Crystal plasticity and crack initiation in a single-crystal nickel-base superalloy
Modelling, evaluation and applications

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Cover:
A FE-simulation of one of the notched test specimens, showing the stress response in the loading direction due to the applied boundary conditions and load (shown in a simplistic form).

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"Why is any object we don’t understand always called a thing?"

Dr. Leonard ’Bones’ McCoy
Abstract

In this dissertation the work done in the projects KME-410/502 will be presented. The overall objective in these projects is to evaluate and develop tools for designing against fatigue in single-crystal nickel-base superalloys in gas turbines. Experiments have been done on single-crystal nickel-base superalloy specimens in order to investigate the mechanical and fatigue behaviour of the material. The constitutive behaviour has been modelled and verified by FE-simulations of the experiments. Furthermore, the microstructural degradation during long-time ageing has been investigated with respect to the material’s yield limit. The effect has been included in the constitutive model by lowering the resulting yield limit. Moreover, the fatigue crack initiation of a component has been analysed and modelled by using a critical plane approach in combination with a critical distance method. Finally, as an application, the derived single-crystal model was applied to all the individual grains in a coarse grained specimen to predict the dispersion in fatigue crack initiation life depending on random grain distributions.

This thesis is divided into three parts. In the first part the theoretical framework, based upon continuum mechanics, crystal plasticity, the critical plane approach and the critical distance method, is derived. This framework is then used in the second part, which consists of six included papers. Finally, in the third part, details of the used numerical procedures are presented.
Sammanfattning


Denna avhandling är indelad i tre delar. I den första delen har det teoretiska ramverket, baserat på kontinuumsmekanik, kristallplasticitet, kritisk planmodell och kritisk distansmetod, härdtats. Detta ramverk används sedan i den andra delen, som består av sex artiklar. Slutligen, i den tredje delen, presenteras de använda numeriska rutinerna.
In this dissertation, the following papers have been included:


Own contribution

In all of the listed papers I have been the main contributor for the modelling and writing, except in the second paper where Johan Moverare and I shared the main writing and this is also the case in the sixth paper where David Aspenberg, David
Gustafsson and I shared the main writing. All the experimental work has been carried out by Johan Moverare, Sten Johansson and Mikael Segersäll.

Papers not included in this dissertation:

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Part I

Theory and background
Due to increasing demands for electricity on the global market, the need for higher efficiency and larger power supply is strong. This sets pressure on the development and design of new power generating equipment, e.g. driven by gas turbines. In gas turbines the operating temperature is very high. The higher the operating temperature is the higher efficiency of the gas turbine is received. The temperature is so high that, for instance, steels will begin to deteriorate (i.e. by creep and oxidation). Therefore, an often used material in gas turbines are nickel-base superalloys, which are able to manage the high temperatures.

The historical development of superalloys started prior to the 1940s [1–3]. These superalloys were iron-based and cold wrought. In the 1940s the investment casting was introduced on cobalt-based superalloys, by which the operating temperature could be raised significantly. These were mainly used in aircraft jet engines and land turbines. During the 1950s the vacuum melting technique was developed allowing a fine control of the chemical composition of the superalloys, which in turn led to a revolution in processing techniques such as directional solidification of alloys and single-crystal superalloys. In the 1970s powder metallurgy was introduced to develop certain superalloys, leading to improved property uniformity due to the elimination of micro segregation and the development of fine grains. In the later part of the 20th century the superalloys had become commonly used for many applications.

Nickel-base superalloys are commonly used in aircraft and industrial gas turbines for blades, disks, vanes and combustors. Superalloys are also used in rocket engines, space vehicles, submarines, nuclear reactors, military electric motors, chemical processing vessels, and heat exchanger tubings.

The superalloys treated in this study are single-crystal nickel-base superalloys, which have even better properties against temperature than their coarse-grained polycrystal cousins. The thermal efficiency increases with the operating temperature of a gas turbine and therefore the temperature is increasing with every gas turbine that is developed or redesigned. With increasing temperature, the components of the gas turbine will be more exposed to creep, oxidation and thermomechanical
CHAPTER 1. INTRODUCTION

fatigue. An extra risk with single-crystal materials is that after initiation, a fatigue crack may propagate through a whole component with much less resistance compared to conventional polycrystal materials. The designer wants to produce better and more efficient gas turbines which can manage higher and higher temperatures. This requires that during the development or redesign of gas turbines there are tools and criteria available which take all of these aspects into consideration.

How do the components of the turbine handle certain temperatures and load conditions? How does the material behave under these loadings? How long is the life of the components? When will a crack initiate and propagate? These are all questions that need to be addressed in order to develop and manufacture a gas turbine. In the initial development phase of a new gas turbine or redesigning an existing gas turbine one needs constitutive and life prediction models for the material in question that can handle all of these aspects.

Siemens Industrial Turbomachinery AB in Finspång, Sweden, develops and manufactures gas turbines for a wide range of applications. Siemens is participating in a research programme that aims at solving material related problems associated with the production of electricity based on renewable fuels and at contributing in the development of new materials for energy systems of the future. This programme, called Konsortiet för Materialteknik för termiska Energiprocesser (KME), was founded in 1997 and presently 7 industrial companies and 18 energy companies are participating through Elforsk AB in the KME programme [4]. Elforsk AB, owned jointly by Svensk Energi (Swedenergy) and Svenska Kraftnät (The Swedish National Grid), started operations in 1993 with the overall aim to coordinate the industry’s joint research and development and is financially supported through Energimyndigheten (The Swedish Energy Agency).

"Our mission is to promote the development of Sweden’s energy system so that it will become ecologically and economically sustainable. This means that energy must be available at competitive prices and that energy generation must make the least possible impact on people and the environment. In simple words, a smarter use of energy.”

Energimyndigheten [5]

The work presented here has been carried out within the following projects of the KME-programme; KME-410 Thermomechanical fatigue of notched components made of single-crystal nickel-base superalloys and KME-502 Fatigue in nickel-based superalloys under LCF and TMF conditions. These projects have been jointly funded by Siemens Industrial Turbomachinery AB and Energimyndigheten.
1.1 Aim

The aim of the KME-410/502 projects is to improve the knowledge regarding the mechanisms that govern crack initiation and propagation in single-crystal nickel-base superalloys under thermomechanical fatigue conditions and to develop models that can be used to predict the service life of components in gas turbine applications. Furthermore, the mechanical behaviour of the single-crystal nickel-base superalloy need to be investigated and modelled to obtain an accurate response due to the loading conditions.

These projects have a strong industrial connection, as the work done in the projects will be beneficial to the design/redesign process of gas turbines as a simulation based design tool.
2.1 Gas turbines

The function of a gas turbine is to supply electric power, to propel heavy machinery or transport vessels such as ships and aircrafts. A gas turbine basically consists of a compressor, a combustor and a turbine, see Figure 1. The incoming air is compressed in the compressor to increase the pressure of the air. The compressed air then enters the combustion chamber, where it is mixed with the fuel and ignited. These hot gases will then flow through the turbine and by doing so make the turbine rotate. The temperature of the turbine components can range from 150°C and up to 1500°C [1]. The turbine drives the compressor by a shaft. In jet engines the hot gases then pass through a nozzle, giving an increase in thrust as it is returned to normal atmospheric pressure. For stationary power generating gas turbines there is, instead, a power turbine, which in turn, drives, for instance, an electric generator.

![Figure 1: The interior of the stationary power generating gas turbine Siemens SGT-600. Courtesy of Siemens.](image-url)
Some of the principal advantages of the gas turbine are [6]:

- For its relatively small size and weight the gas turbine is capable of producing large amounts of useful power.
- Its mechanical life is long and the corresponding maintenance cost is relatively low, since the motion of all its major components involve pure rotation (i.e. no reciprocating motion as in a piston engine).
- The gas turbine, which must be started by some external means (a small external motor or other source), can be brought up to peak performance in minutes in contrast to a steam turbine whose start up time takes hours.
- Natural gas is commonly used in land-based gas turbines as fuel while light distillate (kerosene-like) oils power aircraft gas turbines. Diesel oil or specially treated residual oils can also be used, as well as combustible gases derived from blast furnaces and refineries or from the gasification of solid fuels such as coal, wood chips and bagasse. Hence, a wide variety of fuels can be used.
- As a basic power supply, the gas turbine requires no coolant (e.g. water). The usual working fluid is compressed atmospheric air.

2.2 Single-crystal material in gas turbines

In the hottest area, which is the first turbine step, in a gas turbine, it is common to use single-crystal nickel-base superalloys for the turbine blades, due to their good mechanical properties at high temperature, mainly their creep resistance.

As the gas temperature plays a significant role for the efficiency of the gas turbine, it is necessary that the blades contain cooling channels, in which compressed air from the compressor is flowing, to withstand the hot environment. Furthermore, cooling holes are positioned at the surface of the blades to generate a film cooling effect that cools the surface of the blades [7].

To make the blade even more temperature resistant, a so called thermal barrier coating (TBC) can be applied, see e.g. [3,8]. A thin ceramic layer (topcoat), typically composed of yttria-stabilized zirconia, is applied to the surface of the blades. To bind the topcoat to the metallic substrate (the turbine blade) a bond coat is used to account for the adhesion between the materials. The ceramic layer acts as insulation against the heat, lowering the blade temperature, and thus a hotter inlet temperature can be used in the gas turbine, which further yields a higher efficiency of the gas turbine. The TBC is e.g. applied by air/vaccum plasma spraying or by electron beam physical vapor deposition.
2.3 Loading conditions

An example of a single-crystal turbine blade is shown in Figure 2, where one can see a complex structure with many cooling holes. Single-crystal components are manufactured by investment casting, where a single grain is made to grow in the orientation of a seed which was chosen by the grain-selector [1,3]. This is a very delicate process, hence the production is very expensive due to failure of wrongly oriented components.

Figure 2: A single-crystal turbine blade. Courtesy of Siemens.

Typically these single-crystal blades are manufactured with their [001]-orientation along the length direction of the blade, because it is the simplest and cheapest orientation to manufacture and the [001]-orientation yields lower stresses in notches than other orientations for a given strain, due to the lower elastic stiffness response of this orientation.

