FEM-modelling of SSRT
for Corrosion Tests

Bachelor’s Thesis in applied mathematics

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Abstract

This thesis discusses the mathematical formulation and computational treatment of slow strain rate corrosion tests based on nonlinear finite elements methods. The theory is illustrated by a description of classical small strain elastoplasticity theory as implemented in the Comsol Multiphysics 3.2 software package. The possible extension of the theory to finite strain is briefly addressed. Practical simulations and results regarding the evolution of stresses, strains and geometric deformation are also presented and discussed. Experimental data used in simulation were reported by Onchi, Takeo et al. and published in Journal of Nuclear Science and Technology in May 2006.
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1 Introduction

1.1 Stress corrosion cracking
Through the simultaneous action of stresses and a corrosive environment, normally highly ductile and corrosion resistant metals can sometimes experience brittle cracks well below its usual fracture strength. This phenomenon, known as stress corrosion cracking (SCC), can in the worst case cause unexpected failure in structures. The stresses can be due to externally applied forces, or be residual stresses resulting from e.g. welding, cold working or radiation. A very large number of factors can affect the occurrence of SCC, making it difficult to predict.

1.2 Slow strain rate test
When testing for stress corrosion, a slow strain rate tensile (SSRT) test can be performed in a corrosive environment. Often more than one specimen type and several variations of test specimen configuration are tested. To detect initiation of SCC a current can be sent through the specimen body in order to measure the increased resistance when a crack is formed. Knowledge about the geometric changes of a loaded specimen without crack formation is therefore needed. There can also be a need to model local stresses and strains in the specimen.

1.3 Computer simulations
Computer simulations can be used in connection with SSRT to give more or less crude predictions of the outcome. To model a specimen subjected to mechanical loading, conservational laws from continuum mechanics can be combined with equations describing the material itself to form a PDE boundary value problem. The boundary value problem can be discretized and solved numerically using the finite element method (FEM). FEM based simulation can give answers about the local stresses and strains produced during the test, as well as the geometrical shape changes of the specimen. Parameters specific to the material and test environment can be determined from SSRT:s using specimen of more simple shape.

1.4 Aims of this work

- To explore and discuss the possibilities of using simulation with FEM methods as a complement to real SSRT testings. In particular, to explore the possibilities and functionality of the Comsol Multiphysics 3.2 software package.
- To discuss the mathematical formulation of SSRT with ductile metals without cracks and other damage, as well as solution methods and computational methods implemented in solid mechanics software.
- To present and discuss results regarding stresses and strains as well as deformation of a simulated SSRT using some specifically shaped specimen. Interesting results for Studsvik Nuclear are the evolution of local stresses and strains as a function of specimen elongation, as well as overall stress distribution and the propagation of plastic regions. This information is of great importance when planning physical tests.
2 Modeling the SSRT

In this work the modeling of SSRT that does not take the actual crack formation process into account is studied. The test specimen is thus here assumed to be subject to loading in a non-corrosive environment, to be compared with various real tests in corrosive or non-corrosive environments. The simulations are especially useful as crude predictions in the planning stage of testing.

2.1 Test specimen

For the simulations in this work a set square shaped stainless steel (SS) specimen with a rounded corner, a so called hump, has been used, see Figure 1. The hump causes a local stress concentration as a tensile load is applied to the specimen. This shape gives some advantages, for example regarding time efficiency, in practical testing for SCC and other phenomena.

![Figure 1](image)

*Figure 1* Test specimen of a corrosion resistant SS alloy with a hump causing a stress concentration. The grey circles illustrate how the geometry is defined, and has no other physical meaning. The specimen waist including the rounded ends are 29 mm.
2.2.1 Material behavior

A number of assumptions regarding what physics affect the specimen during SSRT can be stated already at this point.

- Inertial effects are negligible.
- Thermal effects, e.g. from temperature variations due to plastic straining are negligible.
- For the range of slow local strain rates appearing during the test, the hardening behavior of the material is strain rate insensitive.
- For the temperature and time scales used, creep effects are negligible.

The last assumptions depends on that test temperature is kept at a sufficiently low fraction of the melting point of the steel used. A rule of thumb says that creep effects in steel become noticeable at about 30% of the melting point – which is higher than is assumed in simulations described later. Also the time scales are rather short in creep terms, measured in hours or days. My conclusion is that these assumptions should not be considered restrictive under the given circumstances.

Next, a further limitation is added to the model: The specimen is not contracting brittle, corrosion induced cracks, yet not reaching stress levels required to cause unstable strain localization or non-ductile failure. This can be formulated as an additional physics property of the test:

- The specimen is only subject to elastic and plastic ductile deformation.

As a result of the above assumptions, the SSRT can mathematically be described as a deforming continuum obeying a simplified form of the four conservational laws used in computational solid thermomechanics, as will be seen in section 3.2. A constitutive law relating the evolution of stress and plastic strain to strain is also needed. The constitutive law is of course highly material and environment dependent. This subject is addressed in section 3.3.
2.2.2 Lagrangian continuum formulation

The specimen can mathematically be defined as an indestructible continuum body, at the initial state of the test occupying a closed domain $\Omega$ in space, with boundary $\Gamma$. In Lagrangian formulation, predominantly used in mathematical descriptions of solid mechanics, the independent variables of the system are $X$ and $t$, where $X = (X_1, X_2, X_3) \in \Omega$ are the coordinates in space for a particle of matter in $\Omega$, and $t$ is time [5]. The gradual deformation of the body subject to loading can then be characterized by the displacement field:

$$u(X, t) = x(X, t) - X,$$  \hspace{1cm} (2.2.1)

where $x = x(X, t)$ are the coordinates at the time $t$ of a particle originally positioned at $X$. In Comsol Multiphysics 3.2 solid mechanics module, a total Lagrange formulation, as opposed to updated Lagrange, is used for problems with large deformations (this should not be confused with the similar but not quite equal notion of large strain, as will be seen later). In the total Lagrange formulation, all derivatives and integrals are computed over the undeformed geometric body [5]. The two different Lagrange formulations are in fact equivalent, leaving the choice to be based on practical or computational considerations.

Deformation can typically depend on over time evolving boundary conditions imposing prescribed displacements or tractions on the geometry surface. At the same time a number of fundamental continuum conservational laws are enforced.

![Figure 3. The symmetry cuts and an additional boundary, all marked in blue, are fixed in order to as far as possible allow for a unique deformation path as the red boundary evolves in the x-direction. This means that displacements in the normal direction of the blue marked boundaries are prohibited throughout the test. The boundary marked in red obeys a time-dependent displacement or traction boundary condition representing the load on the structure.](image-url)
2.2.3 Boundary conditions

The boundary conditions are prescribed values of displacement or surface traction (defined as force/unit area) in each coordinate direction at each point on the boundary of the specimen geometry. In Comsol Multiphysics, the boundary values are by default surface tractions in all directions set to zero at all times.

Now consider the specimen of Figure 1. Because of the two symmetries, it can for the computation be reduced in size by three quarters, see Figure 3 above. This will have a significant impact on performance, as memory requirement increases quadratically with the number of degrees of freedom. To “fix” the specimen in space, three sets of homogenous displacement boundary conditions, are imposed. At each of the blue boundaries in the figure, displacements in the normal direction of the boundary are prohibited. Note that we only fix the boundary in one coordinate direction: in the other two the boundaries still only obey the zero surface traction condition.

To define the load acting on the structure, on the red colored boundary is imposed a prescribed evolution of displacement in the normal direction, governed by a monotonically increasing parameter analogous to time. The system is thus solved for incremental time steps, each time using as initial values data computed at the previous time step. This parametric representation of time is possible for equilibrium (time independent) problems, and the solutions obtained in this way are called incremental solutions [2].

Load could also be defined in terms of prescribed surface tractions in the same way. In the Lagrangian formulation, boundary tractions are prescribed as force per unit of area in the undeformed geometry. However in this example it is unlikely that the red boundary would shrink by any degree as a result of the deformation. For the simulations performed in this report, displacement boundary conditions were used to model load since it results in a more straightforward representation of an SSRT. The traction boundary condition has the advantage that it offers the possibility to easily model subsequent unloading of the specimen.

