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# ANISOTROPIC HYPER-ELASTIC FINITE ELEMENT BASED UPON GENERALIZED STRAIN

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**Abstract.** *This paper presents the mathematical formulation of a finite element model based on the stress-strain constitutive equations derived for anisotropic hyper-elastic materials using logarithmic strain. Assuming a constitutive equation for the specific internal energy the equation governing the Cauchy stress is derived. The dependence of third-order elastic constants on the choice of strain measure is shown. Using the finite element method the equilibrium equation is integrated in the current configuration. Differentiation of the residuum vector, which is a nonlinear function of displacements leads to a complex analytical expression for the tangent stiffness matrix. The particular terms of it are discussed. The paper presents also a numerical example, which demonstrates how nonlinear elasticity together with dislocations induce the surface tension observed in thin layers of crystalline monostructures.*

# 1 Introduction

Many elastic constitutive models are used to describe the nonlinear elastic behaviour of materials. Anisotropic hyperelastic materials compose a narrow group among numerous constitutive models describing elastic behaviour. It is worth emphasizing that the most known *anisotropic* hyperelastic models like the Biot and St.Venant–Kirchhoff models change strongly their (instantaneous) stiffness under large strains. Moreover, such stiffness evolution is often far away from the behaviour of real materials. For example, neglecting an anomalous behaviour, we can expect, regarding molecular effects, that *the instantaneous stiffness of crystalline solids increases under compression and decreases under extension* [1], cf. the hydrostatic and temperature effects [2, 3, 4], as well as the form of interatomic potentials (e.g. Stillinger-Weber, Lennard-Jones) used in molecular dynamics [5]. So, the application of the mentioned constitutive models (St.Venant–Kirchhoff, Biot) behaving just conversely can be the reason of many undesirable effects like the wrong estimation of stress distribution in epitaxial layers, improper proportions in sizes of the extension and compression regions about edge dislocations in crystals, an erroneous calculation of elastic-plastic instability where the correct estimation of the instantaneous stiffness of material takes the fundamental role. Therefore, the use of new hyperelastic models the behaviour of which could be more adapted to the behaviour of real materials is to be desired. Since many years a special attention is focused on the logarithmic strain measure called also the Hencky strain.

The constitutive models based on the logarithmic strain measure were considered in many papers, cf. [6, 7, 8, 9, 10, 11, 12]. Nevertheless, from the viewpoint of nonlinear elasticity, most of the papers devoted to logarithmic strains fall mainly into two categories: (a) isotropic hyperelasticity and (b) isotropic and/or anisotropic *hypo*elasticity. It is worth emphasizing that, contrary to hyperelastic materials the hypoelastic ones ignore the potential character of energy. Therefore, *hypo*elastic models often describe nothing else than a perpetual motion producing or annihilating energy (work) in closed deformation loops — depending on the loop direction. To ascertain whether the given constitutive model describes the hyperelastic (Green) or at least the Cauchy elastic material, additional theorems are studied in *hypo*elasticity cf. [12]. Concerning *anisotropy* the problem is more complicated and, therefore, the respective considerations are often limited only to remarks stating that for anisotropy the stress conjugate to logarithmic strain is not coaxial to the stretch tensor what implies a complex relation between the Cauchy stress and the conjugate stress to logarithmic strain.

In this paper a model for anisotropic hyperelastic material is derived and implemented into a finite element code. First, the constitutive equation is obtained from energy considerations. Lagrangian and Eulerian tensors are simultaneously developed. Two fourth order tensors characterize the respective relations. Next, the discretization into finite elements is briefly presented and, finally, a numerical example illustrates the behaviour of the model.

## 2 Hyperelasticity

According to the polar decomposition theorem the deformation gradient $\mathbf{F}$ can be decomposed into the rotation tensor $\mathbf{R}$ and the right and left stretch tensors $\mathbf{U}$ and $\mathbf{V}$, respectively.

**Definition** *By general Lagrangian and Eulerian strain tensors we mean two tensor functions*

$$\widehat{\boldsymbol{\varepsilon}} \stackrel{df}{=} f(u_{\mathsf{i}})\ \mathbf{u}_{\mathsf{i}} \otimes \mathbf{u}_{\mathsf{i}} \qquad \textit{and} \qquad \boldsymbol{\varepsilon} \stackrel{df}{=} f(v_{\mathsf{i}})\ \mathbf{v}_{\mathsf{i}} \otimes \mathbf{v}_{\mathsf{i}}, \tag{1}$$

*where $u_{\mathsf{i}}, \mathbf{u}_{\mathsf{i}}, v_{\mathsf{i}}, \mathbf{v}_{\mathsf{i}}$ denote respectively the $i$-th eigenvalue and unit eigenvector of the right and left stretch tensors, while $f(\cdot)$ denotes an arbitrarily chosen $C^1$ monotonically increasing function $f(x) : R^+ \ni x \to f \in R$ which satisfies the conditions $f(x)|_{x=1} = 0$ and $\frac{df(x)}{dx}\big|_{x=1} = 1$.*

This definition includes the well-known family of strain measures [13, 7]

$$\widehat{\boldsymbol{\varepsilon}} = \frac{1}{m}(\mathbf{U}^m - \mathbf{1}) \qquad \text{and} \qquad \boldsymbol{\varepsilon} = \frac{1}{m}(\mathbf{V}^m - \mathbf{1}), \tag{2}$$

where $m$ is a real number, and also many others, e.g. $\widehat{\boldsymbol{\varepsilon}} = \frac{1}{4}\mathbf{U}^2 + \frac{1}{2}\mathbf{U} - \frac{3}{4}\mathbf{1}$.