2.3 Loading conditions

As the hot gases flow over the turbine stage the turbine will rotate, thus creating a centrifugal load acting on the turbine components. Considering that the shaft is rotating at an angular velocity of more than 10000 rpm [3], the centrifugal load affecting the blades becomes very high as they are positioned on the disk rim. This leads to high stresses in the fir tree attachment (connecting the blade to the disk) at the root of the blades, which contains notches.

As stated previously the temperature in gas turbines tends to get rather high during operation and during long time exposure in combination with the centrifugal
load this will lead to creep deformation. After long time cyclic loading (by start-
run-stop cycles), small fatigue cracks may initiate, usually at the surface of the 
component. As the components are further loaded these small cracks will start to 
propagate in the material and eventually lead to fatigue failure.

During a normal operation cycle (start-up, steady-state operation and shut-down) 
the components in the hot sections of the gas turbine will be affected by different 
temperatures, and might experience so called thermomechanical fatigue (TMF). 
In this case large temperature changes result in significant thermal expansion and 
contraction and therefore significant strain excursions. These strains are enlarged 
or countered by the mechanical strains associated with the centrifugal load [9]. 
The combination of these events may cause TMF. There are many types of TMF 
cycles, but the two most common cycles are the In-phase and Out-of phase cycles.

- **In-phase cycle**
  This is when the strain and the temperature are cycled in phase, see Figure 
  3(a). A typical example is a *cold spot* in a hotter environment, which at 
  high temperature will be loaded in tension and at low temperature loaded in 
  compression.

- **Out-of phase cycle**
  This is when the strain and the temperature are cycled in counterphase, see 
  Figure 3(b). A typical example is a *hot spot* in a colder environment, which 
  at low temperature will be loaded in tension and at high temperature loaded 
  in compression.

![Figure 3: The thermomechanical fatigue cycles, a) In-phase and b) Out-of phase from a components perspective.](image)

Most turbine blades have a variety of features like holes, interior passages, curves 
and notches. These features may raise the local stress level to the point where 
plastic flow occurs. As engine rotational speed increases, centrifugal forces may 
result in local plastic strains at the fir tree attachment surfaces that can lead to
2.3. LOADING CONDITIONS

Low-cycle fatigue (LCF) damage. LCF is usually characterised by a Coffin-Manson type of expression [10,11] for determining the fatigue life of a specific component.

Also depending on what kind of fuel is used, different oxidative and corrosive elements are present in the hot gases, which affects the components negatively.
3.1 Basic material composition

A superalloy is an alloy that exhibits excellent mechanical strength and creep resistance at high temperatures. A superalloy might also have very good corrosion resistance (depending on the chromium wt.%) and oxidation resistance (depending on the aluminium wt.%). Nickel-base superalloys are alloys which consist mostly of nickel. Nickel is used as the base material on account of its face-centered cubic (FCC) crystal lattice structure [12], which is both ductile and tough, and on account of its moderate cost (compared with other useful materials) and low rates of thermally activated processes (creep). Nickel is also stable in the FCC form when heated from room temperature to its melting point, i.e., there are no phase transformations [3].

There are often more than 10 different alloying elements in a superalloy, each with their specific enhancing property. The alloying materials reside in different phases, which for a typical nickel-base superalloy are [1, 3, 13, 14].

- The $\gamma$-phase. This phase exhibits the FCC crystal lattice structure and forms a matrix phase, in which the other phases reside. Common elements of this phase are iron, cobalt, chromium, molybdenum, ruthenium and rhenium. The narrow channels of the matrix phase have a size smaller than 0.1 $\mu$m.

- The $\gamma'$-phase. This ordered phase is promoted by additions of aluminium, titanium, tantalum, niobium and presents a barrier to dislocations. The role of this phase is to confer strength to the superalloy. $\gamma'$ forms cubical precipitates, whose sides are smaller than 1 $\mu$m. It also exhibits a number of surprising mechanical properties like increase of yield strength with increasing temperature, strong orientation dependence of the yield stress and tension/compression asymmetry.

- The $\gamma''$-phase. The strengthening precipitate in nickel-iron superalloys, used in e.g. turbine disks, is known as the $\gamma''$-phase. This phase occurs in nickel-base superalloys with significant additions of niobium (e.g. Inconel 718) or vanadium; the composition of the $\gamma''$ is then Ni$_3$Nb or Ni$_3$V. The crystal structure of the $\gamma''$-phase is the body-centered tetragonal (BCT) lattice structure.
with an ordered arrangement of nickel and niobium atoms.

- Carbon and boron acts as grain boundary strengthening elements as they segregate to the grain boundaries of the $\gamma$ phase, where they form carbides and borides.

There can also be other phases in the superalloys, e.g. the topologically close-packed (TCP) phases $\mu$, $\sigma$, etc. or the orthorhombic $\delta$-phase, which can be formed in nickel-iron alloys.

In Figure 4 one can see the microstructure of a single-crystal nickel-base superalloy. The cubical shapes are $\gamma'$-particles which are surrounded by a matrix of $\gamma$, thus, constituting a composite structure. Single-crystal superalloys are alloys that consist of only one grain. They have no grain-boundaries, hence grain boundary strengtheners like carbon and boron are unnecessary. Grain boundaries are easy diffusion paths and therefore reduce the creep resistance of the superalloys. Due to the nonexistence of grain boundaries single-crystal superalloys possess the best creep properties of all superalloys.

Figure 4: Microstructure of a single-crystal nickel-base superalloy [15].

3.1.1 Crystal structure

With nickel as the base material the superalloy possesses the FCC crystal lattice structure. The strengthening $\gamma'$-particles consist of Ni$_3$Al with an L1$_2$ ordered structure, where as the disordered $\gamma$-phase consist of a disordered mixture of the alloying compounds [3], see Figure 5.
3.1. BASIC MATERIAL COMPOSITION

The FCC structure is a very close-packed structure with a coordination number of 12 \cite{12}, which is the maximum. The coordination number is the number of atoms surrounding each particular atom in the structure. Inelastically, the material deforms primarily along the planes which are most tightly packed, these are called \textit{close-packed planes} or \textit{discrete slip planes}. The FCC structure has four unique close-packed planes which, in Miller indices, are of the family \{111\}.

\[
\{111\} = \begin{cases} 
(111) \\
(1\bar{1}1) \\
(\bar{1}11) \\
(\bar{1}\bar{1}1)
\end{cases}
\]

The unit cell of the crystal structure, with slip plane (111), is seen in Figure 6. The axes of the unit cell, labelled \(a_1\), \(a_2\) and \(a_3\), define the crystal orientation with respect to the global coordinate system. It is most likely that the crystal orientation does not coincide with the global coordinate system of a structure, as during casting of the components small orientation deviations are to be expected.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{The (111) slip plane in the unit cell.}
\end{figure}
In each of these slip planes there are three slip directions, disregarding the negative directions. These directions are the most close-packed directions in each slip plane. The slip directions are of the family \(\langle 110 \rangle\) and for this crystal structure they coincide with the Burger’s vectors [16].

\[
\begin{align*}
\langle 110 \rangle & \quad \{110\} \quad [110] \\
 & \quad \{101\} \quad [101] \\
 & \quad \{011\} \quad [011]
\end{align*}
\]

These slip directions, in sets of three, are orthogonal against each one of the slip planes defined above. Hence, one has twelve slip systems to take into consideration.

### 3.2 Basic material properties

To get a solid view of the material properties of single-crystal nickel-base superalloys, one needs to examine the mechanical behaviour of the material. Some basic experimental tension and compression tests at room temperature reveal the basic material properties, see Figure 7.

![Figure 7: Results from basic monotonic tension and compression tests [17].](image)

We can note a number of special features from the mechanical response shown in Figure 7:

- Depending on which crystal orientation that is parallel with the axis of the test specimens, different elastic moduli are received. Thus, the material exhibits a significant elastic anisotropy.
3.2 BASIC MATERIAL PROPERTIES

- The yield limits are different for the respective crystal orientations, hence plastic anisotropy is observed.
- The material also has different yield limits in tension and compression for the respective crystal orientation, thus a tension/compression asymmetry is present in the material.
- The hardening found in the yield curves is negligibly small. Hence, an assumption of a perfect plasticity behaviour can be motivated.

3.2.1 Elastic anisotropy

When the component is loaded in different crystal orientations it experiences different elastic stiffness responses, i.e. it has different elastic moduli. The different elastic stiffnesses are correlated to the bonding of the atoms along the different crystal orientations [18].

3.2.2 Plastic anisotropy

When a single-crystal component is deformed inelastically the deformation will take place by shearing of the $\gamma'$-particles and a sliding motion (dislocation motion) along the discrete slip planes will be obtained as the material is distorted, and eventually persistent slip bands (PSB) [19] will start to appear. This sliding motion is referred to as slip, which is generated in the direction of the Burger’s vector [16] on the discrete slip planes, see Figure 6. Depending on the crystal orientation in the loaded component different yield limits are obtained, as seen in Figure 7 the [001]-orientation experiences the lowest yield limit and the [011]-orientation (in compression) experience the highest.

3.2.3 Tension/Compression asymmetry

In experimental studies, e.g. [17, 20], it has been found that single-crystal nickel-base superalloys have different yield limits along different loading axes, these yield limits are also different in tension and compression, which can also be seen in Figure 7. With use of the basic unit triangle from the stereographic projection, shown in Figure 8, the three major directions of the crystal are studied.

The conclusions that can be drawn from these experimental studies are the following:
- The yield limit in tension for [001] is higher than in compression.
Figure 8: The dominating tension/compression yield limit responses contra crystal orientation in the unit triangle of the stereographic projection [13].

- The yield limit in compression for $\{111\}$ is higher than in tension.
- The yield limit in compression for $\{011\}$ is much higher than in tension.

However, the magnitude of this tension/compression asymmetry can vary significantly depending on the chemical composition of the alloy [21].