2.2.3 General overview of the FEM solution procedure

The finite element method (FEM) is a numerical method for solving partial differential equations (PDE) or integral equations approximately. In solid mechanics a PDE arises from the conservation of momentum law - a continuum equivalent of Newton’s second law. This PDE, combined with the boundary conditions and elastic-plastic constitutive laws of the solid, defines a problem of evolution that in general cannot be solved analytically [4]. Due to the importance and characteristics of this equation, FEM is today the most widely used numerical technique to solve almost any problem in solid mechanics [3]. A complete mathematical description of the boundary value problem for a general static solid mechanics system of evolution will be presented in section 3.4.

In the continuum mechanics context, the aim of the FEM is to compute approximate values of the displacement at a finite number of discrete points in the body, so called node points. Because of the nonlinear behavior of the constitutive relations of plasticity, incremental time steps must be used, whereas for a linear elastic body, only one time step is normally required.

By transforming the PDE into a discrete approximation of its weak form, at each time step the problem can be reformulated as a nonlinear system of algebraic equations with the nodal displacement coordinates as the unknowns. This equation is solved iteratively through linearization,
using Newton’s method or some similar approach [2]. The target function is usually called the residual vector:

\[ f(d) = 0 \]  

(2.2.2)

where \( d \) is the vector of nodal displacement coordinates. Using methods based on linearizing the problem, the finite element method applied to metal plasticity owes its success to the establishment of the Jacobian to the residual vector.

\[
\begin{align*}
\text{Figure 4. The discretization of the geometric body into small elements of simple shape, so called meshing.}
\end{align*}
\]

To sum up, a crude sketch of the algorithm applied globally to solve the system at the (n+1):th time step is outlined below. Each step of this algorithm will be elaborated further upon in later sections.

0. \( i = 0, d_{n+1}^0 = d_n \)
1. Based on \( d_{n+1}^i \), compute strains through a strain-displacement relation at a finite number of points, that is connected to the number of nodes.
2. Based on the strains, establish stresses and plastic strains obeying the constitutive law.
3. Establish the residual vector \( f(d_{n+1}^i) \) and its jacobian \( A(d_{n+1}^i) \)
4. Use \( A(d_{n+1}^i) \) to compute the next iteration step \( \Delta d^i \).
5. Set \( d_{n+1}^{i+1} = d_{n+1}^i + \Delta d, i = i + 1 \)
6. Check convergence criterion. If not met: go to step 1. If met, set \( d_{n+1} = d_{n+1}^i \).

### 2.2.4 Solution and analysis

As can be seen in the previous section, the main output of FEM computations is for each time step a vector containing the nodal displacements, as well as computed values of stress and plastic strain.

Perhaps the most useful piece of output data from a FEM simulation of an SSRT is the distribution of the von Mises stress. This can be regarded as a simple three-dimensional generalization of stress states in uniaxial tension [3]. The von Mises stress, defined as a tensor norm of the deviatoric part of the Cauchy stress tensor (see section 3.3) [10], is often used in failure or yield criteria for solids under general stress states [3].
2.2.4 Some sources of error and approximation

This report does in no way aspire to provide with an exhaustive error analysis. However, a brief survey of the approximations used and possible sources of error could be in place.

- An improper constitutive relation is perhaps the most likely cause of error in simulation. When using relatively simple one-way loading paths in metal SSRT, the most probable cause to this comes from the difficulties in determining an initial anisotropic yield condition, taking into account complex previous deformation and residual stresses in the material. Comparison with physical test results in these cases is especially inescapable in order to establish if the model is useful. It should be said that classical elastoplasticity theory might or might not work well in cases where non-ductile damage, for example stress corrosion cracking, is apparent.
- In order to gain more accurate results when strain levels increases above a few percents, software that implements finite strain plasticity theory should be advantageous.
- The stresses in the material is based on interpolation based on a finite number of points where the stress is computed using implicit Euler to solve the constitutive relation. This is where the choice of time steps has its biggest impact, especially so as the derivatives of stress are discontinuous at yield.
- When imposing volumetric constraints on the model, for example to model plastic incompressibility, a problem called volumetric locking arises, due to unbalance in the number of constraints relative to the number of degrees of freedom [11]. This is avoided in this report by simply not imposing such constraints. Unfortunately, there seems not to be an easy way in Comsol Multiphysics to evaluate the consequence of this decision.
- Finally, the PDE is solved using an approximation of its equivalent weak form. Errors from this can be reduced by simply refining the mesh, see chapter 4, and in the end this might turn out to be a relatively minor source of error.

2.3 Material data

A constitutive law for general deformation paths can be constructed using a simple extension of stress-strain behavior in uniaxial tension. Material parameters can thus be extracted from a tensile test with a uniaxially shaped specimen. The sufficiency of knowing the behavior in this special case is however not obvious. It actually requires an assumption not in general supported by phenomenology - that of isotropic, or direction independent, hardening. This assumption is contradictory to the Bauschinger effect (that is, deformation induced anisotropy of plastic yield, more about this effect in the next section), that is often clearly visible when reversing the load. If a considerable Bauschinger effect can be expected to become evident during the test, there is serious cause to doubt if a model only using experimental data from uniaxial tension can be appropriate. Unfortunately, Bauschinger effects can be difficult to forecast correctly if the material has been subject to previous deformation.

The following material parameters are required to model a static metal SSRT assuming isotropic hardening:
Elastic parameters:
• Young’s modulus $E$
• Poisson’s ratio $\nu$.

Plastic parameters:
• Yield stress level $\sigma_Y$.
• A strain hardening function $f_2$.

Experimental results has shown that pressure has little or no effect on $E$, $\sigma_Y$ and $f_2$ of most metals. However, the parameters should be considered temperature and strain rate specific, i.e. specific for slow strain rates in a range where the material is not strain rate sensitive [1].

2.3.1 Uniaxial tensile test

Apart from acquiring a value of elastic modulus $E$ of the material for temperatures used in the test, the uniaxial tensile test can be used to establish a relation between the true stress and the uniaxial plastic strain. This relation can then be generalized to three dimensions in the form of a function between the von Mises stress and the effective plastic strain. The yield stress level can be defined as the point where the curve stops behaving elastically.

In a uniaxial tensile test, a uniformly shaped bar of metal is subjected to a traction of force causing it to extend in some constant rate. The original cross sectional area and length are respectively $A_0$ and $L_0$, and in a given deformed state respectively $A$ and $L$. The axial stretch at some point of time is defined as:

$$\lambda = \frac{L}{L_0} \quad (2.3.1)$$

The axial stretch is assumed to be multiplicatively decomposed into elastic and plastic parts, governed by respectively elastic and plastic constitutive laws [7]:

$$\lambda = \lambda^e \lambda^p \quad (2.3.2)$$

However, the constitutive laws usually relate stresses and strains in the material. In uniaxial tests, curves are normally given as nominal or average stress versus nominal strain, as these are most easily measured:

$$\sigma_{avg} = \frac{F}{A_0} \text{ and } e = \lambda - 1, \quad (2.3.3)$$

where $F$ is the applied force of traction. The nominal strain is a special case ($k = -1$) of the more general Seth-Hill definition of axial strain:

$$e_k = \frac{1}{k} (\lambda^k - 1) \quad (2.3.4)$$

Note that (2.3.2) is equivalent with an additive decomposition of the so called logarithmic axial strain, where $k$ approaches 0 in (2.3.4). The stress in the material depends on the elastic part of deformation through Hooke’s law. Using stress-strain relations, this can be formulated as follows:

$$\varepsilon = \lim_{k \to 0} \frac{1}{k} (\lambda^k - 1) = \ln(\lambda) \quad (2.3.5)$$

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\[ \varepsilon = \varepsilon^e + \varepsilon^p \]  
(2.3.6)

\[ \sigma = E\varepsilon^e = E(\varepsilon - \varepsilon^p), \]  
(2.3.7)

The elastic modulus \( E \) is assumed to be a constant material parameter. As noted in the beginning of this section, the strain hardening function \( f_2 \) relates true stress as a function of logarithmic plastic strain. By using the plastic incompressibility condition and noting that volume change due to elastic deformation is small next to unity, \( f_2 \) can with good approximation be constructed directly from the nominal stress-strain curve using the following transformations:

\[ \sigma = \sigma_{avg}(1 + \varepsilon) \]  
(2.3.8)

\[ \varepsilon = \ln(1 + \varepsilon) \]  
(2.3.9)

\[ \varepsilon^p = \varepsilon - \frac{\sigma}{E} \]  
(2.3.10)

Note that (2.3.9) and (2.3.10) are direct consequences of (2.3.4) and (2.3.7) respectively, whereas (2.3.8) inhibits the incompressibility assumption. True stress and strain in this way is used to characterize ductile hardening until the point of necking, which can be identified as the point of maximal stress in the nominal stress-strain curve.