We will make use of these strain measures later on. Hyperelasticity is based on the fulfillment of the energy balance. In the case of isothermal quasistatic deformation of elastic bodies, the local form of the energy conservation can be reduced to

$$-\rho\dot{\psi} + \boldsymbol{\sigma} : \mathbf{d} = 0, \tag{3}$$

where $\rho, \dot{\psi}, \boldsymbol{\sigma}$ and $\mathbf{d}$ denote respectively the mass density, material derivative of internal energy density per unit mass, Cauchy stress tensor, and the symmetric part of the velocity gradient, i.e.

$$\mathbf{d} \stackrel{df}{=} \frac{1}{2}(\nabla\mathbf{v} + \nabla^T\mathbf{v}) = \frac{1}{2}\mathbf{R}(\dot{\mathbf{U}}\mathbf{U}^{-1} + \mathbf{U}^{-1}\dot{\mathbf{U}})\mathbf{R}^T, \tag{4}$$

where $\mathbf{v}$ denotes the velocity vector. Suppose that the specific internal energy depends on the Lagrangian strain tensor

$$\psi = \psi(\widehat{\boldsymbol{\varepsilon}}). \tag{5}$$

Before we substitute (5) into (3) let us first recall the mathematical relations for the material derivative of the general Lagrangian strain tensor (1a)

$$\dot{\widehat{\boldsymbol{\varepsilon}}} = \widehat{\boldsymbol{\mathcal{A}}} : (\mathbf{R}^T\mathbf{d}\,\mathbf{R}), \tag{6}$$

where the fourth-order tensor $\widehat{\boldsymbol{\mathcal{A}}}$ decomposed in the eigenvector basis $\{\mathbf{u}_{\mathsf{K}}\}$ is represented by the following non-vanishing components

$$\widehat{\mathcal{A}}_{\mathsf{IJIJ}} = \widehat{\mathcal{A}}_{\mathsf{IJJI}} = \begin{cases} \delta_{\mathsf{IJ}}\, u_{\mathsf{I}} f'(u_{\mathsf{I}}) & \text{for } u_{\mathsf{I}} = u_{\mathsf{J}}, \\ \frac{u_{\mathsf{I}} u_{\mathsf{J}}[f(u_{\mathsf{I}}) - f(u_{\mathsf{J}})]}{u_{\mathsf{I}}^2 - u_{\mathsf{J}}^2} & \text{for } u_{\mathsf{I}} \neq u_{\mathsf{J}}, \end{cases} \tag{7}$$

where $f'(u_{\mathsf{I}}) = \frac{df(u)}{du}\big|_{u=u_{\mathsf{I}}}$. A rigorous proof of (7) has been given in [15]. Relation (6) was noted in [7] and re-derived by many authors. Nevertheless, in the further papers, the thermodynamical consequences of this relation for the stress in anisotropic materials were ignored because the *multiplicative* decomposition (6) was immediately replaced by an *additive* one. For example, instead of (6) and (18) the following decomposition was used $\frac{d}{dt}\ln \mathbf{U} = \mathbf{R}^T\mathbf{d}\mathbf{R} + \mathbf{O}(\mathbf{E}^2)$ where $\mathbf{O}(\mathbf{E}^2)$ was neglected as a second order term, cf. [16, 8].

Substituting (5) and (6) into (3) we find

$$-\frac{\rho}{\widehat{\rho}}\,(\widehat{\rho}\frac{\partial \psi}{\partial \widehat{\boldsymbol{\varepsilon}}}) : \widehat{\boldsymbol{\mathcal{A}}} : (\mathbf{R}^T\mathbf{d}\,\mathbf{R}) + \boldsymbol{\sigma} : \mathbf{d} = 0, \tag{8}$$

where $\widehat{\rho} = \rho \det \mathbf{F}$. To balance energy for arbitrarily chosen $\mathbf{d}$, the Cauchy stress has to be governed by the following constitutive equation

$$\boxed{\boldsymbol{\sigma} = \mathbf{R}(\widehat{\boldsymbol{\mathcal{A}}} : \widehat{\rho}\frac{\partial \psi}{\partial \widehat{\boldsymbol{\varepsilon}}})\mathbf{R}^T \det \mathbf{F}^{-1}.} \tag{9}$$

The above equation can be rewritten in the form of the following transformation rule

$$\boldsymbol{\sigma} = \mathbf{R}(\widehat{\boldsymbol{\mathcal{A}}} : \widehat{\boldsymbol{\sigma}})\mathbf{R}^T \det \mathbf{F}^{-1}, \tag{10}$$

where $\widehat{\boldsymbol{\sigma}}$ denotes the stress measure conjugate to the Lagrangian strain tensor $\widehat{\boldsymbol{\varepsilon}}$ calculated as $\widehat{\boldsymbol{\sigma}} \stackrel{df}{=} \widehat{\rho}\,\partial\psi/\partial\widehat{\boldsymbol{\varepsilon}}$.