The tension/compression asymmetry is believed to be attributed by the cross-slip of dislocations from the primary slip plane to the cube slip plane [22–26]. When the dislocations cross-slip to the cube plane so called Kear-Wilsdorf locks [27, 28] are created, which locally pin the dislocation on the primary slip plane. To be able to cross-slip the dislocation needs to contract its core, and when it has cross-slipped it is able to expand its core on the cube plane, this is known as the core width effect. This asymmetry is believed to be affected by the shear stresses acting along different crystallographic directions, see e.g. [13, 14, 20, 29–34].

3.2.4 Hardening

Usually either a softening or hardening response is seen as a material is plastically deformed. According to Suresh [19], a well-annealed FCC single-crystal superalloy experience a hardening behaviour when deformed, but as seen in Figure 7 the hardening is negligibly small for this specific material. Hence, for simplicity a perfect plasticity description can be adopted.

3.3 Microstructural degradation

Superalloys can undergo microstructural degradations when exposed to high temperatures. One such phenomenon is directional coarsening or rafting, which is a temperature-dependent ageing process, in which the strengthening $\gamma'$-particles become elongated in certain directions. The overall response is that the yield limit is
3.3 MICROSTRUCTURAL DEGRADATION

decreasing along with the increase of the rafting [15]. Rafting is governed by the lattice misfit between the $\gamma$- and $\gamma'$-phases and by the type of applied stress, see e.g. [35, 36]. Additionally, it has been reported that rafting can occur in the absence of an applied load if the structure has been subjected to sufficient amount of plastic straining prior to the temperature exposure [37]. Most of the single-crystal superalloys have negative lattice misfit at the operating temperatures, which means that the $\gamma'$-particles experience internal tensile stresses and that the $\gamma$-phase experiences internal compressive stresses prior to deformation, see Figure 9(a), cf. [38]. When the structure is loaded in tension, so that plastic flow occurs, the internal stresses in the microstructure are affected according to Figure 9(b). This leads to an increase in dislocations along the horizontal channels of the $\gamma$-phase, due to the increasing internal compressive stress, which yields the corresponding rafting direction. A typical rafted microstructure can be seen in Figure 10.

![Diagram of internal stresses in microstructure](image.png)

Figure 9: The internal stresses of the microstructure in a) an unrafted condition and b) a rafted condition (LD = Loading Direction) [38].

Several aspects of directional coarsening of $\gamma'$-precipitates, i.e. rafting, during high temperature deformation are still under discussion [39]. However, for a wide range of [001]-oriented nickel-base superalloy specimens, the coalescence results either in uniaxial rods (or needles) of the $\gamma'$-phase oriented parallel to the stress axis, or in biaxial rafts (or plates) within planes perpendicular to it [40], depending on whether the applied stress is compressive or tensile, respectively.
Figure 10: A typical rafted microstructure of a specimen with loading axis in [001], loaded in tension (LD = Loading Direction) [15].
A number of experiments were made to examine the actual material behaviour of the investigated single-crystal nickel-base superalloy. The investigated material is MD2, which has very similar properties as CMSX-4 (a widely used single-crystal nickel-base superalloy), and it has the following chemical composition Ni, 5.1Co, 6.0Ta, 8.0Cr, 8.1W, 5.0Al, 1.3Ti, 2.1Mo, 0.1Hf, 0.1Si (in wt.%). These tests formed the basis for the development of the models reported in this dissertation. The following experimental tests have been carried out:

- Tension and compression tests of four [001], four [011] and four [111]-oriented specimens at room temperature, see [17].
- Tension and compression tests of four [001], four [011] and four [111]-oriented specimens at room temperature after microstructural degradation (rafting), see [15].
- Tension and compression tests of two [001], two [011] and two [111]-oriented specimens at 500° C, see [41].
- LCF tests of four [001], four [011] and four [111]-oriented specimens at 500° C, smooth geometry at $R_e = -1$, see [41].
- LCF tests of seven [001]-oriented specimens at 500° C, notched geometry at $R_e = 0$, see [41–43].

The main testing was conducted at Siemens Industrial Turbomachinery AB in Finspång, using an MTS810 servo-hydraulic testing machine, see Figure 11. The heating of the test specimens was done by an induction coil, which heated the material very rapidly to the desired temperature. The cooling was performed by a focused flow of compressed air. A strain gauge applied over the center of the test specimen measured the strain in the specimen and controlled the displacement of the servo-hydraulic testing machine grips so that the correct strain or strain range was reached. Strain gauges with gauge lengths of 12, 12.5 and 15 mm were used.

The test specimens used in the experiments were manufactured by investment casting with the longitudinal axis parallel to the nominal [001], [011] and [111] crystal directions, respectively. When the test specimens are manufactured it is very hard to get the crystallographic directions perfectly parallel to the axes of the
CHAPTER 4. EXPERIMENTS

Figure 11: The MTS810 servo-hydraulic testing machine. Courtesy of Siemens.

specimens; due to this the test specimens experience a small misalignment from the ideal directions. The misalignments are defined according to Figure 12. These misalignments were taken into consideration in all the developed models to get a correct compliance with the experimental tests.

For the degraded test series the test specimens were first loaded in tension and compression at room temperature to ∼ 0.7% plastic strain, the specimens were then placed in a furnace for 1100 h at 1025°C. After this long temperature exposure the test specimens were again loaded in tension and compression to see how the
degradation effected the yield limits. To find out how much the test specimens had degraded/rafted the specimens were cut and analysed with scanning electron microscopy (SEM). The average distance between the \( \gamma \)-channels of the material were then measured along three crystal orientations, see Figure 13. This average distance was then normalised with the distance found in the virgin state, thus defining a coarsening parameter which are used in the developed material model.

![Figure 13: Measured distance between the \( \gamma \)-channels [15].](image)

The LCF testing of the smooth specimens were performed on twelve specimens with the nominal [001], [011] and [111] crystal directions in the loading direction. The specimens were loaded under displacement control with different nominal strain ranges, ranging from 0.4% to 1.799%. The number of cycles to fatigue crack initiation was determined by a 5% load-drop from the trend line describing the maximum stress in the cycle versus the number of load cycles.

The test series of the notched specimens were conducted with seven specimens which had the nominal [001] crystal direction parallel to the loading direction. The top of the test specimens, at the smooth state, were investigated to find one of the secondary crystal orientations. The notch was then machined so that the horizontal projection of the found secondary crystal orientation was aligned with it, see Figure 14.

The notched specimens were also loaded under displacement control with different nominal strain ranges, ranging from 0.4% to 0.598%, but different strain gauges were used; one with length 12.5 mm and one with 15 mm. The number of cycles to fatigue crack initiation was determined by optical inspection using an CCD-camera. After the testing had been completed the footage was manually inspected by going backwards to find the cycle at which no crack could be seen, the corresponding
cycle is thus the cycle to fatigue crack initiation. The specimens were then pulled apart and the fracture surface was investigated by microscopy to determine which crystallographic plane the crack initiated on, see Figure 15.

Figure 14: The location of the secondary crystal orientation (SCO) with reference to the notch [42].
Figure 15: The opened test specimens after loading, showing the crystallographic plane which they initiated on [43].
For describing the stress state in a structure, subjected to small deformations, the following expression is used

\[ \sigma = C^e \cdot \varepsilon^e \]  
(1)

where \( C^e \) is the elastic stiffness tensor and \( \varepsilon^e \) is the elastic part of the strain.

The total strain is divided into an elastic part and a plastic part as follows

\[ \varepsilon = \varepsilon^e + \varepsilon^p \]  
(2)

The plastic strain needs an evolution law to be updated correctly.

Now in the single-crystal case, we might experience large deformations when the structure is loaded. Hence, one cannot use the above stated expressions, instead one needs to use other stress and strain measures, and the elastic stiffness tensor needs to be defined in such a way that it can describe the different stiffnesses in the different crystal orientations (an anisotropic fourth order tensor). To define the large deformation stress and strain measures, we first have to set up the appropriate kinematics which they are based upon.

5.1 Kinematics

When a body is deformed its configuration is changed. As seen in Figure 16, the body undergoes a deformation from the reference configuration (\( \Omega_0 \)) to the current configuration (\( \Omega \)). Instead of taking the direct way, with the use of the total deformation gradient tensor \( F \), the other way through the intermediate configuration (\( \bar{\Omega} \)) is preferable [44]. The first step is performed by shearing of the lattice, described by the plastic deformation gradient tensor \( F^p \), and finally, the lattice is both elastically stretched and rotated by the elastic deformation gradient tensor \( F^e \).

The total deformation gradient tensor is thus divided into an elastic part and a plastic part, through the following multiplicative decomposition [45]

\[ F = F^e F^p \]  
(3)
The velocity gradient tensor $L$ can then also be expressed in an elastic part and a plastic part by insertion of Equation (3)

$$L = \dot{F}F^{-1} = \dot{F}^e F^{e^{-1}} + \dot{F}^p F^{p^{-1}} F^{e^{-1}}$$

(4)

From Equation (4) the following quantities can be defined

$$L^e = \dot{F}^e F^{e^{-1}}$$

(5)

$$L^p = \dot{F}^p F^{p^{-1}} F^{e^{-1}}$$

(6)

$$\dot{L}^p = \dot{F}^p F^{p^{-1}}$$

(7)

where $L^e$, $L^p$ are the elastic and plastic velocity gradient tensors, respectively, defined in the current configuration ($\Omega$) while $\dot{L}^p$ is the plastic velocity gradient tensor defined in the intermediate configuration ($\bar{\Omega})$. The velocity gradient can be divided into one symmetric part and one skew-symmetric part.

$$L = \frac{1}{2} (L + L^T) + \frac{1}{2} (L - L^T) = D + W$$

(8)
where \( D \) is the rate of deformation tensor (symmetric) and where \( W \) is the spin tensor (skew-symmetric). These two can each be divided into an elastic part and a plastic part, according to an additive split

\[
D = D^e + D^p \tag{9}
\]

\[
W = W^e + W^p \tag{10}
\]

where

\[
D^e = \frac{1}{2} \left( L^e + L^e^T \right), \quad D^p = \frac{1}{2} \left( L^p + L^p^T \right) \tag{11}
\]

\[
W^e = \frac{1}{2} \left( L^e - L^e^T \right), \quad W^p = \frac{1}{2} \left( L^p - L^p^T \right) \tag{12}
\]

The elastic Green-Lagrange strain tensor \( \bar{E}^e \) measured relative the intermediate configuration is defined as

\[
\bar{E}^e = \frac{1}{2} \left( F^e^T F^e - I \right) \tag{13}
\]

The relationship between the elastic rate of deformation tensor \( D^e \) defined in the current configuration and the elastic Green-Lagrange strain rate tensor \( \dot{\bar{E}}^e \) defined in the intermediate configuration is given by either a push-forward or a pull-back operation [46]

\[
D^e = F^e^{-T} \dot{\bar{E}}^e F^e^{-1}, \quad \dot{\bar{E}}^e = F^e T D^e F^e \tag{14}
\]

The second Piola-Kirchhoff stress tensor \( \bar{S} \) defined in the intermediate configuration can be expressed by a pull-back of the Kirchhoff stress tensor \( \tau \) from the current configuration

\[
\bar{S} = F^e^{-1} \tau F^e^{-T} \Rightarrow \tau = F^e \bar{S} F^e^T = J \sigma \tag{15}
\]

where \( J = \det F^e \). As can be seen, in order to receive the Cauchy stress tensor \( \sigma \) the Kirchhoff stress tensor is scaled by the Jacobian determinant [46].