Next, the curve can be fitted to an analytical function. This is optional; plotted values from measurements can be interpolated directly to define the hardening function. Mostly all models of microscopic hardening predicts a parabolic hardening function though, and it can be convenient to view the measured values as slight deviations from a general trend, given by a smooth analytical function. The most common analytical approach uses Ludwik’s equation:

\[ \sigma = \sigma_y + K(\varepsilon^p)^n \]  
(2.3.11)

\( K > 0 \) and \( 0 < n < 1 \) are material constants that can be determined from a plot of \( \ln(\sigma - \sigma_y) \) versus \( \ln(\varepsilon^p) \). Ludwik’s equation then predicts:

\[ \ln(\sigma - \sigma_y) = \ln K + n\ln(\varepsilon^p) \]  
(2.3.12)

That is, in the Ludwik approach the resulting plot predicts a linear functional curve with slope \( n \), crossing the \( y \)-axis at \( K \) (by extrapolation, since \( \varepsilon^p \) is highly unlikely to come close to 1 for metals). Linear least squares can be used to obtain numerical values of \( K \) and \( n \). Assembling the RHS and LHS of equation (2.3.12) for a number of tabulated values in vectors \( x \) and \( y \) respectively, the linear least squares method yields:

\[ (\ln K \ n)^T = (x^T x)^{-1} x^T y \]  
(2.3.12)

In section 5.1.2 the above procedure is illustrated with Matlab code, using numerical values from a uniaxial nominal stress-strain curve.

This section is enclosed with a short discussion about the assumption of isotropic hardening for this special case of uniaxial deformation.

Plastic straining of isotropically hardening solids results in an elevated yield stress level equal to the applied stress. That is, if the specimen is unloaded, the amount of tensile or compressive stress...
required to cause further plastic deformation is equal to the new elevated yield stress. This is however not in general in accordance with metal phenomenology, where it can be seen that the centre of the elastic range (compressive stress is regarded as negative) is moved in the direction of plastic flow. That is, less compressive than tensile stress is required to cause further plastic deformation. This is the typical situation where the Bauschinger effect is clearly visible. As long as the stress is never reversed however, there is no longer a fundamental reason to raise objections against using an isotropic hardening assumption.

3 Continuum formulation

The mathematical treatment of solid mechanics can be almost completely separated into two main problem formulations:

- The PDE problem arising from the continuum balance equations.
- A sub problem to the above where a constitutive law governs the evolution of stress in the material.

The global treatment of the PDE problem remains largely the same when using different metal constitutive laws. Variations for example in the computation of the jacobian of the residual vector rest on practical considerations to assure fast convergence. As long as the solutions converge, these differences does not affect the accuracy.

A few comments about the matrix and tensor notation used in this report are in place.

- Second order tensors, such as stress and strain measures (in this report only the various elastic modulus tensors are of higher order), can conceptually be thought of as square matrices.

- In computation, also the elastic or plastic modulus tensors are treated as linear matrices mapping the six independent components of symmetric stress or strain tensors. This matrix treatment is called Voigt notation.

- If an index is repeated in the same term in any expression, it should be interpreted as summation over the range of the index. Tensor indices for example are in this way summed over the number of dimensions.

- Second order tensors (in the form for example of numerous stress and strain measures) form a vector space with the following frequently used inner product:

  \[ \mathbf{A} : \mathbf{B} = A_{ij}B_{ji} = \text{tr}(\mathbf{A}^T\mathbf{B}) \]

- Differentiation or integration over tensor valued functions is carried out componentwise.

- An accented dot over a variable denotes (componentwise) differentiation with respect to time, i.e.

  \[ \dot{\mathbf{A}} = \frac{d\mathbf{A}}{dt} \]
3.1 Stress and strain measures

The stretch in (2.3.2) can be straightforwardly generalized to the general multiaxial deformation state through the deformation gradient, which is correspondingly assumed to be multiplicatively decomposed into an elastic and a plastic part.

\[ F_{ij} = \frac{\partial x_i}{\partial X_j} \]  
\[ F = F^eF^p \] (3.1.1) (3.1.2)

The determinant of the deformation gradient is used to quantify changes in volume [3].

\[ J = \det (F) \] (3.1.3)

The important law of momentum balance for a continuum is usually expressed in terms of stresses and strains. In linear geometric analysis, the different stress and strain measures defined in the next section are assumed to be approximately equal (They share the linear term of their Taylor series; this term is used as strain measure and is called the infinitesimal strain tensor).

3.1.1 Nonlinear geometry

If changes in shape of the geometry are taken into account when setting up the equation of motion and strain-displacement relation at different times, the geometry is said to be nonlinear. Geometric nonlinearity is used when deformations large enough to cause unacceptable error when making no distinction is expected. This deformation can be in the form of both large strains and (maybe local) rigid body rotation. When using a nonlinear geometric treatment, it becomes necessary to distinguish between different stress and measures depending on which geometry (basically either the current or the original undeformed) is considered at the moment. Different measures can appear in different equations depending on which choice gives the simplest expressions.

3.1.2 Stress

The Cauchy’s stress tensor, \( \sigma \) as defined by Cauchy’s law, is the “true” physical measure of internal forces in a body. Its components are the forces inside the body per unit area of the deformed solid, normal and shear, acting on each of the coordinate planes [3]. Other measures of stress are used in the equations of nonlinear Lagrange formulations. These always relate the forces to the undeformed geometry. The different stress measures used are interrelated through simple transformations using the deformation gradient.

\[ \sigma = J^{-1}PF^T = J^{-1}FSF^T \] (3.1.4)

The evolution the stress measure S (called the second Piola-Kirchhoff or PK2 stress) is given through the constitutive law, while partial derivatives of PK1 stress P are found in the formulation of the momentum equation. The updated Lagrange formulation on the contrary only uses the Cauchy stress, making it more appropriate for finite strain constitutive theory formulated in Cauchy stress rates, since it avoids unnecessary transformations [2].
### 3.1.3 Strain

An extension of the concept of strain to general deformation states in three dimensions is given by the Seth-Hill definition of strain in analogy with (2.3.4), replacing stretch with the deformation gradient. Like in uniaxial tension, the different strain measures relate changes in length of short material fibers between the undeformed and the deformed state, this time with orientation.

\[
E_k = \frac{1}{k} (U^k - I), \quad \text{where} \quad U = (F^T F)^{1/2}
\]  
(3.1.5)

The Green-Lagrange strain \( (k = 2) \) inhibits for large deformations important property of being invariant under rigid body rotation. Also it has the computational advantage in that it can be established directly through the deformation gradient without performing a root operation. For example, the logarithmic strain tensor \( (k \to 0) \) inhibits only the former advantage but not the latter. The Green-Lagrange strain is for this reason the absolutely dominating choice of strain measure in nonlinear geometry formulation of solid mechanics.

In large strain constitutive relations, an alternative rate measure of strain is used - the rate of deformation, \( \mathbf{D} \). This measure can be obtained through a transformation of the time derivative of the Green-Lagrange strain - a so called push-forward operation. Details of large strain constitutive theory will only be very briefly addressed in this work. However, as pointed out earlier, only the constitutive theory needs normally be changed at all when reformulating the problem for large strains.

### 3.2 The conservational laws

The fundamental governing equations in computational thermomechanics, where the only sources of energy are mechanical work and heat, arises from four conservational laws of continuum mechanics, also known as the balance laws [2]. Because of the assumptions introduced in section 2.2.1, the equations can be somewhat simplified from their general forms.

#### 3.2.1 Balance equations

For the special case of a static (time-independent), constant temperature system in a total Lagrangian formulation, the four balance equations in terms of stresses and strains are reduced to the below forms. Note that the PK1 stress is used in the balance equations, and the PK2 stress as the target function of the constitutive relation. This should not cause confusion since they either measure can be transformed into the other through the deformation gradient. For simplicity, body forces like gravity are here assumed to be negligible, though the addition of body forces to the system would not cause much extra complication.