### 2.1 Second-order elastic constants

Let us consider the hyperelastic material governed by the constitutive equation for the specific internal energy in the form

$$\psi = \frac{1}{2\widehat{\rho}}\,\widehat{\boldsymbol{\varepsilon}} : \widehat{\mathbf{c}} : \widehat{\boldsymbol{\varepsilon}}\ , \tag{11}$$

where $\widehat{\mathbf{c}}$ is the fourth-order elastic stiffness tensor. Substitution into (9) leads to

$$\boldsymbol{\sigma} = \mathbf{R}(\widehat{\boldsymbol{\mathcal{A}}} : \widehat{\mathbf{c}} : \widehat{\boldsymbol{\varepsilon}})\mathbf{R}^T \det \mathbf{F}^{-1}. \tag{12}$$

The above equation can be rewritten in terms of tensorial measures referred to the current configuration. Then we find

$$\boldsymbol{\tau} = \boldsymbol{\mathcal{A}} : \mathbf{c} : \boldsymbol{\varepsilon}, \tag{13}$$

where $\boldsymbol{\tau}$ denotes the Kirchhoff stress and

$$\boldsymbol{\tau} = \boldsymbol{\sigma} \det \mathbf{F}, \qquad c^{klmn} = R^k{}_K R^l{}_L R^m{}_M R^n{}_N\, \widehat{c}^{KLMN}, \tag{14}$$

$$\boldsymbol{\varepsilon} = \mathbf{R}\widehat{\boldsymbol{\varepsilon}}\mathbf{R}^T, \qquad \mathcal{A}_{\mathsf{ijij}} = \begin{cases} \delta_{\mathsf{ij}}\, v_{\mathsf{i}} f'(v_{\mathsf{i}}) & \text{for } v_{\mathsf{i}} = v_{\mathsf{j}}, \\ \frac{v_{\mathsf{i}} v_{\mathsf{j}}[f(v_{\mathsf{i}}) - f(v_{\mathsf{j}})]}{v_{\mathsf{i}}^2 - v_{\mathsf{j}}^2} & \text{for } v_{\mathsf{i}} \neq v_{\mathsf{j}}, \end{cases} \tag{15}$$

The components $\mathcal{A}_{ijij}$ are referred to the vector basis composed of eigenvectors $\mathbf{v}_i$ of $\mathbf{V}$, cf. (7). Equation (13) can be rewritten in the following incremental form

$$\overset{\nabla}{\boldsymbol{\tau}} = \boldsymbol{\mathcal{A}} : \mathbf{c} : \overset{\nabla}{\boldsymbol{\varepsilon}} + \left( \frac{\partial \boldsymbol{\mathcal{A}}}{\partial \boldsymbol{\varepsilon}} : \overset{\nabla}{\boldsymbol{\varepsilon}} \right) : \mathbf{c} : \boldsymbol{\varepsilon}, \tag{16}$$

where $\nabla$ denotes the Zaremba-Jauman derivative corresponding to the rigid rotation rate $\mathbf{w} = \dot{\mathbf{R}}\mathbf{R}^T$, i.e. $\overset{\nabla}{\boldsymbol{\tau}} = \dot{\boldsymbol{\tau}} - \mathbf{w}\boldsymbol{\tau} + \boldsymbol{\tau}\mathbf{w}$. This form is very simple in comparison to other incremental descriptions adapted to hyperelasticity, cf. [12].

**Logarithmic hyperelasticity** The constitutive equations discussed above concern many constitutive models. Logarithmic strain tensors are defined as

$$\widehat{\boldsymbol{\varepsilon}} \overset{df}{=} \ln \mathbf{U} \qquad \text{and} \qquad \boldsymbol{\varepsilon} \overset{df}{=} \ln \mathbf{V}. \tag{17}$$

Assuming the internal energy function in the form (11) the stress-strain constitutive equation for anisotropic hyperelastic model takes the form of (12) and (13). Then, for the generally anisotropic logarithmic hyperelastic model the representation of the fourth-order tensors $\widehat{\boldsymbol{\mathcal{A}}}$ in the eigenvector basis $\{\mathbf{u}_I\}$ takes the form

$$\widehat{\mathcal{A}}_{IJIJ} = \begin{cases} \delta_{IJ} & \text{for } \widehat{\varepsilon}_I = \widehat{\varepsilon}_J, \\ \dfrac{(\widehat{\varepsilon}_I - \widehat{\varepsilon}_J)}{e^{\widehat{\varepsilon}_I - \widehat{\varepsilon}_J} - e^{\widehat{\varepsilon}_J - \widehat{\varepsilon}_I}} & \text{for } \widehat{\varepsilon}_I \neq \widehat{\varepsilon}_J. \end{cases} \tag{18}$$

Since $\varepsilon_i = \widehat{\varepsilon}_I$, we find $\mathcal{A}_{ijij} = \widehat{\mathcal{A}}_{IJIJ}$.

### 2.2 Third-order elastic constants

Third-order elastic constants can be determined by measuring small changes of ultrasonic wave velocities in stressed crystals. Usually, they are determined for the constitutive relation between the second Piola-Kirchhoff stress and the Green strain called often the Lagrangian strain, see [17, 18, 19, 20] among many others. So, let us assume here that a hyperelastic material satisfies a specific energy function of the form

$$\psi(\widehat{\boldsymbol{\varepsilon}}) = \frac{1}{\widehat{\rho}} \left[ \frac{1}{2!} \widehat{c}^{ijkl} \widehat{\varepsilon}_{ij} \widehat{\varepsilon}_{kl} + \frac{1}{3!} \widehat{C}^{ijklmn} \widehat{\varepsilon}_{ij} \widehat{\varepsilon}_{kl} \widehat{\varepsilon}_{mn} \right], \tag{19}$$

where $\widehat{\mathbf{c}}$ and $\widehat{\mathbf{C}}$ are tensors of the second- and third-order elastic constants determined in relation to a particular strain measure of the family (2). Obviously, we can rewrite (19) by using another strain measure, say

$$\widehat{\boldsymbol{\varepsilon}}' = \frac{1}{m'} (\mathbf{U}^{m'} - \mathbf{1}). \tag{20}$$