The internal power \( \mathcal{P}^{int} \), when a body is deformed, is defined as

\[
\mathcal{P}^{int} = \int_{\Omega} \sigma : D dV \tag{16}
\]

The internal power can be divided into an elastic part and a plastic part by the additive decomposition of \( D \)

\[
\mathcal{P}^{int} = \int_{\Omega} \sigma : D^e dV + \int_{\Omega} \sigma : D^p dV \tag{17}
\]
 CHAPTER 5. MODELLING

The elastic part is transformed by a regular pull-back to the intermediate configuration, according to

\[ \int_{\Omega} \sigma : D_e \, dV = \int_{\bar{\Omega}} \bar{\sigma} : \bar{E}_e \, dV \]  

(18)

while the plastic part can be shown to obey the following transformation

\[ \int_{\Omega} \sigma : D_p \, dV = \int_{\bar{\Omega}} \bar{\sigma} : \bar{L}_p \, dV \]  

(19)

where \( \sigma \) is the so called Mandel stress tensor, given by the following expression

\[ \sigma = F^{-T} \tau F^{-T} \]  

(20)

Thus, the Mandel stress tensor is a non-symmetric tensor and it is defined in the intermediate configuration. The above relation can be further developed with the insertion of Equation (15), such that it includes the Kirchhoff stress tensor

\[ \sigma = F^{-T} \tau F^{-T} \]  

(21)

5.2 Elastic behaviour

Nickel-base superalloys are elastically anisotropic when in single-crystal form. Hence, the elastic stiffness is dependent on the crystal orientation relative the loading direction, e.g. the elastic stiffness tensor of a [001]-oriented component has the following appearance in Voight notation [46]

\[
\mathbf{C}^e = \begin{bmatrix}
C_1 & C_2 & C_2 & 0 & 0 & 0 \\
C_2 & C_1 & C_2 & 0 & 0 & 0 \\
C_2 & C_2 & C_1 & 0 & 0 & 0 \\
0 & 0 & 0 & C_3 & 0 & 0 \\
0 & 0 & 0 & 0 & C_3 & 0 \\
0 & 0 & 0 & 0 & 0 & C_3
\end{bmatrix}
\]  

(22)

Consequently, components machined from single-crystal specimens in different crystallographic orientations display different elastic behaviours, see e.g. [3]. A way to describe this elastic anisotropy is to divide the elastic stiffness tensor into an isotropic part and an anisotropic part [17,47], where the latter is described by using so called structural tensors \( \mathbf{M}_1 \) and \( \mathbf{M}_2 \), cf. [48], according to

\[
\mathbf{C}^e = \lambda I \otimes I + \mu (I \otimes I + I \otimes I) + 2\eta (\mathbf{M}_1 \otimes \mathbf{M}_1 + \mathbf{M}_2 \otimes \mathbf{M}_2 + \mathbf{M}_1 \otimes \mathbf{M}_2 - I \otimes \mathbf{M}_1 - I \otimes \mathbf{M}_2)_{MS}
\]  

(23)
where $\lambda$, $\mu$ are the Lamé constants, $\eta$ is an additional third elastic constant and the subscript $MS$ stands for major symmetry. The structural tensors are dependent on the crystallographic orientations in the following way:

$$M_1 = a_1 \otimes a_1$$

$$M_2 = a_2 \otimes a_2$$

(24)  

(25)

Thus, with the above defined stiffness tensor, the second Piola-Kirchhoff stress tensor in the intermediate configuration can be calculated by the following expression

$$\bar{S} = C^{ce} : \bar{E}^e$$

(26)

Hence, we get different stress components depending on the crystal orientation.

5.3 Basic crystal plasticity

In a tension test of a single-crystal component the axial load that initiates plastic flow depends on the crystal orientation. In order for this to happen, a sufficiently large shear stress acting in a slip direction on a discrete slip plane, must be produced by the axial load. It is this shear stress, called the resolved shear stress ($\tau_{pb}^\alpha$), that in the simplest case initiates the plastic deformation. It is expressed by Schmid’s law, with the Kirchhoff stress tensor in the current configuration, as

$$\tau_{pb}^\alpha = s^\alpha \cdot n^\alpha$$

(27)

where $\alpha$ denotes the slip system, and where $s^\alpha$ and $n^\alpha$ denotes the associated slip direction and normal direction of the slip plane, respectively. The subscript $pb$ indicates that $\tau_{pb}^\alpha$ is acting in the direction of the Burger’s vector on the primary slip plane, further details will follow below. Slip occurs on the slip systems that exhibit the greatest resolved shear stress. If only one slip system is active, the other slip systems have a smaller resolved shear stress than the critical stress and due to this slip does not occur on these systems.

During monotonic deformation of a structure, either in tension or compression, the crystal orientation will rotate. As seen in Figure 17 the normal direction $\bar{n}^\alpha$ will rotate away from the axial axis in tension and towards it in compression [49]. If the structure would have been deformed as a result of fully reversed cyclic loading, then no such rotation would be present [19].

The slip directions may be transformed from the intermediate configuration into the current configuration by

$$s^\alpha = F^e s^\alpha$$

(28)
Since the slip direction $\vec{s}^\alpha$ and the normal of the slip plane $\vec{n}^\alpha$ defined in the intermediate configuration, cf. Figure 16, are unit vectors and orthogonal to each other it follows that

$$\vec{n}^\alpha \cdot \vec{s}^\alpha = n^\alpha \cdot s^\alpha = 0 \quad (29)$$

Hence, the transformation for the normal vector can be defined as

$$n^\alpha = F_{e}^{-T} \vec{n}^\alpha \quad (30)$$

where $s^\alpha$ and $n^\alpha$ might no longer be unit vectors. To verify this result, we note that

$$n^\alpha \cdot s^\alpha = F_{e}^{-T} \vec{n}^\alpha \cdot F_{e}^{-1} \vec{s}^\alpha = \vec{n}^\alpha \cdot F_{e}^{-1} F_{e} \vec{s}^\alpha = \vec{n}^\alpha \cdot \vec{s}^\alpha \quad (31)$$

As mentioned above, plastic deformation occurs due to slip on the active slip systems [50], which can be expressed in the current configuration as

$$L^p = \sum_{\alpha} \dot{\gamma}^\alpha s^\alpha \otimes n^\alpha \quad (32)$$

where $\dot{\gamma}^\alpha$ is the inelastic shear strain rate on the slip system $\alpha$. With the use of Equation (28) and (30) the plastic deformation can be expressed in the intermediate
configuration as
\[ \bar{L}^p = \sum_{\alpha} \dot{\gamma}^\alpha \bar{s}^\alpha \otimes \bar{n}^\alpha \] (33)

For a detailed description of how the plastic deformation gradient tensor is coupled to the inelastic shear strain rate and iteratively updated see Appendix A.

The plastic part of the internal power in the current configuration can be expressed with Equation (32), taking into account that \( dV = J \cdot \bar{dV} \), as

\[ \int_{\Omega} \sigma : \bar{L}^p \, dV = \int_{\bar{\Omega}} \sum_{\alpha} \dot{\gamma}^\alpha \mathbf{T} : (s^\alpha \otimes n^\alpha) \, d\bar{V} = \int_{\bar{\Omega}} \sum_{\alpha} \dot{\gamma}^\alpha \tau^\alpha_{pb} \, d\bar{V} \] (34)

or in the intermediate configuration, cf. Equation (19), using Equation (33), as

\[ \int_{\bar{\Omega}} \mathbf{C} : \bar{L}^p \, d\bar{V} = \int_{\bar{\Omega}} \sum_{\alpha} \dot{\gamma}^\alpha \mathbf{C} : (\bar{s}^\alpha \otimes \bar{n}^\alpha) \, d\bar{V} = \int_{\bar{\Omega}} \sum_{\alpha} \dot{\gamma}^\alpha \tau^\alpha_{pb} \, d\bar{V} \] (35)

where \( \tau^\alpha_{pb} \) is the resolved shear stress. As Equation (34) and (35) yields the same result, the resolved shear stress can be expressed from both of them, as

\[ \tau^\alpha_{pb} = \mathbf{T} : (s^\alpha \otimes n^\alpha) = \mathbf{C} : (\bar{s}^\alpha \otimes \bar{n}^\alpha) \] (36)

It can be shown from Equation (36) that the following is true

\[ \tau^\alpha_{pb} = s^\alpha \cdot \mathbf{T} n^\alpha = \bar{s}^\alpha \cdot \mathbf{C} \bar{n}^\alpha \] (37)

which represents the resolved shear stress in both the current- and the intermediate configuration. One can also see this as a projection of the macroscopic stress state down onto the slip plane in the slip direction of slip system \( \alpha \).