1. \( \rho = \rho_0 \mathbf{I} \), where \( \rho_0 \) is the initial density \hspace{1cm} (Balance of mass) \hspace{1cm} (3.2.1)
2. \( \frac{\partial \rho \mathbf{u}}{\partial x_j} = 0 \) \hspace{1cm} (Balance of linear momentum) \hspace{1cm} (3.2.2)
3. \( \mathbf{FP} = \mathbf{P}^\mathbf{T} \mathbf{F}^\mathbf{T} \) or, equivalently, \( \mathbf{S} = \mathbf{S}^\mathbf{T} \) \hspace{1cm} (Balance of angular momentum) \hspace{1cm} (3.2.3)
4. \( \rho_0 \frac{\partial w^{int}(\mathbf{X}, \mathbf{t})}{\partial t} = \mathbf{F} : \mathbf{P} \ (= \ \mathbf{E} : \mathbf{S} = \mathbf{D} : \mathbf{\sigma}) \) \hspace{1cm} (Balance of energy) \hspace{1cm} (3.2.4)
A few comments about these equations:

- (3.2.1) will simply define the density distribution of the computed solution, which hopefully should be close to $\rho_0$, due to the plastic incompressibility used in the constitutive theory.
- (3.2.2) is the important balance of moment equation for the special case of a mechanical body without inertial forces acting on it. For this reason it is often called the *equilibrium equation*.
- Eq. 3 is enforced in the constitutive laws through the elastic stress-strain relation (2.3.6) as a result of symmetry of both the Green-Lagrange strain tensor and the elastic modulus.
- In the absence of heat sources and heat flux, eq. 4 is reduced to a *definition* of the rate of work done by stresses per unit volume of undeformed solid, or the *internal energy rate*. Depending of the nature of the deformation, the work done by stresses is either transformed into elastic stored energy or dissipated as heat [3]. With this definition in mind, the pairs $(\mathcal{F}, P)$, $(\mathcal{E}, \mathbf{S})$ and $(\mathbf{D}, \sigma)$ are called *power conjugates*. This power conjugacy is later used to formulate a weak form of Eq. 2.

### 3.3 The constitutive law

In the classical theory of elastoplasticity, it is assumed that elastic deformation is due to lattice distortion, and that all plastic deformation originates from slip on crystallographic planes [9]. The theory is however used with success to model polycrystalline plasticity on macroscopic levels also where there are other more complicated sources of plastic deformation, such as in alloys [9].

In analogy with the one-dimensional case, isotropic hardening means that the yield surface simply expands when plastic flow occurs, while phenomenology shows that the center also translates in the direction of plastic flow, introducing anisotropy to the yield condition. As long as the material is free of previous deformation and the loading path is not reversed, the isotropic model is often regarded as sufficient [9]. Extending the model to include a Bauschinger effect may not add much extra complication mathematically, but will demand more experimental knowledge about the material, in SSRT most importantly about the initial state.

The Cauchy and PK2 stress tensors can be additively split up into two components: one which acts to change the volume of the body, and one which acts to distort the shape. The former are called *hydrostatic* and the latter *deviatoric* stress, here denoted $\tau$. The same notation is used here because in the constitutive law for large deformation and small strain is the same as for small deformation, just replacing the Cauchy stress with the PK2 stress in the former [6]. The hydrostatic stress tensor equals one third of the trace of the stress tensor times a unit tensor. An experimentally well established fact for metals is that plastic deformation occurs with no appreciable volume changes on the body [9]. The interpretation of this is that only the deviatoric part of the stress affect plastic deformation.

### 3.3.1 Elastic stress-strain relation, small strains

The linear elastic response is given by the generalized Hooke’s law. When using small strain large deformation analysis it relates PK2 stress with elastic Green-Lagrange strain through Hooke’s operator of linear elasticity $\mathbf{C}$. The elements of $\mathbf{C}$, called the elastic moduli, are all functions of $E$ and $\nu$. In constitutive relations, the elastic response is given in rate form:
\[
\dot{\mathbf{S}}_{ij} = C_{ijkl}(\dot{\mathbf{E}}_{kl} - \dot{\mathbf{E}}_{kl}^{p})
\]  
(3.3.1)

However, this additive decomposition of the strain tensor increments into an elastic and a plastic term is an approximation, assuming that the total magnitude of strain in the test is small next to unity. For total strains of more than a few percent in magnitude, errors due to the small strain assumption are likely to become unacceptable in many applications.

### 3.3.2 J2 metal plasticity

In the von Mises theory of metal plasticity, the yield stress level from the uniaxial state is generalized to a hypersphere in deviatoric stress space, called the yield surface. The process of plastic deformation causing the yield surface to change in shape is called plastic flow. The yield surface can be visually be interpreted in the space of eigenvalues of the deviatoric stress as a cylinder centered on the hydrostatic axis (the axis on which all eigenvalues are equal). As mentioned earlier, the scalar generalization of true stress to three dimensions in this theory is the von Mises effective stress. Remember that \( \tau \) is here the deviatoric part of PK2 stress:

\[
\Phi(\mathbf{S}) = \frac{3}{2} \| \mathbf{\tau} \| = \frac{3}{2} \langle \mathbf{\tau} : \mathbf{\tau} \rangle
\]  
(3.3.2)

The scalar before the tensor norm is chosen so that, in the special case of uniaxial tension, the only nonzero eigenvalue of the symmetric tensor \( \sigma \) will equal the von Mises stress. In other words, it is chosen so that it exactly corresponds to the true stress in uniaxial tension. The tensor norm is sometimes called the second invariant of the deviatoric stress, denoted \( J_2 \). It forms, together with the hydrostatic stress \( \langle \mathbf{\tau} \rangle \) and a third measure an invariant set. This theory is therefore called \( J_2 \) plasticity, because the third invariant is ignored. There is solid experimental support of a flow criterion based only on von Mises stress for ductile metals [9]. For a previously undeformed solid, the von Mises yield criterion predicts that plastic deformation starts when the von Mises stress reaches a certain critical value.

When plastic flow is modeled as isotropic, it causes the yield surface to expand uniformly, while remaining centered on the origin. Just as in the one-dimensional case, this takes no account of the Bauschinger effect, and is generally only suitable for relatively simple, non-reversed loading paths.

### 3.3.2 Associativity

Whether the model is based on small strain or some large strain theory; the plastic deformation given in rate form needs to be specified in terms of both magnitude and direction (a tensor value). In order to use the one-dimensional hardening function, a scalar measure corresponding to the uniaxial logarithmic strain, called the effective plastic strain, is added to the model. In the small strain case, this measure has the concrete physical meaning of accumulated plastic strain:

\[
\alpha = \int \frac{3}{2} \| \mathbf{E}^p \| \, dt
\]  
(3.3.3)

The direction of plastic flow can be specified by some arbitrary potential function. However, plastically deforming solids are often assumed to obey the so called Drucker’s material stability condition. An important result of this postulate is that plastic flow is always normal to the yield surface. That is, whenever non-zero, the rate of plastic deformation (whether as \( \mathbf{D}, \mathbf{E} \) or \( \mathbf{e} \)) is proportional to the normal direction of the yield surface (in deviatoric stress space). The plastic flow
direction is then said to be associative. It can also be shown that plasticity models based on associative plastic flow direction are stable for small strains [2]. Also, non-associative flow tends to be difficult to treat in computation. Drucker's postulate is formulated for small strains, but associativity is regarded an appropriate choice of flow direction for many materials in general, and is predominantly used to describe metal plasticity [2].

Due to the link between stress and plastic flow direction, an auxiliary variable \( \gamma \), called the consistency variable, is introduced in the constitutive law. This consistency variable can be regarded as the target variable of the resulting problem of evolution.

### 3.3.3 Constitutive equations

The constitutive theory for an associative von Mises metal with isotropic hardening can be formulated in the form of a set of equations of evolution. This particular formulation using nonlinear geometry together with a small strain assumption will only eliminate one of the two sources of approximations in small deformation theory. As discussed in section 4.1.5, the problem can be numerically treated through a succession of convex optimization problems, requiring increments in total strain to be given at the start of each time step.