On solving (20) with respect to $\mathbf{U}$ and substituting into (2a) we find the following isotropic tensor function

$$\widehat{\boldsymbol{\varepsilon}}(\widehat{\boldsymbol{\varepsilon}}') = \frac{1}{m} \left[ (m' \widehat{\varepsilon}'_i + 1)^{\frac{m}{m'}} - 1 \right] \mathbf{u}_i \otimes \mathbf{u}_i, \tag{21}$$

| m | $C_{111}$ | $C_{112}$ | $C_{123}$ | $C_{144}$ | $C_{155}$ | $C_{456}$ | $c_{11}$ | $c_{12}$ | $c_{44}$ | Exptl |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | -1076 | -315 | 36 | -23 | -340 | -30 | 106 | 60 | 28 | [21] |
| 0 | -440 | -195 | 36 | 37 | -201 | 12 | 106 | 60 | 28 | |
| -1.384 | 0 | -112 | 36 | 79 | -105 | -1 | 106 | 60 | 28 | |

Table 1: Dependence of elastic constants [GPa] on different strain measures for aluminium crystal.

where $\widehat{\varepsilon}'_{\mathsf{i}}$ is the $i$-th eigenvalue of $\widehat{\boldsymbol{\varepsilon}}'$ while $\mathbf{u}_{\mathsf{i}}$ is the eigenvector of both $\widehat{\boldsymbol{\varepsilon}}'$, $\widehat{\boldsymbol{\varepsilon}}$ and $\mathbf{U}$. Let us decompose the specific internal energy function into a power series

$$\psi(\widehat{\boldsymbol{\varepsilon}}(\widehat{\boldsymbol{\varepsilon}}')) = \frac{1}{\widehat{\rho}}\left[\frac{1}{2!}\widehat{c}'^{ijkl}\widehat{\varepsilon}'_{ij}\widehat{\varepsilon}'_{kl} + \frac{1}{3!}\widehat{C}'^{ijklmn}\widehat{\varepsilon}'_{ij}\widehat{\varepsilon}'_{kl}\widehat{\varepsilon}'_{mn} + \cdots\right], \tag{22}$$

where

$$\mathbf{c}' = \frac{1}{\widehat{\rho}\,2!}\left.\frac{\partial^2\psi(\widehat{\boldsymbol{\varepsilon}}(\widehat{\boldsymbol{\varepsilon}}'))}{\partial\widehat{\boldsymbol{\varepsilon}}'\partial\widehat{\boldsymbol{\varepsilon}}'}\right|_{\widehat{\boldsymbol{\varepsilon}}'=\mathbf{0}}, \qquad \mathbf{C}' = \frac{1}{\widehat{\rho}\,3!}\left.\frac{\partial^3\psi(\widehat{\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}'))}{\partial\widehat{\boldsymbol{\varepsilon}}'\partial\widehat{\boldsymbol{\varepsilon}}'\partial\widehat{\boldsymbol{\varepsilon}}'}\right|_{\widehat{\boldsymbol{\varepsilon}}'=\mathbf{0}}, \qquad \cdots. \tag{23}$$

Substitution of (22) and (21) into (23) followed by use of the known formula for derivatives of an isotropic proper-symmetric fourth-order tensor function of a symmetric second-order tensor yields

$$\widehat{c}'^{ijkl} = \widehat{c}^{ijkl}, \tag{24}$$

$$\widehat{C}'^{ijklmn} = \widehat{C}^{ijklmn} + (m-m')\left[\mathcal{J}^{ijkl}{}_{ab}\widehat{c}^{abmn} + \mathcal{J}^{klmn}{}_{ab}\widehat{c}^{abij} + \mathcal{J}^{mnij}{}_{ab}\widehat{c}^{abkl}\right], \tag{25}$$

where the representation of $\boldsymbol{\mathcal{J}}$ written in any chosen orthonormal coordinate set takes the form

$$\begin{aligned}\mathcal{J}_{\mathsf{ijklmn}} =& \frac{1}{8}(\delta_{\mathsf{ik}}\delta_{\mathsf{jm}}\delta_{\mathsf{ln}} + \delta_{\mathsf{ik}}\delta_{\mathsf{jn}}\delta_{\mathsf{lm}} + \delta_{\mathsf{il}}\delta_{\mathsf{jm}}\delta_{\mathsf{kn}} + \delta_{\mathsf{il}}\delta_{\mathsf{jn}}\delta_{\mathsf{km}} \\ &+ \delta_{\mathsf{im}}\delta_{\mathsf{jk}}\delta_{\mathsf{ln}} + \delta_{\mathsf{im}}\delta_{\mathsf{jl}}\delta_{\mathsf{kn}} + \delta_{\mathsf{in}}\delta_{\mathsf{jk}}\delta_{\mathsf{lm}} + \delta_{\mathsf{in}}\delta_{\mathsf{jl}}\delta_{\mathsf{km}}),\end{aligned} \tag{26}$$

cf. eqns (3.5.33-34) in [14]. Since the strains and stress are symmetric, only six among nine components are independent therefore it is convenient to use the Voight notation reducing the number of subscripts $11 \to 1$, $22 \to 2$, $33 \to 3$, $23 \to 4$, $13 \to 5$, $12 \to 6$. Then, for cubic symmetry, equation (25) gives the following relations between the third-order elastic constants determined for two different strain measures (2) and (20),

$$\widehat{C}'_{111} = \widehat{C}_{111} + (m-m')3\widehat{c}_{11}, \qquad \widehat{C}'_{144} = \widehat{C}_{144} + (m-m')\frac{1}{2}\widehat{c}_{12}, \tag{27}$$

$$\widehat{C}'_{112} = \widehat{C}_{112} + (m-m')\widehat{c}_{12}, \qquad \widehat{C}'_{155} = \widehat{C}_{155} + (m-m')[\widehat{c}_{44} + \frac{1}{4}\widehat{c}_{12} + \frac{1}{4}\widehat{c}_{11}], \tag{28}$$

$$\widehat{C}'_{123} = \widehat{C}_{123}, \qquad \widehat{C}'_{456} = \widehat{C}_{456} + (m-m')\frac{3}{4}\widehat{c}_{44}. \tag{29}$$

In table 1 the third- and second-order elastic constants determined experimentally for the Green strain [20, 22, 23, 21, 19] have been recalculated to elastic constants corresponding to the logarithmic strain measure ($m = 0$) and to another strain which has been such chosen as to vanish the elastic constant $C_{111}$.