5.4 Modelling the mechanical behaviour

As the mechanical behaviour of single-crystal nickel-base superalloys are rather complex one can not just describe it with Schmid’s law. In order to have a more realistic description of the material behaviour one also needs to take non-Schmid effects into account (capable of representing e.g. tension/compression asymmetry). This is done by further projections of the macroscopic stress state, i.e. in other directions and on other planes than that of the resolved shear stress. In this work the following non-Schmid stresses have been considered, cf. Equation (37) and Table 1

\[ \tau^\alpha_{cb} = \bar{s}^\alpha \cdot \mathbf{C}^{\text{dev}} \bar{n}^\alpha \] (38)


\[ \tau_{sb}^\alpha = \hat{s}_b^\alpha \cdot \mathbf{\tau}^{\text{dev}} n_s^\alpha \]  
\[ \tau_{pe}^\alpha = \hat{s}_e^\alpha \cdot \mathbf{\tau}^{\text{dev}} n_p^\alpha \]  
\[ \tau_{sc}^\alpha = \hat{s}_e^\alpha \cdot \mathbf{\tau}^{\text{dev}} n_s^\alpha \]  
\[ \sigma_{\mu 0}^\alpha = n_p^\alpha \cdot \mathbf{\tau}^{\text{dev}} n_p^\alpha \]

where \( \mathbf{\tau}^{\text{dev}} = \mathbf{\tau} - \frac{1}{3} \text{tr} (\mathbf{\tau}) \mathbf{I} \) is the deviatoric part of the Mandel stress tensor. The motivation of only taking the deviatoric part of the Mandel stress tensor into account is that we do not want to have a pressure dependant plastic behaviour. The reason for using these stress components can be found in the discussion regarding tension/compression asymmetry in Chapter 3.2.3 and below.

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The expansion/contraction of the core of the superpartial (core width effect) is affected by the shear stresses acting on the primary and the secondary slip planes in the direction of the edge component of the superpartial \( (\tau_{pe}^\alpha, \tau_{sc}^\alpha) \), see Figure 18.

When the core of the dislocation is fully contracted it may cross-slip on to another slip plane, which usually is a cube slip plane. The effect is that the dislocation movement is hindered on the primary slip plane which the dislocation cross-slipped from, and the core is allowed to expand on the cube slip plane and the dislocation is free to move on this plane. This cross-slip is likely to be affected by the shear stress acting on the cube slip plane in the direction of the Burger’s vector, \( \tau_{cb}^\alpha \).

The normal stress \( \sigma_{\mu 0}^\alpha \) on the primary slip plane may make it easier or harder for the material to undergo slip, depending on its sign. This can readily be seen in Figure 19, which represents two atomic layers loaded in tension and compression, respectively, showing the effect of the normal stress. In tension the atomic layers will move apart, making it easier for sliding, thus increasing the shear strain rate.
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In compression the atomic layers will be pressed together, making it harder for sliding, thus decreasing the shear strain rate.

Figure 19: Atomic layers loaded in a) tension and b) compression.

An equivalent stress, influenced from the work of [31–34, 51–54], was set up to incorporate all these stresses which describe a specific phenomenon. The following equivalent stresses were defined for slip systems $\alpha = 1, \ldots, 12$

$$\sigma_{\alpha} = |\tau_{pb}| + \kappa_1 |\tau_{cb}| + \kappa_2 |\tau_{se}| + \kappa_3 |\tau_{pe}| + \kappa_4 \tau_{sd} + \kappa_5 \sigma_{pn}$$  \hspace{1cm} (43)

In these equivalent stresses we find the resolved shear stress $\tau_{pb}$ as well as the five non-Schmid stresses $\tau_{cb}, \tau_{se}, \tau_{pe}, \tau_{sd}$ and $\sigma_{pn}$. The $\kappa$-values defines how much...
each of the non-Schmid stresses affect the equivalent stresses. The κ-values are
determined from experimental yield limits where the deviation in orientation in
the specimens are to be taken into consideration. With the use of these equivalent
stresses the model is able to predict the tension/compression asymmetry seen in
the experiments. The first three terms defines the level of the yield curve by the
use of the absolute sign, with the condition that κ₁, κ₂ > 0, and the three last
terms adjust the level corresponding to the sign of the applied load, hence ten-
sion/compression asymmetry is received, see [17] regarding further details.

The equivalent stresses are used in the following yield functions to determine if the
slip systems are plastically activated

\[ f^\alpha = \sigma^\alpha_e - G_r \]  
(44)

where \( G_r \) is the slip resistance on the slip planes. As one can see, the slip resistance
act as a type of yield limit for the slip planes.

The following non-associated flow rule is adopted

\[ \dot{\gamma}^\alpha = \dot{\lambda}^\alpha \frac{\partial g^\alpha}{\partial \tau^\alpha_{pb}} \]  
(45)

with the flow being in the direction of the slip

\[ g^\alpha = |\tau^\alpha_{pb}| \]  
(46)

Thus, with the flow direction inserted in Equation (45) one gets the following flow
rule

\[ \dot{\gamma}^\alpha = \dot{\lambda}^\alpha \text{ sgn}(\tau^\alpha_{pb}) \]  
(47)

The magnitude of the flow is finally given by the following viscoplastic relation

\[ \dot{\lambda}^\alpha = \dot{\gamma}_0 \left( \left( \frac{\sigma^\alpha_e}{G_r} \right)^m - 1 \right) \]  
(48)

where \( \dot{\gamma}_0 \) and \( m \) are regularization parameters that have been given the values
\( \dot{\gamma}_0 = 0.1 \) and \( m = 10 \). A backward-Euler approximation, see e.g. [46], in combi-
nation with a Newton-Raphson iterative scheme, was used for the implicit stress
update algorithm, for further details regarding the numerics of the stress update
see Appendix B.

5.5 Modelling the degradation effect

In order to also include the effect of degradation, and more specifically rafting
(coarsening), a scalar coarsening parameter, \( x \), has been incorporated into the ma-
terial model. Based on how much the specimen has degraded, we can calculate how
this affects our stress/strain state in the component. Thus, no evolution law for the coarsening has been developed and only the instantaneous degradation after the aging process has been considered.

As seen in the second included paper, the long temperature exposure (rafting) lowers the yield limit of the material. Hence, this motivates as a first approximation a reduction of the slip resistance by an isotropic degradation function $f_D(x)$, which is depending on the coarsening parameter. Thus, a modified viscoplastic relation for the magnitude of the flow is used according to

$$\dot{\lambda}^\alpha = \dot{\gamma}_0 \left( \frac{\sigma_\alpha^e}{f_D(x) G_e} \right)^m - 1$$  \hspace{1cm} (49)

The degradation function was determined from experiments before and after the ageing. Yield limit ratios were calculated from the experiments as $f_D^* = \frac{\rho_{deg}}{\rho_{vir}}$, and these were subsequently plotted versus the corresponding coarsening parameter, see Figure 20. The virgin condition has no reduction in yield limit, hence $f_D^* = 1$, and from the work of Nazmy et al. [38] it could be concluded that a fully rafted structure has a value of $f_D^* = 2/3$.

![Figure 20: Reduction in yield limit versus the coarsening parameter, yielding the degradation function by curve adaption [15].](image)

A curve fit was made to the points in the figure and the following expression was found

$$f_D(x) = \frac{2}{3} + \frac{1}{3} e^{- \left( \frac{x - 1}{2.4} \right)^{6.3}}$$ \hspace{1cm} (50)

Hence, when analysing a component an estimation of the microstructural state and thus the value of the coarsening parameter is necessary. Having obtained such a value, the model lowers the slip resistance according to the degradation function, thus yielding a lower yield limit.
5.6 Fatigue crack initiation

As previously mentioned, the single-crystal superalloys have an internal structure of well defined crystal planes and slip directions, and the inelastic deformation will primarily take place along these planes and directions, creating so called persistent slip bands. It seems then reasonable to assume that a fatigue crack may initiate along such a persistent slip band, created due to cyclic loading. A way to describe the fatigue crack initiation is by use of the critical plane approach [55–57], which can use the already defined internal structure of slip planes in the material.

From the material model the total shear strain ranges at the component’s surface are determined for each slip plane and slip direction. The maximum total shear strain range is then used in a fatigue life function, which determines the number of cycles to fatigue crack initiation, see [41]

\[ \Delta \gamma_{\text{tot}}^{\text{max}} = f(N_i) \] (51)

The life function follows a Coffin-Manson type of expression [10,11], which has the following appearance

\[ f(N_i) = a(N_i)^b \] (52)

where the parameters \(a\) and \(b\) are determined from experiments.

5.7 Notch correction

The prediction of the fatigue crack initiation lives obtained by the critical plane approach will be too conservative if the lives are evaluated at notch surfaces. To obtain a better estimate in fatigue life in such situations, one need to address the importance of the effect of the notch, such as stress/strain gradients. A way to deal with the stress/strain gradients is to apply the theory of critical distances [58, 59]. This relatively new approach assumes that failure will take place when the stress/strain reaches the fatigue limit at a certain distance (the critical distance) into the material under investigation, e.g. underneath the surface of a notch.

A relationship between the strain range underneath the notch and the distance is determined by a curve fit from the extracted entities of the structure under consideration by the following function

\[ \Delta \gamma_{\text{tot}} = cr^l \] (53)

where \(r\) is the distance underneath the surface. An example of this can e.g. be seen in Figure 21, where the shear strain range is plotted versus the distance into
Figure 21: The total shear strain range versus the distance underneath the notch [42].