- **Elastic response:**
  \[
  \dot{S}_{ij} = C_{ijkl}(\dot{E} - \dot{E}^p)_{kl} \tag{3.3.4}
  \]

- **Elastic region:**
  \[
  e_S = \{(S, \alpha) : f(S, \alpha) \leq 0\}, \tag{3.3.5}
  \]
  \[
  f(S, \alpha) = \Phi(S) - (\sigma_\tau + f_2(\alpha)), \tag{3.3.6}
  \]
  \[
  f_2(\alpha) = K(\alpha)^n \tag{3.3.7}
  \]

- **Flow rule and hardening law:**
  \[
  \dot{\alpha} = : \dot{\gamma} \tag{3.3.8}
  \]
  \[
  \dot{E}^p = \dot{\gamma}\nabla f(S) = \ldots = \dot{\gamma} \sqrt{\frac{3}{2||\nabla||}} \tag{3.3.9}
  \]

- **Kuhn-Tucker conditions:**
  \[
  \dot{\gamma} \geq 0, \quad f(S, \alpha) \leq 0, \quad \dot{\gamma} f(S, \alpha) = 0 \tag{3.3.10}
  \]

- **Evolution of the consistency parameter:**
  \[
  \dot{\gamma} = \frac{\nabla f(S) : C : \dot{E}}{f'(\alpha) + \nabla f(S) : C : \nabla f(S)} \tag{3.3.11}
  \]

The elastic moduli in \( C \) depend only on the material parameters \( E \) and \( \nu \), while \( f_2 \) is obtained experimentally from the uniaxial test as described in the previous chapter. (3.3.11) above follows by differentiating (3.3.6) with the chain rule and setting the result to zero, as \( f \) is constant (zero) when \( \dot{\gamma} \) is nonzero, according to (3.3.10).

One more result from the constitutive theory is needed later in the FEM implementation. That is an expression relating the evolution of stress to the evolution of total strain, similar to (3.3.1) above.
In the case of associative, isotropic von Mises plasticity, the elastoplastic tangent modulus \( C^{ep} \) can be shown after some work to take the following expression [4]:

\[
C_{ijkl}^{ep} = C_{ijkl} - \frac{9E^2}{4(1 + \nu)^2} \Phi(S) \left( \frac{3E}{2(1 + \nu)} + f'(\alpha) \right)^{-1} \tau_{ijkl}
\]  

As a final comment it can be seen above that the plastic incompressibility condition is only implicitly included in the constitutive law. In the numerical treatment it will not be exactly satisfied and later not enforced explicitly in the FEM solution either. This would require additional constraints on the systems, causing volumetric locking. This is not a trivial problem to overcome in practice, so in this work it is avoided by simply not enforcing plastic incompressibility.

### 3.3.4 Finite strain

No additional material parameters are needed to straightforwardly extend the above constitutive model to finite strains. For example, the hardening function is already defined to be valid on the entire stress-strain curve up unto necking.

In most finite strain plasticity formulations, the rate of deformation tensor \( D \) is used as strain rate measure. An additive decomposition of \( D \) into elastic and plastic parts can be constructed using (2.3.7). The plastic term does however, non-rigorously speaking, not inhibit the usual structure of the rate of deformation gradient, and this decomposition has been subject to objection on fundamental grounds [2]. There are mainly two rate formulations of finite strain plasticity based on \( D \) in use today. In the hypoelastic-plastic formulation, the additive decomposition of the rate of deformation tensor \( D \) is adopted. A hypoelastic (rate form) elastic response is used.

The hyperelastic-plastic formulation on the other hand uses explicitly the multiplicativity of the deformation gradient (2.3.7). This leads to the introduction of an intermediate virtual geometric configuration where the additive decomposition of \( D \) has better motivation. The hyperelastic treatment has several advantages, especially for problems involving large rotations or stress reversal. For monotonically loaded structures, experience shows that implementation of the two models produce the same results [2]. It seems that a hyperelastic-plastic constitutive theory would be the most suitable framework for simulating the complex and severe deformation of the specimen considered here.
4 Implementation with FEM

4.1 Formulation of the BVP

4.1.1 Summary of governing equations

For the remainder of this report it is assumed that the problem is driven by over time evolving displacement boundary conditions, as described in chapter 2. Associated with each of the (Cartesian spatial) coordinate directions, the part of the geometry boundary $\Gamma$ which has prescribed displacements $\bar{u}_i(X, t)$ in the $i$-direction is denoted $\Gamma_{u_i}$, and the surface traction in the $i$-direction outside $\Gamma_{u_i}$ is set to be zero. The outward normal vector to the boundary is denoted $n$. With this notation, the complete boundary value problem (BVP) to be solved by the FEM can finally be stated.

1. $\frac{\partial P_{ji}}{\partial x_j} = 0$ (Balance of linear momentum) \hspace{1cm} (4.1.1)
2. $n_j P_{ji} = 0$ on $\Gamma - \Gamma_{u_i}$ (Traction boundary conditions) \hspace{1cm} (4.1.2)
3. $u_i(X, t) = \bar{u}_i(X, t)$ on $\Gamma_{u_i}$ (Displacement boundary conditions) \hspace{1cm} (4.1.3)
4. $\mathbf{S} = \mathbf{S}(\mathbf{E})$, $\mathbf{S} \in C(\Omega)$ (Constitutive law) \hspace{1cm} (4.1.4)

Equations (4.1.1) and (4.1.2) together form the so called the strong form of the problem. The stress can actually be allowed to be discontinuous along planes, for example at material interfaces, but this case is not considered here. The main point of the continuity is that Gauss theorem can be used later in the derivation of the weak form.

4.1.2 The weak form

The first step in solving the BVP of the last section with FEM is to transform the strong form into an equivalent relation called the weak form, a form that can be discretized and solved.

As a first step in the derivation of the weak form, a class of displacement-like functions that vanishes on $\Gamma_{u_i}$, called test functions or virtual displacement functions, is defined. The test functions are also required to be piecewise continuously differentiable on $\Omega$ in order to make all subsequent steps well defined [2].

$$U = \{ C^0(X) \ni \delta u : \Omega \times t \to \mathbb{R}^3 \mid \delta u_i(X, t) = 0 \text{ on } \Gamma_{u_i} \} \hspace{1cm} (4.1.6)$$

The weak form is developed by first multiplying equation (4.1.1) by an arbitrary test function $\delta u \in U$ and then integrating over $\Omega$:

$$\int_{\Omega} \delta u_i \frac{\partial P_{ji}}{\partial x_j} d\Omega = 0 \hspace{1cm} (4.1.6)$$

Using the derivative product rule followed by Gauss theorem (in equations (4.1.7) and (4.1.8) respectively), the derivatives of stress can be removed altogether from (4.1.6):
\[ \int_{\Omega} \delta u_i \frac{\partial P_j}{\partial x_j} d\Omega = \int_{\Omega} \frac{\partial}{\partial x_j} (P_j \delta u_i) d\Omega - \int_{\Omega} \frac{\partial (\delta u_i)}{\partial x_j} P_j d\Omega \quad (4.1.7) \]

\[ \int_{\Omega} \frac{\partial}{\partial x_j} (P_j \delta u_i) d\Omega = \int_{\Gamma} n_j (P_j \delta u_i) d\Gamma \quad (4.1.8) \]

Because \( \delta u_i = 0 \) on \( \Gamma_{ui} \), and \( n_j P_j = 0 \) on \( \Gamma - \Gamma_{ui} \) according to (4.1.2), the last expression in (4.1.8) vanishes. Using the notation

\[ \delta F_{ij} = \frac{\partial (\delta u_i)}{\partial x_j}, \quad (4.1.8) \]

the weak form finally emerges as:

\[ \int_{\Omega} \delta F^T : \mathbf{p} d\Omega = 0 \quad (4.1.9) \]

In a similar straightforward way it can be shown also that equation (4.1.9) implies the strong form. Thus, if (4.1.9) is satisfied for all test functions \( \delta u \in U \), then this is equivalent with the strong form. This weak form is sometimes called the principle of virtual work, which is in line with the notion of power conjugacy from the energy equation (3.2.4), here regarding the test functions as virtual displacement fields. What remains now is a method to solve the weak form numerically in a way that also satisfies equations (4.4.3) and (4.4.4).