## 3 Finite element model

The physical model presented in the previous section has been implemented within the finite element method. As a result, a computational tool for analyzing non-standard problems, namely those involving large-strain deformation processes of anisotropic hyperelastic materials has been developed. The general discretization patterns used in the finite element method have been followed, but accounting for the special features of the present problem.

We start considering the weighted equilibrium equation in its weak form, where, following the Galerkin method, the weighting functions are equal to the shape functions $\mathbf{N}$ in terms of which the displacement field is discretized ($\mathbf{u} = \mathbf{N}^{\mathrm{T}}\mathbf{a}$)

$$\int_v N_{\mathsf{k}}\sigma_{ij,j}\mathrm{d}v = \int_v N_{\mathsf{k}} f_j \mathrm{d}v, \tag{30}$$

where $v$ is the discretized domain in the current configuration and $f$ is volume distributed forces. By integrating by parts the left-hand side of Eq. (30) we can write

$$\int_v N_{\mathsf{k},j}\sigma_{ij}\mathrm{d}v = -\int_v N_{\mathsf{k}} f_j \mathrm{d}v + \int_{\partial v} N_{\mathsf{k}}\sigma_{ij} n_j \mathrm{d}(\partial v), \tag{31}$$

where $n_j$ is the outward normal vector to the boundary $\partial v$. In the above system of equations it is the discretized displacement $a_{\mathsf{i}}$ that it is solved for. The actual configuration and the stress tensor (through the strain tensor and the proper transformation) are functions of them. Since Eq. (31) is non-linear in the discretized variables, it is solved by iterations. To this aim we write it in residual form as

$$\mathbf{P}(\mathbf{a}) = \int_v N_{\mathsf{k},j}\sigma_{ij}\mathrm{d}v + \int_v N_{\mathsf{k}} f_j \mathrm{d}v - \int_{\partial v} N_{\mathsf{k}}\sigma_{ij} n_j \mathrm{d}(\partial v) \tag{32}$$

To arrive at the solution of Eq. (32) we require

$$||\mathbf{P}(\mathbf{a})|| < \delta, \tag{33}$$

where $\delta$ is a convergence tolerance. To meet this condition we calculate the correction to the solution vector $\mathbf{a}$ so as to zero a one term series expansion of the residual at $\mathbf{a}$. Denoting with a right upper index the iteration number, we require that

$$\mathbf{P}(\mathbf{a}^{\omega+1}) = \mathbf{P}(\mathbf{a}^{\omega}) + \frac{\partial \mathbf{P}(\mathbf{a}^{\omega})}{\partial \mathbf{a}}(\mathbf{a}^{\omega+1} - \mathbf{a}^{\omega}) = \mathbf{0} \tag{34}$$

from which we solve for $(\mathbf{a}^{\omega+1} - \mathbf{a}^{\omega})$ using the so-called tangent matrix as the system matrix

$$\begin{aligned}
\mathbf{K} &= \frac{\partial \mathbf{P}}{\partial \mathbf{a}} = \frac{\partial \int_v \boldsymbol{\nabla}\mathbf{N}\boldsymbol{\sigma}(\mathbf{a})dv}{\partial \mathbf{a}} = \frac{\partial \int_V \boldsymbol{\nabla}\mathbf{N}\boldsymbol{\sigma}(\mathbf{a})\frac{dv}{dV}dV}{\partial \mathbf{a}} = \int_V \frac{\partial[\boldsymbol{\nabla}\mathbf{N}\boldsymbol{\sigma}(\mathbf{a})\frac{dv}{dV}]dV}{\partial \mathbf{a}} = \\
&= \int_V \frac{\partial(\boldsymbol{\nabla}\mathbf{N})}{\partial \mathbf{a}}\boldsymbol{\sigma}(a)\frac{dv}{dV}dV + \int_V \boldsymbol{\nabla}\mathbf{N}\frac{\partial[\boldsymbol{\sigma}(\mathbf{a})\frac{dv}{dV}]}{\partial \mathbf{a}}dV = \\
&= \int_v \frac{\partial(\boldsymbol{\nabla}\mathbf{N})}{\partial \mathbf{a}}\boldsymbol{\sigma}(a)dv + \int_V \boldsymbol{\nabla}\mathbf{N}\frac{\partial[\boldsymbol{\sigma}(\mathbf{a})\frac{dv}{dV}]}{\partial \mathbf{a}}\frac{dV}{dv}dv
\end{aligned} \tag{35}$$

On the other hand the first member in the last equation involves the derivative of the shape function. It is easy to note that this derivative changes sign many times within a single element. Due to the convergence of the Newton-Raphson method for large deformations, when the configuration searched for is far away from the initial one, this term has been dropped. This assumption only affects the solution procedure, but not the system of equations we are solving, defined by the residual $\mathbf{P}(\mathbf{a})$, equation (34). Summing up we have employed the following tangent matrix

$$K_{\mathrm{ij}} \approx \int_v \boldsymbol{\nabla}\mathbf{N}_{\mathrm{i}} \frac{\partial[\boldsymbol{\sigma}(\mathbf{a})\det\mathbf{F}]}{\partial \mathbf{a}_{\mathrm{j}}} \det\mathbf{F}^{-1} dv = \int_v \boldsymbol{\nabla}\mathbf{N}_{\mathrm{i}} \frac{\partial[\boldsymbol{\sigma}(\mathbf{a})\det\mathbf{F}]}{\partial \mathbf{F}} \frac{\partial \mathbf{F}}{\partial \mathbf{a}_{\mathrm{j}}} \det\mathbf{F}^{-1} dv \quad (36)$$

The constitutive model has been implemented into the FEAP program [24] as a new user element.

