf{F}} F^T + \frac{\partial \tau}{\partial \mathbf{F}} \frac{\partial \mathbf{F}}{\partial \mathbf{F}} (F_{trial})^T \] (B.4)

However, since the material is assumed to be plastic incompressible the identity \(J = J^e\) holds. By introducing the quantity \(F_{trial}^e = FF_n^{-1}\) one obtains by use of the chain rule

\[ \frac{\partial \tau}{\partial \mathbf{F}} F^T = \frac{\partial \tau}{\partial J^e} \frac{\partial J^e}{\partial \mathbf{F}} F^T + \frac{\partial \tau}{\partial b^{e,i}} \frac{\partial b^{e,i}}{\partial \mathbf{F}} F_{trial}^e (F_{trial})^T + \frac{\partial \tau}{\partial \mathbf{F}} \frac{\partial \mathbf{F}}{\partial \mathbf{F}_{trial}} (F_{trial})^T \] (B.5)

The first term is evaluated by straightforward differentiation, whereas the other two terms require further investigation. By considering the local residual function the following relation is obtained

\[ \mathcal{R}(\mathbf{Y}(F_{trial}^e), F_{trial}^e) = 0 \quad \forall F_{trial}^e \] (B.6)

Differentiation of (B.6) with respect to \(F_{trial}^e\) and post multiplying with \((F_{trial}^e)^T\) gives

\[ \frac{\partial \mathbf{Y}}{\partial F_{trial}^e} (F_{trial}^e)^T = -\left[\frac{\partial \mathcal{R}}{\partial \mathbf{Y}}\right]^{-1} \frac{\partial \mathcal{R}}{\partial F_{trial}^e} (F_{trial}^e)^T \] (B.7)

Where the terms from the right hand side is evaluated as

\[ \frac{\partial \mathcal{R}}{\partial F_{trial}^e} (F_{trial}^e)^T = I \otimes \mathbf{b}_{trial}^e + \mathbf{b}_{trial}^e \otimes I \] (B.8)

\[ \frac{\partial \mathcal{R}}{\partial F_{trial}^e} (F_{trial}^e)^T = I \otimes \mathbf{v}_{trial}^{(s)} \]

i.e. \(F_{trial}^e\) is not needed explicitly. From the definition of \(\mathbf{Y}\) it is clear that all quantities involved in the derivation of the algorithmic tangential stiffness can be obtained.
References