### 4.2 Discrete equations

#### 4.2.1 Meshing

Solving the BVP of section 4.1.1 with FEM requires the discretization of space as well as of time. Based on the geometric body of the specimen, a so-called mesh is created. The mesh is a union of smaller volume elements that approximates the total geometric body of the specimen. The point of this is that on these simple volume elements, the weak form can be integrated symbolically, effectively transforming the problem from a PDE boundary value problem into a set of algebraic equations.

The mesh elements share interfaces, edges and corner points with each other. The corner points are especially important as the values of displacement at these points constitute the degrees of freedom of the discretized problem.

For the remainder of this chapter, \( \Omega \) is used to denote the approximate geometry resulting from taking the union of all mesh elements, rather than the actual geometry.

#### 4.2.3 The interpolated displacement field

In order to integrate the weak form over the mesh elements, the displacement field is approximated using polynomial interpolation. For each mesh node point, a time-independent interpolant, called shape function, is defined. The shape functions are exactly one at the parent node, and exactly zero at all other nodes. In addition, the sum of all shape functions is one everywhere. Assuming that the
displacements are known at all mesh node points, the defining property of the shape functions becomes clear:

\[ u_i(X, t) \approx u_{il}(t)N_l(X), \]  

(4.2.1)

where

\[ u_{il}(t) = u_i\text{ (nodepoint } l, t) \quad l = 1, ..., m \]  

(4.2.2)

The level of accuracy of course depends on the resolution of the mesh. In order to follow the remaining development it is probably sufficient to know that (4.2.1) constitutes an approximation of the displacement field using polynomial interpolation of known values at the mesh nodes. Comsol Multiphysics 3.2 implements by default a quadratic Lagrange interpolation technique.

4.2.4 Discrete approximation of the weak form

The key equation to the numerical treatment arises when applying the weak form on the meshed geometry, thus combining equations (4.1.9) and (4.2.1).

\[ 0 = \int_\Omega \delta u_i^T \mathbf{P} d\Omega \approx \delta u_{il} \int_{\Omega^l} \frac{\partial N_j}{\partial X_j} P_{ji} d\Omega =: \delta u_{il} f_{il}^{\text{int}}, \]  

(4.2.3)

where \( \Omega^l \) is the meshed geometry, \( f_{il}^{\text{int}} \) is called the nodal force in the \( i \)-direction at node \( l \). Because \( \delta u_{il} \) is arbitrary outside \( \Gamma - \Gamma_{ui} \),

\[ f_{il}^{\text{int}} = 0 \]  

(4.2.4)

is then true for all node points \( l \) where displacement in the \( i \)-direction is not prescribed. Note that the test functions are at this point not anymore included. When traction boundary conditions are used, the internal nodal forces should vanish except in coordinates where non-zero traction is prescribed. In the latter, the internal nodal force must instead equal the so called external nodal forces, corresponding to the prescribed value of traction.

Equation (4.2.3) is of course equally valid on all subsets of \( \Omega^l \), and especially on individual mesh elements. Thanks to the polynomial structure of the approximated displacement field, the nodal forces can be integrated exactly over these using Gauss quadrature. This method only requires the computation of stress at a small number of so called Gauss quadrature points inside the element. The total internal nodal force of a mesh node can in this way be computed by simply adding the terms resulting from each individual element in the mesh.

Note that this method can give rise to some error due to the discontinuous derivatives of stress at the borders of plastically deformed areas. Using higher order interpolation can increase the theoretical accuracy, but likely it will instead lead to increased stiff behavior, making it an unsuitable choice in general [2].
4.2.5 Constitutive update algorithm

By applying an implicit Euler method, the numerical treatment of the problem in section 3.1.3 can be transformed into a convex optimization problem with discrete Kuhn-Tucker conditions [3]. The standard method of solving this problem is the popular radial return algorithm, which in the FEM implementation must be solved at all element Gauss points for each discrete time step [3]. These computations account for the most part of computational time in FEM plasticity modeling. It is regarded the central problem of computational plasticity, as it directly corresponds to the crucial role of a satisfying constitutive theory [3]. As discussed in [3], the finite strain theory using (2.3.7) with an intermediate configuration leads to a straightforward extension of the radial return mapping of the small strain theory.

4.3 Iterative solution procedure

4.3.1 Newton’s method

The assembly of all nodal forces in a vector \( f \) results exactly in the residual vector seen in the solution sketch of section 2.2.3. Indeed, at time step \( n + 1 \), (4.1.10) becomes a nonlinear algebraic equation in the \( 3 \cdot m \) components of nodal displacement, using values computed at time step \( n \):

\[
f(d) = 0, \tag{4.3.1}
\]

where \( d \) is a vector containing the nodal displacements. To solve equation (4.3.1) at some given point of time while imposing (4.1.3), a modification of Newton’s method using Lagrange multipliers can be implemented. If \( \bar{u}_{n+1} \) is the vector containing the prescribed nodal displacements at time step \( n + 1 \), then (4.1.3) can be stated in matrix form as

\[
Dd = \bar{u}_{n+1}, \tag{4.3.2}
\]

where \( D_{c \times 3m} \) has exactly one nonzero component (= 1) on each of its rows; \( c \) is here the total number of nodal constraints.

Optimization theory with Lagrange multipliers can be used to produce a linearization of (4.3.1) subject to (4.3.2). This is done by considering a modified differential of energy that vanishes at equilibrium points satisfying (4.3.2). After some work the following equation emanates [2]:

\[
f + D^T \lambda = 0, \tag{4.3.3}
\]

where \( \lambda \) is a vector of (free) Lagrange multipliers. Linearizing (4.3.3) around \( d^k \) and adding (4.3.2) explicitly to the system yields the following linear equation system:

\[
\begin{pmatrix}
A(d^k) & D^T \\
D & 0
\end{pmatrix}
\begin{pmatrix}
d - d^k \\
\lambda - \lambda^k
\end{pmatrix} =
\begin{pmatrix}
-f(d^k) - D^T \lambda \\
Dd^k - \bar{u}^{k+1}
\end{pmatrix}, \tag{4.3.4}
\]

where \( A(d) \) is the jacobian of the residual, i.e:

\[
A_{kl}(d) = \frac{\partial f_k}{\partial d_l} \tag{4.3.5}
\]
Solving (4.3.4) for \( \mathbf{b} \) then provides the next iterate \( \mathbf{b}^{k+1} \). The only remaining difficulty is to correctly establish the jacobian, which forms the subject of the concluding section of this chapter.

### 4.3.2 Computing the jacobian

The jacobian (4.3.5) can relate *time* derivatives of the nodal forces to the nodal displacements by the chain rule. This leads to an alternative definition, equivalent to (4.3.5):

\[
\dot{\mathbf{f}} = A \mathbf{b}
\]

(4.3.6)

Taking the time derivative of a nodal force component by the definition in (4.2.3), then applying the product rule then yields the following result:

\[
\dot{f}_{il} = \int_{\Omega} \frac{\partial N_i}{\partial x_{ij}} \dot{p}_{ij} \, d\Omega = \int_{\Omega} \frac{\partial N_i}{\partial x_{ij}} (S_{ik} F_{jk} + S_{lk} F_{jk}) \, d\Omega
\]

(4.3.7)

A time derivative of PK2 stress is provided by the constitutive law through (3.3.4) and (3.3.5). The remaining development of the jacobian then reduces to the technical problem of translating (4.3.7) into a matrix expression. For this end, a number of new definitions are first needed.

\[
\mathbf{f}_i = (f_{i1} f_{i2} f_{i3})^T, \quad i = 1, \ldots, m
\]

(4.3.12)

\[
\mathbf{b}_i = \left( \frac{\partial N_i}{\partial x_1} \frac{\partial N_i}{\partial x_2} \frac{\partial N_i}{\partial x_3} \right)
\]

(4.3.12)

\[
\mathbf{B}_i = \begin{pmatrix}
\frac{\partial N_i}{\partial x_1} \frac{\partial u_1}{\partial x_1} & \frac{\partial N_i}{\partial x_1} \frac{u_2}{\partial x_1} & \frac{\partial N_i}{\partial x_1} \frac{u_3}{\partial x_1} \\
\frac{\partial N_i}{\partial x_2} \frac{u_1}{\partial x_2} & \frac{\partial N_i}{\partial x_2} \frac{u_2}{\partial x_2} & \frac{\partial N_i}{\partial x_2} \frac{u_3}{\partial x_2} \\
\frac{\partial N_i}{\partial x_3} \frac{u_1}{\partial x_3} & \frac{\partial N_i}{\partial x_3} \frac{u_2}{\partial x_3} & \frac{\partial N_i}{\partial x_3} \frac{u_3}{\partial x_3}
\end{pmatrix}
\]