According to (36) the process of calculating the tangent matrix has been split into two steps: the first one concerning the constitutive relations and the second concerning the nonlinear geometry relations. The first term rewritten in an orthonormal coordinate set is composed by the following analytical terms

$$\begin{aligned}\frac{\partial(\sigma_{ij}\det\mathbf{F})}{\partial F_{kl}} = &\left(\frac{\partial R_{im}}{\partial F_{kl}} R_{jn} + R_{im}\frac{\partial R_{jn}}{\partial F_{kl}}\right)\widehat{\mathcal{A}}_{mnpr}\widehat{c}_{prst}\widehat{\varepsilon}_{st} \\ &+ R_{im}R_{jn}\left(\frac{\partial \widehat{\mathcal{A}}_{mnpr}}{\partial F_{kl}}\widehat{c}_{prst}\widehat{\varepsilon}_{st} + \widehat{\mathcal{A}}_{mnpr}\widehat{c}_{prst}\frac{\partial \widehat{\varepsilon}_{st}}{\partial F_{kl}}\right). \end{aligned} \quad (37)$$

From the viewpoint of Fortran programming this analytically advanced dependence has been implemented together with the constitutive equation (9) into a single subroutine,

`subroutine sigma(F,`$m, \widehat{\mathbf{c}}, \boldsymbol{\sigma}, \frac{\partial(\boldsymbol{\sigma}\det\mathbf{F})}{\partial\mathbf{F}}$`,isw)`. This subroutine, on the basis of the deformation gradient, strain parameter, and elastic constants, calculates the Cauchy stress and optionally (for `isw` =3) the respective derivative of the Kirchhoff stress needed to determine the matrix equation. Due to the complex dependencies on $\mathbf{F}$ the mentioned derivative has been calculated numerically.

The second term takes the form, cf. [25],

$$\frac{\partial F_{kl}}{\partial a_{\mathrm{i}j}} = F_{km}[g_{mj}\, F_{nl}\nabla_n N_{\mathrm{i}} + u_m N_{\mathrm{i},jn}]F_{nl}. \quad (38)$$

Let us consider how the presented scheme works for elastic-plastic deformation. Let the total deformation gradient describing the deformation of crystal lattice be decomposed into the rigid rotation of material microstructure together with the elastic stretch of crystal lattice and plastic deformation according to

$$\mathbf{F} = \underbrace{\mathbf{R}\mathbf{U}}_{\mathbf{F}_{\mathrm{lt}}}\mathbf{F}_{\mathrm{p}}. \quad (39)$$

Then, independently of the constitutive equations for plastic deformation flow the calculation of the derivative discussed above can be divided into two parts

$$\frac{\partial[\boldsymbol{\sigma}(\mathbf{a})\frac{dv}{dV}]}{\partial\mathbf{F}} = \frac{\partial[\boldsymbol{\sigma}(\mathbf{a})\frac{dv}{dV}]}{\partial\mathbf{F}_{\mathrm{lt}}}\frac{\partial\mathbf{F}_{\mathrm{lt}}}{\partial\mathbf{F}}, \quad (40)$$

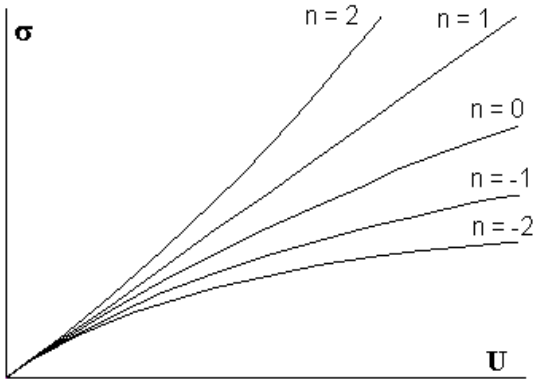


Figure 1: Cauchy stress versus various strain measures applied in (12) for isotropic elastic material.

where

$$\frac{\partial(\sigma_{ij}\det\mathbf{F}_{\rm lt})}{\partial F_{{\rm lt}kl}} = \left(\frac{\partial R_{im}}{\partial F_{{\rm lt}kl}}R_{jn} + R_{im}\frac{\partial R_{jn}}{\partial F_{{\rm lt}kl}}\right)\widehat{\mathcal{A}}_{mnpr}\widehat{c}_{prst}\widehat{\varepsilon}_{st} + R_{im}R_{jn}\left(\frac{\partial\widehat{\mathcal{A}}_{mnpr}}{\partial F_{{\rm lt}kl}}\widehat{c}_{prst}\widehat{\varepsilon}_{st} + \widehat{\mathcal{A}}_{mnpr}\widehat{c}_{prst}\frac{\partial\widehat{\varepsilon}_{st}}{\partial F_{{\rm lt}kl}}\right), \tag{41}$$

$$\frac{\partial F_{{\rm lt}kl}}{\partial F_{mn}} = g_{km}F^{-1}_{{\rm p}nl} \tag{42}$$

what means that the same subroutine as previously can be now employed to determine the main component of the tangent matrix, `subroutine sigma(`$\mathbf{F}_{\rm lt}, m, \widehat{\mathbf{c}}, \boldsymbol{\sigma}, \frac{\partial(\boldsymbol{\sigma}\det\mathbf{F}_{\rm lt})}{\partial\mathbf{F}_{\rm lt}}$`,isw)`.