It was concluded from the set of tested specimens that the critical distance is cycle dependent, which has e.g. been showed by Susmel and Taylor [60], thus to acquire the fatigue crack initiation life of a component the following non-linear equation system need to be solved

\[
\begin{align*}
\Delta \gamma_{tot} &= a (N_i)^b \\
N_i &= c r^d \\
\Delta \gamma_{tot} &= e r^f
\end{align*}
\]

where the second equation governs the cycle dependency and it has been obtained by a curve fit in a plot of critical distances versus experimental fatigue crack initiation lives obtained from the set of investigated test specimens. The starting value of \( N_i \) is the value received at the surface of the notch. The constants in the two first equations (\( a, b, c, d \)) are non-changeable and the constants in the last equation (\( e, f \)) are changed depending on the structure investigated.
6.1 Constitutive material model

The constitutive material model has been implemented as a user-defined material model for the FEM-softwares LS-DYNA, version 971 [61], and Abaqus, version 6.10 [62], the coding was made in FORTRAN. The material model was implemented with an adapter routine for each of the used FEM-softwares to make it non-software-dependent, as e.g. the Voight-notation and how certain entities are handled are different between LS-DYNA and Abaqus. If the model is to be used for other FEM-softwares it is just to add an appropriate adapter routine.

The constitutive material model needs a number of material parameters as input data. The bulk and shear modulus are mandatory in the LS-DYNA keyword deck for the user-defined material. They are only needed for calculating an estimate of the critical time step in an explicit analysis. Furthermore, the Lamé constants \( \lambda, \mu \) and the additional elastic parameter \( \eta \) (used to define the elastic stiffness tensor), the slip resistance \( G_r \), the regularization parameters \( m \) and \( \dot{\gamma}_0 \) (used in the viscoplastic relation for the magnitude of the flow) are needed. The three components of the respective crystal orientation of \( a_1 \) and \( a_2 \) need to be specified so that the analysed component has the correct crystal orientation relative the global coordinate system in the used FEM-software. The five \( \kappa \)-values for the equivalent stresses and the coarsening parameter for the degradation are also input data to the material model. The density of the material is also set in the input data file, but it is not actively used in the material model.

6.2 Fatigue crack initiation model

After an FE-analysis has been carried out with the above constitutive material model a post-process is performed to determine the fatigue crack initiation life of the analysed component. The fatigue crack initiation model needs two constant input parameters for the fatigue life function \( (a, b) \) and from the performed FE-analysis it needs the maximum total shear strain range \( (\Delta \gamma_{\text{tot}}^{\text{max}}) \), which has been
6.3 Notch correction model

The above mentioned fatigue crack initiation model can be used in conjunction with a notch correction model, a critical distance approach. The method is basically an extraction (data from the FE-analysis) and evaluation (critical distance, fatigue life) function, where the extraction code was implemented in FORTRAN and the evaluation code in MATLAB\textsuperscript{®} [63]. The model need the cycle dependent critical distance curve parameters ($c, d$) and, of course, the fatigue life function parameters ($a, b$) to solve the equation system in Equation (59).

See Appendix C for flowcharts of the above stated implementations.
When examining a gas turbine component made of coarse grained material, one will see that the size of the grains can be of the same order as of stress raising features in the component, and thus, realise that this will affect the mechanical response during loading. For instance, in the coarse grained turbine blade in Figure 22, we can see that the grains at the fir tree attachment are rather large with respect to the geometrical features of the component (even though they decrease in size towards the top).

![Coarse grained turbine blade](image)

Figure 22: A coarse grained turbine blade, showing the size of the grains in comparison to the stress raising features [64].

In an industrial context it can be reasonable to consider a coarse grained material as isotropic, with a general elastic and plastic behaviour, due to the computational cost. Depending on the size of the grains and the features of the structure analysed this can of course be a proper approach, but as the grains are getting larger and the features of the structure are getting smaller, then such an approximation may
no longer hold, and one needs to utilise other approaches. One way to handle this is to see the individual grains as separate single-crystals with their unique crystal orientations and to define the FE-model accordingly to incorporate the grains as individual parts, where the developed crystal plasticity model can be applied.

The above approach will describe a response which is dependent on the crystal orientation and the placement of the grains in the FE-model. As the components are manufactured by casting, the grains will be randomly located and oriented throughout the structure, hence a central question is how will this random grain placement and orientation affect the mechanical response and fatigue life. Thus, this calls for a statistical procedure.
8.1 FE-model

In order to get a good correlation with the experimentally obtained data realistic FE-models are needed. The developed material model was tested by FE-models of the test specimens used in the experimental testing and in the simulation based analysis of the coarse grained application. Three FE-models were made in the mesh-software TrueGrid® [65], one smooth specimen and two notched specimens. All the models consisted of a mapped mesh of brick elements and the models of the round test specimens had a butterfly mesh, see the included papers for more details regarding the models.

8.2 Simulation basis

In order to handle the non-associated flow rule adopted in Chapter 5.4 the initial stiffness method [66] is used, in which the stiffness tensor is never updated. This implies a longer time to find equilibrium compared to using an updatable stiffness tensor, but as a powerful Linux-cluster containing eight quad-core processors and the supercomputer at the National Supercomputer Centre [67] were available for the simulations, the time was of less significance in this matter.

Results from the FE-simulations of the performed monotonic tension and compression tests can be seen in Figure 23. One can see a good agreement with the experimental results in Figure 7, the properties as different stiffness in the different crystal orientations, the perfect plasticity response, the different yield limits for the different crystal orientations and the big tension/compression asymmetry in the [011]-direction and the small asymmetry in the other directions are all present and accurately described. For more results concerning the simulations of the tension and compression tests see the first two included papers.

To determine the constant values $a$ and $b$ in the fatigue life function, Equation (52),
a series of LCF-tests with smooth specimens were simulated with a matching setup as in the experiments. From each of these simulations the $\Delta \gamma_{\text{tot}}$ value was found in an element at the surface and plotted against the corresponding experimentally obtained number of cycles to fatigue crack initiation in a log-log scaled graph. A curve fit was made to approximate a straight line through the points, thus yielding the wanted constants, for more details see the third included paper.

A large deviation between the experimentally obtained fatigue crack initiation lives and the predicted ones was seen when the life was evaluated at the surface of the notch, see Figure 24(a). Thus, a notch correction was needed. A critical distance approach was adopted in which the maximum total shear strain range from the most highly loaded element and orthogonally inwards over a distance of five elements was evaluated, the values $e$ and $f$ was obtained by a curve fit. The received critical distance was plotted versus the experimental life and a curve fit was made to determine $c$ and $d$ in Equation (59). Based on this procedure a more accurate fatigue crack initiation life prediction could be made of the notched test specimens, see Figure 24(b). Furthermore, the slip planes which the components initiated on were observed and compared to the real slip planes as seen in Figure 15. From this comparison it could be concluded that out of the seven tested components only one critical plane differed. For a more thorough description see the fourth and fifth of the included papers.

In a coarse grained structure the placements and crystal orientations of the grains are not known, as during the casting process the grains are randomly scattered
over the whole component. Thus, as a consequence, such a structure is likely to yield different mechanical responses depending on the grain distribution. To investigate this a Monte Carlo analysis containing 100 FE-simulations was performed, thus mimicking the randomness of the casting process of coarse grained material. The optimisation software LS-OPT [68] was used to handle the responses from the FE-simulations performed in the Monte Carlo analysis. The interest of this investigation lies in the obtained dispersion of the fatigue crack initiation lives. Each of the 100 FE-simulations received its unique setup of random grain distributions and was cyclicly loaded at $R_e = -1$, afterwards the fatigue crack initiation life was evaluated by the previously described critical plane model. The obtained maximum total shear strain ranges and the corresponding fatigue lives are plotted in Figure 25. For further details see the sixth included paper.

Figure 25: The distributions of the obtained a) shear strain range and b) fatigue life [64].
At the start of this project a number of interesting tasks were set up to be studied. As the work progressed some new interesting matters were found and investigated, which lead to some deviations from the initially prepared plan.

One of the major aims of the project has been to study the TMF behaviour of the material in question. The start-up, steady-state and shut-down cycle of a gas turbine give rise to both mechanical and temperature loads. As the turbine blades operates in the hottest area of the gas turbine, the component will as a consequence be affected by both creep and rafting. The creep deformation of a turbine component is essential for the TMF behaviour, as the single-crystal material is highly temperature dependent. Consequently, a robust and reliable creep law is needed to yield correct responses in a TMF context. There are a number of different creep laws available, but which one will yield the most satisfying response? Furthermore, one needs creep experiments, preferably experiments that have been carried out in a near reality load case, to accurately model the creep behaviour.

Some basic work has been made on rafting, but there are much more to be done here. As an example, in a TMF cycle with holdtime the component will as stated above be exposed to rafting at the high temperature, which will alter the microstructure of the material and successively decrease the yield limit. To take care of this one needs evolution laws for the rafting to account for the microstructural changes. Do we need to perform micromechanical simulations or can we directly include the effects in a macromechanical description or perhaps a multiscale analysis? There are many questions that need to be answered in order to fully understand the complex nature of rafting, likely a key point in another Ph.D. project.

At high temperature the mechanical responses of the material will be different from that described in the presented work. If we exclude creep and rafting, one of the major differences is that the tension and compression asymmetry will diminish more and more as the temperature increases and will eventually disappear. The plastic anisotropy, different yield limits for the crystal orientations, will also be different at the high temperature. How are these temperature dependencies to be included in the model?
Different approaches regarding the evaluation of the fatigue crack initiation can be used. Instead of using a point based critical distance approach a more physically motivated approach can be to use the found critical plane (slip plane) and to evaluate the strains on this plane by the area based critical distance approach. Alternatively, a totally different approach, such as a stress/strain gradient method, could be adopted. Which of these approaches is the most suitable one?

The fatigue crack initiation behaviour at low temperatures has been extensively elaborated in this work, but the propagation of a crack has not been dealt with. A reason for this is that most of the life of a single-crystal component is spent in the fatigue initiation phase and that the propagation phase is rather short in comparison. In an industrial context a single-crystal component has failed when it reaches the initiation life, as the next loading cycle probably will lead to a crack which span over a larger part or the whole component. Thus, is it relevant from an industrial point of view to consider crack propagation in these materials? Is there an academical relevance?