(4.3.10)

Thanks to the symmetry of \( \mathbf{S}, \mathbf{E} \) and \( \mathbf{C}^{\text{ep}} \), the tensor relation (3.3.4) can alternatively be expressed in matrix form using so called Voigt transformation. Then the six independent components of stress and strain are related by the 6 \( \times \) 6 *matrix of elastoplastic moduli:*
\[ \{ S \} = (S_{11} \ S_{22} \ S_{33} \ S_{23} \ S_{13} \ S_{12})^T \]  \hfill (4.3.9)
\[ \{ E \} = (E_{11} \ E_{22} \ E_{33} \ 2E_{23} \ 2E_{13} \ 2E_{12})^T \]  \hfill (4.3.9)
\[ \{ S \} = [C^{ep}]\{ E \} \]  \hfill (4.3.8)

Note that \([C^{ep}]\) is constructed using the elements of \(C^{ep}\). It can also easily be shown that

\[ \{ E \} = B_I d_I \]  \hfill (4.3.9)

Using the definitions above, (4.3.7) applied to all nodes in the system becomes after some work:

\[
f_I = \left( \int_{\Omega_I} B_I^T [C^{ep}] B_I d\Omega + \int_{\Omega_I} b_I^T S b_I (d\Omega) \right) d := A_{II} \right) \frac{d}{d_I},
\]  \hfill (4.3.8)

which finally yields the jacobian as:

\[ A = \begin{pmatrix} A_{11} & \cdots & A_{m1} \\ \vdots & \ddots & \vdots \\ A_{1m} & \cdots & A_{mm} \end{pmatrix} \]  \hfill (4.3.11)
5 Simulations

The results of three computer simulations are presented and discussed in this chapter. The geometry of the specimen used in simulation is specified in figure 1, using a hump radius of respectively 0.25, 0.50 and 1.00 mm. Because of the similarities between the three simulations apart from hump dimension, values corresponding to the simulations with 0.5 and 1.00mm hump are sometimes given in parenthesis after the value corresponding to the 0.25mm hump.

The theory assumes isotropic initial yield condition, no initial deformation (fully solutions annealed) as well as pure ductile deformation. The simulations where performed in Comsol Multiphysics 3.2. Using the features available in the software interface, simulations are based on small strain classical strain hardening elastoplasticity with isotropic hardening, using a nonlinear total Lagrange geometry formulation.

5.1 Material properties

The material data was taken from a uniaxial tension test of an SS steel carried out in a 290°C water process. In the oxygenated water environment the curve deviated by a small percent from a similar test performed in inert gas, which suggests that non-ductile cracking in water affected fracture by a small degree [8]. The conditions as it seems deviate from the assumption of pure ductile deformation of a solid free of previous deformation. It is still possible however that the uniaxial test can be used to simulate SSRT under the same material and environmental conditions with some accuracy.

A plot with numerical values from the nominal stress-strain curve of the uniaxial test was provided by Studsvik Nuclear, and is shown in Figure 5 below. Below is also illustrated in Matlab code how the analytical Ludwik hardening function can be constructed based on the plot. The (nominal) yield stress level was given as 168 Mpa, which saves the trouble of establishing this value. The computations are based on theory from section 2.3 of this thesis.

<table>
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</table>

Figure 5
To begin with, the numerical values of nominal stresses and strains past yield were collected into two vectors, x and y. Young’s modulus $E$ could be determined by dividing true stress with true strain at the closest point before yield. Fortunately, the nominal stress at yield was provided in the report as $168 \text{ MPa}$, which saved some work to determine the point of yield [8]. True stress at yield could then be obtained through $E$, the nominal yield stress and the true strain at yield.

\[
x = 1 \times 10^6 \cdot [181.03 \ 205.6 \ \ldots \ 393.1]^T; \quad \text{nominal stresses above yield until the ultimate stress.}
\]

\[
y = 1 \times 10^{-2} \cdot [3.05 \ 5.12 \ \ldots \ 47.48]^T; \quad \text{corresponding nominal strains}
\]

\[
E = 164.22 \times 10^6 \cdot (1.0207)/\log(1.0207); \quad \text{($\approx 8181 \text{ MPa}$), Young’s modulus}
\]

\[
ey = 168^*/(E - 168); \quad \text{($\approx 0.0210$, true strain at yield)}
\]

\[
sy = 168e6*(1+ey); \quad \text{($\approx 172 \text{ MPa}$, true stress at yield)}
\]

Next, the nominal values were transformed as in equations (2.3.9) and (2.3.10):

\[
u = [x \cdot (y + \text{ones}(1,18))] - sy;
\]

\[
v = [\log(y + \text{ones}(1,18))] - u ./ E
\]

The resulting plot is shown in figure 6a.

\[
p = \log(u2);
\]

\[
q = \log(v2);
\]

\[
\text{plot}(v2,u2);
\]

The last plot is shown in figure 6b. It can be seen that the points are scattered around an approximately straight curve. The last two values however, as we approach the ultimate stress, seem to deviate suspiciously from the linear curve. This could be a sign of some material instability (necking) or crack growth, and data from these points are for safety excluded. The hardening function should model pure ductile behavior in homogenous uniaxial tension to be consistent with theory. This decision implies that simulations yielding von Mises stresses above $385.34 \cdot 1.4127 \approx 545 \text{ MPa}$ should not be considered. The constants $n$ and $K$ can now be obtained using the linear least squares method.

\[
p = p(1:14); \quad q = q(1:14);
\]

\[
X = [\text{ones}(14,1) \ q(1:14)];
\]

\[
b = (X' \cdot X) \cdot (X' \cdot p(1:14)); \quad \text{solution vector b of } X^T X b = X^T p(1:14)
\]

\[
K = b(1); \quad n = b(2); \quad \text{($K \approx 1139 \text{ MPa}, n \approx 0.8737$)}
\]

The analytic hardening function based on Ludwik’s equation with the computed constants is shown in figure 6c.
Figure 6. Graphs resulting from the three plot commands of the matlab code.
5.1 Building the model in Comsol Multiphysics

In this section is described how the simulations can be carried out step by step with the software.

5.1.1 Geometry

The specimen geometry was drawn using the graphical CAD (computer-aided design) environment of Comsol Multiphysics 3.2. To draw fully three dimensional geometries in the CAD environment, two dimensional figures can be drawn and extruded from arbitrary planes into the global coordinate system. This, together with set operations, was sufficient to draw the test specimen as specified in figure 1. Boundaries, edges and corner points are automatically defined and numbered by the software. The spatial coordinates can be used as variables anywhere in the model.

5.1.2 Hardening function

In order to define a hardening function from section 5.1, select Functions from the Options menu. Click the new button and create the new function \( f_2 \) as an interpolation function using values from table. Rather than using the analytic Ludwik function, a cubic spline interpolation function was created based on values from the analytic Ludwik function. The derivative of the analytic Ludwik function approaches infinity at zero, which indicates a deviation from physics, and will also cause problems in the numerical treatment of the constitutive law.

![Figure 7](image-url)
5.1.3 Physics settings

1. Select Properties from the Physics menu, and check the box Large Deformations. Now the software will use a total lagrangian finite element formulation.

2. Select Subdomain Settings from the Physics menu. This is where the material properties of the specimen body are set. Specify $E$ and $\nu$ in the respective fields. Poissons ratio was in the simulations set as 0.3, which is a typical value for any steel [1]. Then click the Elasto-plastic material data button and specify $\sigma_y$, check the hardening function box and enter $f_2(epe)$ in the field next to the box.

3. Select Boundary Settings from the Physics menu. Select the the boundary marked in red in figure 1, and enter para*1e-6 in the $R_x$ field. For each parameter increase, that boundary will move 1µm in the x direction. For the blue marked boundaries, check respectively the $R_x$, $R_y$ and $R_z$ boxes, corresponding with the normal direction of the boundary planes.