## 4 Numerical results

In this paper our interest is focused on the nonlinear elastic behaviour of the hyperelastic constitutive model based on logarithmic strain measure. Figure 1 shows the stress-strain behaviour of isotropic hyperelastic constitutive models based upon so-called generalized strain measure. This nonlinear elastic effect is responsible for many important phenomena. For example the tension and compression stress fields around an edge dislocation do not take the mirror distributions what manifests the local volume expansion induced by a single edge dislocation in the crystal lattice. In the example presented below this effect is analysed for the logarithmic hyperelastic model.

**Example** In this example we analyse the volume change effect induced by edge dislocations situated in [001] crystal plane in an aluminium crystal. Their Burgers vector takes value $\pm\frac{1}{2}$[110], see Fig. 2. To input the dislocations into crystal lattice we have assumed a source (plastic) distortion field which has been such chosen that its volume effect vanish. To do it the respective source distortion corresponding to $F^u_{\rm p11} = 1.1328$ has been assumed locally in the upper row of elements and $F^l_{\rm p11} = 1/F^u_{\rm p11}$ in the

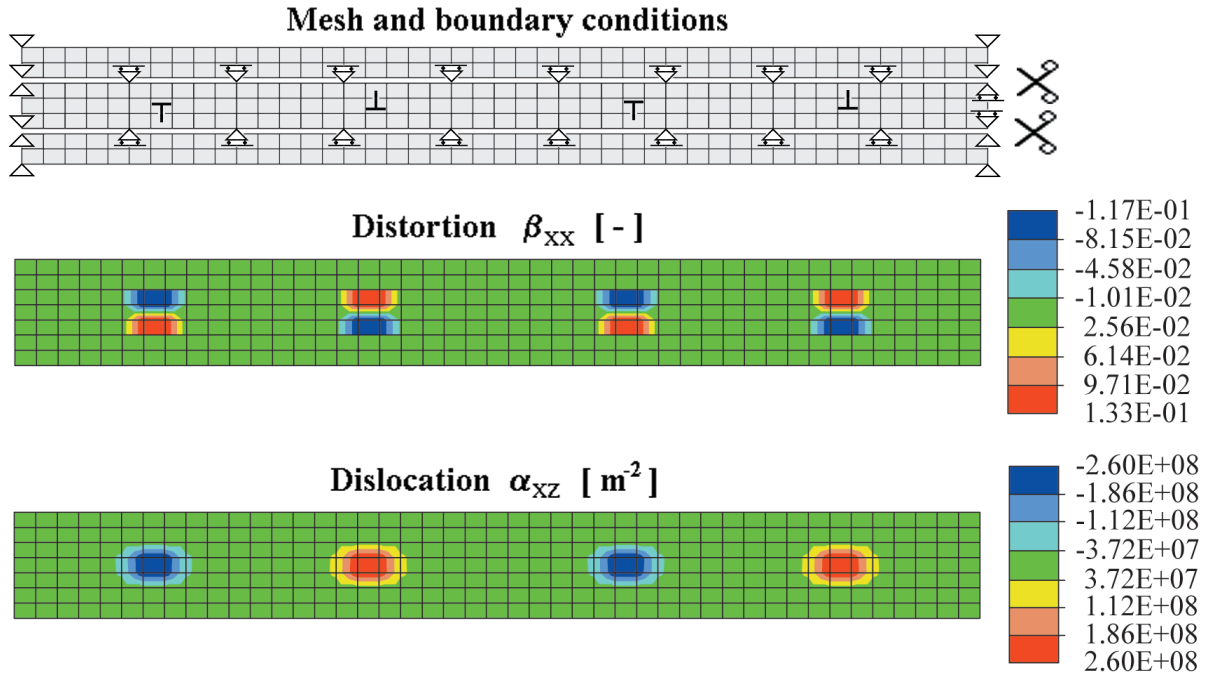


Figure 2: Initial FE mesh and the source distortion assumed.

lower one. The proportion between the upper and lower source distortions have been such chosen as to preserve the constant volume change, $\int_V \det \mathbf{F}_{\mathrm{p}} dV = 0$. With respect to the bilinear shape function the true Burgers vector can be determined as

$$\widehat{b}_1 = \int_{x^u_{n-2}}^{x^u_{n+1}} F_{\mathrm{p}11} dx - \int_{x^l_{n-2}}^{x^l_{n+1}} F_{\mathrm{p}11} dx. \tag{43}$$