The industry is always interested in obtaining more accurate results, but the downside is that if a phenomenon is to be thoroughly analysed the cost will increase. The computational cost will increase, the man hours put into the effort will increase, thus the total economical cost will increase. The industry need to compare the effort put into the demanding work in relation to the economical benefits that hopefully will be received. Finally, one of the most important quere, taking into account all the work reported in this dissertation, is if the industry will refine and implement the presented methods into their normal working routines or will they fall into oblivion?
Paper I

Room temperature yield behaviour of a single-crystal nickel-base superalloy with tension/compression asymmetry

In the first paper the yield behaviour of a single-crystal nickel-base superalloy was analysed and modelled. A series of uniaxial tension and compression tests were performed at room temperature. These tests showed a large tension/compression asymmetry for the different tested crystal orientations. To model the mechanical behaviour a viscoplastic flow function was developed, which takes the elastic and plastic anisotropy and the tension/compression asymmetry into account. The same series of tests were simulated using LS-DYNA, and the results corresponded well with the experimentally obtained ones.

Paper II

Tension/compression asymmetry of a single-crystal superalloy in virgin and degraded condition

The microstructural degradation effects on the yield behaviour is investigated in the second paper. The tested specimens from the first paper were exposed to long time ageing in a furnace, by which the microstructure became degraded. The test specimens were then retested in tension and compression. The ratio between the yield limits of the degraded and virgin condition was determined. The test specimens were cut and analysed with SEM, and a coarsening parameter was determined, basing on how much the $\gamma'$-particles had elongated in the three crystal orientations. The ratios and the coarsening parameters were used to define an isotropic degradation function lowering the slip resistance, and, in turn, also the...

\footnote{Note: In the paper the continuum-mechanical notation is somewhat different from the one used in this dissertation and also the elastic stiffness tensor needs a major symmetry (MS) subscript.}
yield limit of the material. A comparison of the simulations with the experiments shows a good correlation.

Paper III

Fatigue crack initiation in a notched single-crystal superalloy component

In the third paper the fatigue crack initiation behaviour of a single-crystal superalloy component was investigated. LCF tests at 500°C on smooth test specimens were performed with \( R_\varepsilon = -1 \). From these tests the number of cycles to fatigue initiation was determined for specific strain ranges. A critical plane model, based on the total shear strain range, was developed in which a Coffin-Manson type of expression was fitted to the experimental results. In addition, notched test specimens were loaded in LCF with \( R_\varepsilon = 0 \), also at 500°C, and simulations were carried out to determine the number of cycles to fatigue crack initiation by use of the developed critical plane model\(^2\).

Paper IV

A combined critical plane and critical distance approach for predicting fatigue crack initiation in notched single-crystal superalloy components

The fourth paper is a direct sequel of the third paper where the notch effect was addressed. The notch effect is handled by use of a critical distance method in combination with the critical plane approach. The location in the notch which experienced the maximum total shear strain range was found, by the same technique as in third paper, and from this point and orthogonally inwards the shear strain range was plotted versus the distance into the material. From experiments the critical distance could be determined for each of the specimens from the obtained strain-distance plots by using the experimentally obtained fatigue lives. Two critical distance approaches where utilised; a mean value approach and a cycle dependent approach. These two approaches were compared to the experimentally obtained fatigue crack initiation lives and it was concluded that the latter one gave the most satisfying result.

\(^2\)Note: In the paper the notation for the maximum total shear strain range (\( \Delta \gamma_{\text{max}} \)), should be written with a superscript \( \text{tot} \) according to \( \Delta \gamma_{\text{tot, max}} \).
Paper V

Evaluation of fatigue crack initiation in a notched single-crystal superalloy component

The fracture surfaces of the investigated test specimens in the third and fourth paper were analysed and evaluated in the fifth paper. The test specimens were pulled apart and analysed by microscopy to determine the actual crystallographic plane which the specimens had initiated on. These were then compared with the crystallographic planes obtained by the FE-simulations to see how good the correlation was. It turned out that six out of seven specimens matched the experiments. The one that differed had the corresponding right plane in the elements before and after the evaluated element, where the evaluated elements were situated at the critical distance.

Paper VI

The effect of random grain distributions on fatigue crack initiation in a notched coarse grained superalloy specimen

The sixth and last paper in this dissertation is an application of the material and fatigue initiation models. The paper deals with how to perform an analysis of a coarse grained superalloy specimen with a notch. The large grains may be of the size of the notch, hence the material can not be seen homogeneous. Instead an approach where each grain in the notch is considered to be a single-crystal with its own unique crystal orientation and placement has been used. A Monte Carlo analysis of 100 FE-simulations has been performed, which randomised the placement and crystal orientation of the grains. The analysis was evaluated with respect to the obtained dispersion in fatigue crack initiation life.
Bibliography


Part III

Numerical procedures
The plastic velocity gradient tensor is given by

\[
\bar{L}^p = \dot{F}^p F^{p^{-1}}
\]

\[
\bar{L}^p = \sum_{\alpha} \dot{\gamma}^\alpha \bar{s}^\alpha \otimes \bar{n}^\alpha
\]  

(55)

Applying a backward-Euler scheme on Equation (55), thus yielding

\[
\begin{align*}
\Delta t_{n+1} \bar{L}^p_{n+1} &= \Delta F^p_{n+1} F^{p^{-1}}_{n+1} = (F^p_{n+1} - F^p_{n}) F^{p^{-1}}_{n+1} = I - F^p_{n} F^{p^{-1}}_{n+1} \\
\Delta t_{n+1} \bar{L}^p_{n+1} &= \sum_{\alpha} \Delta \gamma_{n+1}^\alpha \bar{s}^\alpha \otimes \bar{n}^\alpha
\end{align*}
\]  

(56)

By setting the two equations equal to each other we get the following expression

\[
I - F^p_{n} F^{p^{-1}}_{n+1} = \sum_{\alpha} \Delta \gamma_{n+1}^\alpha \bar{s}^\alpha \otimes \bar{n}^\alpha
\]  

(57)

With further manipulations we receive the updated plastic deformation gradient tensor, which is

\[
F^p_{n+1} = \left(I - \sum_{\alpha} \Delta \gamma_{n+1}^\alpha \bar{s}^\alpha \otimes \bar{n}^\alpha \right)^{-1} F^p_{n}
\]  

(58)
For stability reasons a fully implicit stress update algorithm was chosen. This was done by a Newton-Raphson iterative scheme\(^1\).

\[
\begin{align*}
\dot{\gamma}^\alpha &= \dot{\lambda}^\alpha \text{sgn}(\tau_{pb}^\alpha) \\
\lambda^\alpha &= \phi(\sigma_{e}^\alpha)
\end{align*}
\] 

(59)

where \(\phi\) is the size of the flow. Applying a backward-Euler scheme on Equation (59), which gives

\[
\begin{align*}
\Delta \gamma_{n+1}^\alpha &= \Delta \lambda_{n+1}^\alpha \text{sgn}(\tau_{pb,n+1}^\alpha) \\
\Delta \lambda_{n+1}^\alpha &= \Delta t_{n+1} \phi_{n+1} = \Delta t_{n+1} \phi(\sigma_{e,n+1}^\alpha)
\end{align*}
\] 

(60)

From this it follows that

\[
0 = \frac{\Delta \gamma_{n+1}^\alpha}{\gamma_{n+1}^\alpha - \gamma_n^\alpha - \Delta t_{n+1} \phi(\sigma_{e,n+1}^\alpha) \text{sgn}(\tau_{pb,n+1}^\alpha)} 
\] 

(61)

The residuals (which are to be equal to zero) are then specified and given an iteration number, \(i\)

\[
R^{\alpha,i}_{\gamma,n+1} = \gamma_{n+1}^\alpha - \gamma_n^\alpha - \Delta t_{n+1} \phi(\sigma_{e,n+1}^\alpha) \text{sgn}(\tau_{pb,n+1}^\alpha) 
\] 

(62)

and expanded by a Taylor-series

\[
0 = R^{\alpha,i+1}_{\gamma,n+1} = R^{\alpha,i}_{\gamma,n+1} + \frac{\partial R^{\alpha}_{\gamma,n+1}}{\partial \gamma_{n+1}^\alpha} \delta_{\gamma,n+1}^\beta \bigg|_{i} 
\] 

(63)

where \(\tau_{pb}^\alpha\) is affected by the shear strain from all of the slip systems, hence \(\gamma^\beta\).

\(^1\)See e.g. Belytschko T., Liu W.K., Moran B., *Nonlinear Finite Elements for Continua and Structures*, John Wiley & Sons Ltd, Chichester, 2000.
More in detail this yields

\[ 0 = \mathbf{R}_{\gamma,n+1}^{\alpha,i+1} = \mathbf{R}_{\gamma,n+1}^{\alpha,i} + \sum_{\delta} \mathbf{\delta}_{\gamma,n+1}^{\beta,i+1} \]

\[ - \Delta t_{n+1} \, \text{sgn} \left( \tau_{pb,n+1}^{\alpha,i+1} \right) \left[ \begin{array}{c} \partial \phi \\ \partial \tau_{pb,n+1}^{\alpha,i+1} \\ \vdots \\ \partial \tau_{n+1}^{\alpha,i+1} \\ \vdots \\ \partial \tau_{se,n+1}^{\alpha,i+1} \end{array} \right] + \]

\[ + \left( \begin{array}{cccc} \frac{\partial \phi}{\partial \tau_{pb,n+1}^{\alpha,i+1}} & \frac{\partial \phi}{\partial \tau_{cb,n+1}^{\alpha,i+1}} & \cdots & \frac{\partial \phi}{\partial \tau_{se,n+1}^{\alpha,i+1}} \end{array} \right) \]

\[ \times \left( \begin{array}{c} \frac{\partial \tau_{pb,n+1}^{\alpha,i+1}}{\partial \gamma_{\alpha,i+1}^{\beta,i+1}} \\ \frac{\partial \tau_{cb,n+1}^{\alpha,i+1}}{\partial \gamma_{\alpha,i+1}^{\beta,i+1}} \\ \vdots \\ \frac{\partial \tau_{se,n+1}^{\alpha,i+1}}{\partial \gamma_{\alpha,i+1}^{\beta,i+1}} \end{array} \right) \]

\[ = \mathbf{R}_{\gamma,n+1}^{\alpha,i+1} \]

where summation is to be done over different indices when in differential (\( \alpha, \beta \)). This Taylor-series can be written in matrix form (Newton-Raphson multidimensional method) as follows

\[ \frac{\partial \mathbf{R}}{\partial \mathbf{A}} \mathbf{A} = -\mathbf{R} \]  \hspace{1cm} (65)

where

\[ \mathbf{R} = \left[ \mathbf{R}_{1}^{\gamma} \ldots \mathbf{R}_{n_{ass}}^{\gamma} \right]^T \]  \hspace{1cm} (66)

\[ \mathbf{A} = \left[ \gamma_{1} \ldots \gamma_{n_{ass}} \right]^T \]  \hspace{1cm} (67)

where \( n_{ass} \) is the number of active slip systems, i.e. all slip systems that fulfill \( f^\alpha > 0 \).