5.1.4 Meshing

The highest resolution of the mesh is needed in areas where the best values of stresses and strains are desired. Small geometric details of course need a better resolution to make correct account for. The number of degrees of freedom, a direct function of the mesh resolution, is a good measure of the computer capacity required to solve the model. The limiting factor to the problem size is the memory capacity needed to solve the linear equation systems resulting from linearization, roughly in the order of the number of degrees of freedom. A good overall resolution may be needed to trace the electrical resistance with minimum error, which of course depends of the overall deformation. The mesh creation is automatic in the graphical interface of Comsol Multiphysics. A number of parameters affecting the resolution are however accessible by the user.

- Select Mesh Parameters from the Mesh menu.

For the different simulations, the parameters where chosen to produce approximately the same number of degrees of freedom, a number that could be handled by the computer used (with 1Gb in memory).

- Choose predefined mesh sizes as fine, this will set all parameters to a new default value. For the specimen with 1mm hump radius these parameters where not changed, however with smaller humps, there was a need to increase the local mesh resolution to maintain a comparable number of elements within the hump.
- Press the boundary mesh parameters button and select the boundary corresponding to the hump surface. Check the maximum element size and enter 1.2e-4 (0.75e-4), this will put an upper limit to the size of the elements at this boundary.
- In order to create a smooth transition from the high resolution in the hump, change the Element growth rate parameter to 1.40 (1.50).

5.1.5 Solving

Choosing good time step sizes is an important detail of the modeling process, as it has significant impact on both accuracy and computational time. Because of the linear behavior prior to yield, only one step is necessary on the entire elastic range. This initial step can be found by trial. The global parameter corresponding to time was named para, and corresponded to half the elongation in micrometer of the full size specimen including symmetries.
Past yield, small parameter steps were chosen to correctly model the abrupt transition into the plastic range of the most interesting area, that is, the hump. As a rule of thumb, the accuracy of computed local results depends on the resolution of the mesh in the immediate neighborhood [5].

- Select **Solver Parameters** from the **Solve** menu.
- Choose **solver** as **parametric nonlinear**.
- Enter **para** in the **Parameter name** field. In the **List of parameter values** field, enter:

\[
0 \ 64:2:70 \ 75:5:100 \ 110:10:410 \\
(0 \ 75:3:90 \ 100:10:500) \\
(0 \ 95:5:120 \ 132:12:660)
\]

5.1.6 **Postprocessing**

After running the simulation, the **Plot Parameters** window can be opened from the **Postprocessing** menu. From this window a large number of plot tools to view the solution data graphically can be reached. To create a numerical plot of nodal quantities like the one seen in Figure 9, the following steps can be used:

- Select **Domain Plot Parameters** from the **Postprocessing** menu.
- Choose **point plot** and select the corner point found in the middle of the hump surface. Enter **epeGp_smsld** in the **Expression** field to plot the effective plastic strain over time, or **misesGp_smsld** to plot the von Mises stress (Gp = Gauss point variable).
- Press **Ok**. Press the **expression** button to specify the x-axis parameter, and enter in the **Expression** field: \((para*2e-6)/(29*e-3)\), that is the increase in percentage from the undeformed to the deformed total length of the specimen. The default value here is the global time parameter **para**.
- Finally press “create plot” button to produce the plot. In order to plot functions from several different models in the same figure, the **Keep current plot** box in the **Domain Plot Parameters** window can be checked before opening the new model and creating the new plot.

5.1.7 **Electrical resistance**

Through the computed displacements, it would of course be possible to follow the change of electrical resistance in the specimen, assuming constant resistivity of the steel. However this might require additional scripting by the user, depending on functionality of the software interface. In Comsol Multiphysics 3.2, a rather cumbersome procedure involving couplings with the ALE (arbitrary lagrangian-eulerian) and static current applications can be used. Without scripting, this procedure it seems must be manually performed at each iteration step.

To obtain numerical values of electrical resistance, the following steps can be performed after running the simulation as described in the preceding sections:
• Open the **Solver Manager** window from the **Solve** menu, and press the **store solution** button. Then check the **stored solution** box for initial value, and choose one parameter value from the list. The remaining steps will obtain a value of electrical resistance for this parameter value.

• Go to the **solve for** tab, and mark only **Moving mesh** and **Electric potential**. The displacements are already stored and will be used as initial values to the moving mesh application.

• Open the **Model Navigator** window from the **Multiphysics** menu.

• Choose **Deformed Mesh – Static Analysis** from the model navigator and press the **Add** button. Then choose **Electromagnetics – Conductive Media DC** from the same list and press **Add** again.

• Select **Subdomain Settings** from the **Physics** menu, and load material **Steel AISI 4340**, or enter the electrical conductivity for the specific alloy manually.

• Select **Boundary Settings** from the **Physics**. First mark all boundaries, choose **normal current inflow** and set **current density** to zero. Then mark the boundary corresponding to the cut through the middle of the hump, and choose **ground**. Finally mark the boundary opposite to the latter, choose **electric potential** and enter 1 in the corresponding field. Now the electromagnetic settings are completed.

• Select **ALE moving mesh** from the **Multiphysics** menu.

• Select **Subdomain Settings** from the **Physics** menu. Specify initial conditions to be **Physics induced displacements** and enter respectively **u**, **v**, and **w** in the three corresponding fields. This will couple the displacements computed during the regular elastoplastic simulation to the initial displacements of the moving mesh application.

• Select **Solver Parameters** from the **Solve** menu and enter 0 in the **List of parameter values** field. Finally press the **solve** button! The computation should only take a couple of seconds.

• Select **Boundary Integration** from the **Postprocessing** menu, and integrate **Current density outflow** over the boundary corresponding to the cut through the middle of the hump. The inverted value this integral is by Ohm’s law the sought value of electrical resistance.
5.2 Results

Many failure criteria are based on the von Mises stress, or equivalently the accumulated effective plastic strain, which makes these values interesting to study [4]. Not so surprisingly, the maximal values of stresses and strains were, except for a few early parameter values, consistently found at the very center point of the hump surface. This was also a predefined corner point of the geometry, making it easily available by plotting tools in the user interface. In Figure 8, these values in the center point are plotted as functions of the total elongation in percent of the specimen waist, see also Figure 1. Note the almost linear stress curve past yield. However, using a more appropriate finite strain material model, a corresponding curve must be expected to deviate more than slightly from the one in figure 9 for the higher strain regions.

![Figure 8](image-url)

Figure 8.
Figure 9. The von Mises stress and accumulated plastic strain at the very center point of the hump surface, plotted versus the elongation in percent of the specimen waist. The waist including the rounded ends is 29mm long in original shape, see Figure 1. The red, blue and green curves correspond to specimen with a hump radius of respectively 0.25, 0.5 and 1.0 mm.
Figure 10: The propagation of plastically deformed areas in the specimen with a 0.5mm hump. The three color levels correspond to accumulated effective plastic strains exceeding 0%, 10% and 20% respectively. The three different plots in turn correspond to an elongation 2.34%, 2.90% and 3.45% respectively.
6 Discussion and conclusions

Due to the relatively large values of strain occurring in SSRT of the type studied in this work, software implementing finite strain elastoplasticity should be preferable over the small strain theory. Essentially only the theory in section 3.3 would need to be revised when implementing for example a hyperelastic-plastic constitutive theory. Particularly the material parameters and other inputs to the software would remain the same, as the true stress-strain curve used is already defined to be meaningful for large strains.

When working with relatively simple outward loading SSRT of initially fully annealed metallic solids, isotropic hardening is likely to be as good as any other hardening hypothesis. The advantage of this hypothesis is that simple uniaxial stress-strain curve can be used to define material behavior, in accordance with a well-tried theoretical foundation.

The effects of residual stresses and previous deformation (cold work, welding etc) in the material are likely to be difficult to take correct account to in simulation. Apart from difficulties in correctly establishing initial stress and plastic strain, anisotropy in the yield stress level required to cause further plastic deformation is a possibility. Since plastic yield is path dependent, this anisotropy would not in general be a direct function of the current state of deformation, whether using tensorial strain or other hardness measures.

In the end, because of the complexity of the physical processes involved, only comparison with physical tests could confirm or reject any constitutive theory used in simulation. One cannot rule out the possibility that an isotropic model, or perhaps some simple modification of it, would indeed work sufficiently well describing tests with previously deformed (that is, not fully solutions annealed) metals. Note that the simulations described in the previous chapter implemented isotropic hardening without any modification.
7 Bibliography


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