In the upper row elements the $F^u_{\mathrm{p}11}$ takes a triangle distribution from zero in $x_{n-2}$ till 1.1328 in node $x_{n-1}$ next it takes the constant value in the element with nodes $x_{n-1}$ and $x_n$ and finally takes a triangle distribution in the element with nodes $x_n$ and $x_{n+1}$. The integration (43) over the Lagrangian configuration gives $\widehat{b}_1 = (1.1328 - 1/1.1328) * 2\sqrt{2}\widehat{a} \approx \frac{\sqrt{2}}{2} * \widehat{a}$. The components $\alpha_{13}$ of the dislocation distribution tensor is determined here by $\boldsymbol{\alpha} = \mathbf{F} \operatorname{grad} \mathbf{F}_{\mathrm{p}}^{-1} \dot{\times} \mathbf{F}_{\mathrm{lt}}^{-1}$ where $\dot{\times}$ denotes the double product the scalar one over the first indices and cross one over seconds, see e.g. [26, 27]. For the mentioned component this formula rewritten in the orthonormal coordinate set is used in FE code and gives $\alpha_{13} = F_{11} F^{-1}_{\mathrm{p}11,2} F^{-1}_{\mathrm{lt}11} e_{213}$, where the comma denotes differentiation over the actual (current) configuration of the crystal lattice while the alternating tensor component is $e_{213} = -1$. The obtained deformation of the crystal lattice is shown in Fig.3. The nonlinear elasticity gives different sizes for tension and compression regions what manifests the volume expansion of crystal lattice leading to elongation of the dislocated region. This elongation was possible here with respect to the fictitious cutting assumed. In real materials due to nonlinear elastic effects the interfacial dislocations introduce a local surface compression in the interfacial atomic layers, what leads simultaneously to tension in the neighbouring atomic layers. The thermodynamic foundations of this effect was discussed from the viewpoint of continuum thermodynamics of anisotropic hyperelasticity in [28].

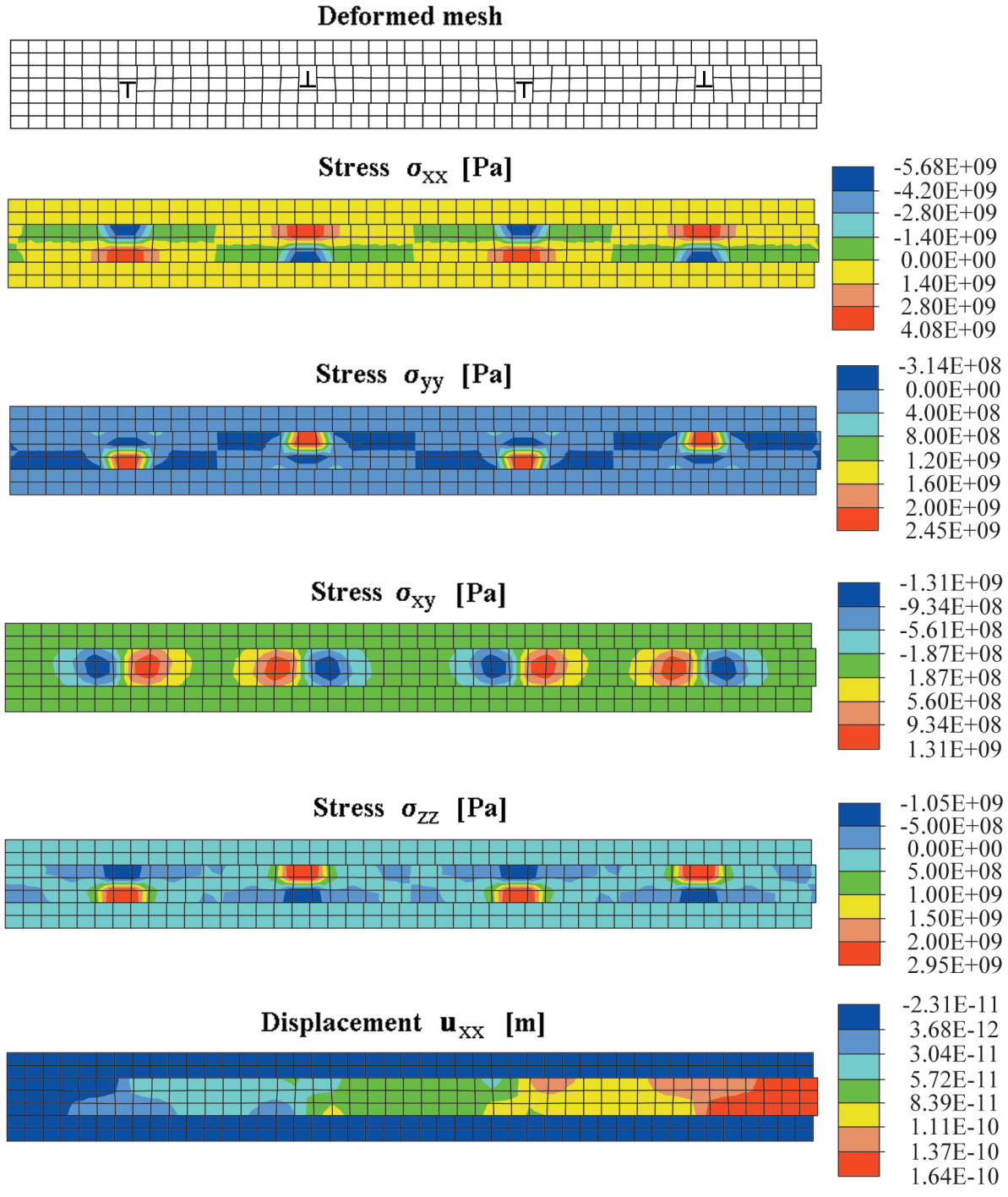


Figure 3: FE mesh deformed, resultant stress and displacement distribution.

## 5 Summary

A new FE algorithm for solving boundary value problems for anisotropic hyperelastic materials has been presented. The constitutive equations applied are based on the generalized strain measure and take into account the second- and third-order elastic constants. The equations have been derived from the thermodynamic balance of the elastic energy. In the example presented it has been shown that the nonlinear elasticity taking into account elastic softening for tension and elastic stiffening for compression influences on the local volume expansion of an elastic continuum including an edge dislocation. When a group of edge dislocations is situated on a given surface this effect results in the surface tension observed in thin layers of crystalline structures.

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