Since the size of the flow has the following form

\[ \phi \left( \sigma_{e,n+1}^{\alpha} \right) = \gamma_0 \left( \frac{\sigma_{e,n+1}^{\alpha}}{G_e} \right)^m - 1 \]  \hspace{1cm} (68)

the partial derivatives, which are used in Equation (64), have the following form

\[ \frac{\partial \phi}{\partial \tau_{pb,n+1}^{\alpha,i+1}} = \frac{\gamma_0 m}{G_e} \left( \frac{\sigma_{e,n+1}^{\alpha}}{G_e} \right)^{m-1} \text{sgn} \left( \tau_{pb,n+1}^{\alpha} \right) \]  \hspace{1cm} (69)

\[ \frac{\partial \phi}{\partial \tau_{cb,n+1}^{\alpha,i+1}} = \frac{\gamma_0 m}{G_n^{\alpha}} \left( \frac{\sigma_{e,n+1}^{\alpha}}{G_n^{\alpha}} \right)^{m-1} \kappa_1 \text{sgn} \left( \tau_{cb,n+1}^{\alpha} \right) \]  \hspace{1cm} (70)
\[ \frac{\partial \phi}{\partial \tau_{sb,n+1}} \bigg|_{i} = \dot{\gamma}_m \left( \frac{\sigma_{\alpha e,n+1}}{G_r} \right)^{m-1} \kappa_1 \text{sgn}(\tau_{sb,n+1}) \] (71)

\[ \frac{\partial \phi}{\partial \tau_{pe,n+1}} \bigg|_{i} = \dot{\gamma}_m \left( \frac{\sigma_{\alpha e,n+1}}{G_r} \right)^{m-1} \kappa_3 \] (72)

\[ \frac{\partial \phi}{\partial \tau_{se,n+1}} \bigg|_{i} = \dot{\gamma}_m \left( \frac{\sigma_{\alpha e,n+1}}{G_r} \right)^{m-1} \kappa_4 \] (73)

\[ \frac{\partial \phi}{\partial \sigma_{\alpha p,n+1}} \bigg|_{i} = \dot{\gamma}_m \left( \frac{\sigma_{\alpha e,n+1}}{G_r} \right)^{m-1} \kappa_5 \] (74)

The derivatives of the crystallographic stress components with regard to the shear strain in Equation (64) are evaluated as follows. In order to facilitate matters, the elastic deformation gradient will in the stress update be assumed equal to unity, which is also reasonable for the applications found in this dissertation. It is to be noted that this only affects the speed of convergence and not the accuracy, hence

\[ F^e = I \Rightarrow C^e = F^{eT}F^e = I \] (75)

From the multiplicatively decomposition of the deformation gradient tensor \( F = F^e F^p \) it follows that (in the plastic corrector step)

\[ \frac{\delta F}{\delta t} = \delta F^e F^p + \frac{F^p}{I} \delta F^p \Rightarrow \delta F^e = -\delta F^p F^{p^{-1}} \] (76)

A small increment in the elastic Green-Lagrange strain tensor then yields

\[ \delta E^e = \frac{1}{2} \delta \left( F^{eT} F^e \right) = \frac{1}{2} \left( \delta F^{eT} \frac{F^e}{I} + \frac{F^e}{I} \delta F^e \right) = \frac{1}{2} \left( \delta F^{eT} + \delta F^e \right) = -\frac{1}{2} \left( F^{eT} \delta F^p + \delta F^p F^{p^{-1}} \right) \] (77)

The plastic velocity gradient is given by

\[ \bar{L}^p = F^p F^{p^{-1}} \] (78)

This is applied on a small timestep \( \delta t \)

\[ \delta t \bar{L}^p = \delta t \dot{F}^p F^{p^{-1}} = \delta F^p F^{p^{-1}} \] (79)

With Equation (79) inserted into Equation (77) this yields

\[ \delta E^e = -\frac{\delta t}{2} \left( \bar{L}^{pT} + \bar{L}^p \right) \] (80)
APPENDIX B. STRESS UPDATE

The incremental resolved shear stress acting on each slip system is expressed as
\[
\delta \tau_{\alpha}^{pb} = \bar{s}^\alpha \cdot \delta \mathbf{C} \mathbf{n}^\alpha, \quad \text{Eq. (75)}
\]
\[
= -\frac{\delta t}{2} \bar{s}^\alpha \cdot \left[ \mathbf{C}^{\varepsilon} \left( \bar{L}^{pT} + \bar{L}^{p} \right) \right] \bar{n}^\alpha \quad \text{Eq. (80)}
\]

Due to slip on the active slip systems the plastic velocity gradient can be expressed as
\[
\bar{L}^{p} = \sum_{\kappa} \dot{\gamma}^\kappa \bar{s}^\kappa \otimes \bar{n}^\kappa \quad \text{(82)}
\]

This inserted into Equation (81) yields
\[
\delta \tau_{\alpha}^{pb} = -\frac{\delta t}{2} \bar{s}^\alpha \cdot \left[ \mathbf{C}^{\varepsilon} \left( \sum_{\kappa} \dot{\gamma}^\kappa \left( \bar{n}^\kappa \otimes \bar{s}^\kappa + \bar{s}^\kappa \otimes \bar{n}^\kappa \right) \right) \right] \bar{n}^\alpha =
\]
\[
= -\frac{1}{2} \bar{s}^\alpha \cdot \left[ \mathbf{C}^{\varepsilon} \left( \sum_{\kappa} \delta \gamma^\kappa \left( \bar{n}^\kappa \otimes \bar{s}^\kappa + \bar{s}^\kappa \otimes \bar{n}^\kappa \right) \right) \right] \bar{n}^\alpha \quad \text{(83)}
\]

Finally, the searched derivative becomes
\[
\frac{\delta \tau_{\alpha}^{pb}}{\delta \gamma^\beta} = -\frac{1}{2} \bar{s}^\alpha \cdot \left[ \mathbf{C}^{\varepsilon} \left( \bar{n}^\beta \otimes \bar{s}^\beta + \bar{s}^\beta \otimes \bar{n}^\beta \right) \right] \bar{n}^\alpha \quad \text{(84)}
\]

which is the wanted result. This derivative contains only constant terms, so it can be derived at the start of the algorithm (once per timestep). The other derivatives follow the form given above but are projected a little bit differently, cf. Equations (38) - (42).
The flowcharts of the different developed models are presented below. They are written in *pidgin code*, i.e. a mixture between pseudocode, equations and natural language.

Flowchart of the material model

Initiating constant material parameters from the input deck
Define crystal orientation vectors
Calculate $C^e$
if degradation/rafting analysis is performed
  Calculate $f_D(x)$
  $G_r = f_D(x) G_r$
end if
loop, $\alpha : 1 \rightarrow 12$
  loop, $\beta : 1 \rightarrow 12$
    Calculate $\frac{\delta \tau^{ab}}{\delta \gamma^3}, \frac{\delta \tau^{ab}}{\delta \gamma^3}, \frac{\delta \tau^{ab}}{\delta \gamma^3}, \frac{\delta \sigma^{ab}}{\delta \gamma^3}$ and $\frac{\delta \sigma^{ab}}{\delta \gamma^3}$
  end loop
end loop
Initiating values $\gamma_0 = 0, \gamma_{i=0} = 0, F_{p,i}^{n+1} = F_p^n$
loop, $i : 0 \rightarrow convergence$
  $F_{e}^{n+1} = F_{e,n+1} F_{e,n+1}^{-1}$
  $\bar{E}_{e}^{n+1} = \frac{1}{2} (F_{e,n+1}^{\top} F_{e,n+1} - I)$
  $\bar{S}_{n+1} = C^e \bar{E}_{e}^{n+1}$
  $\bar{M}_{n+1} = F_{n+1}^{e} F_{e,n+1}^{e} S_{n+1}$
\( \mathbf{\sigma}_{n+1}^{\text{dev}} = \mathbf{\sigma}_{n+1} - \frac{1}{3} \text{tr} (\mathbf{\sigma}_{n+1}) \mathbf{I} \)

loop, \( \alpha : 1 \rightarrow 12 \)

Calculate \( \tau_{\alpha}^{\text{pb},n+1}, \tau_{\alpha}^{\text{cb},n+1}, \ldots \) and \( \sigma_{\alpha,n+1} \)

\[
\sigma_{\alpha,n+1} = \tau_{\alpha}^{\text{pb},n+1} + \kappa_1 \tau_{\alpha}^{\text{cb},n+1} + \kappa_3 \tau_{\alpha}^{\text{sc},n+1} + \kappa_4 \tau_{\alpha}^{\text{se},n+1} + \kappa_5 \sigma_{\alpha,n+1}
\]

\[
f_{\alpha,n+1} = \sigma_{\alpha,n+1} - G_r
\]

end loop

\[
\bar{\mathbf{E}}_{n+1} = \frac{1}{2} (\mathbf{F}_n^T \mathbf{F}_n - \mathbf{I})
\]

\(
\bar{\mathbf{E}}_n^\text{tot} \mathbf{n}_n^\alpha \cdot \bar{\mathbf{E}}_n^\text{tot} \mathbf{d}_n^\alpha \) are calculated and stored in the history variables

Determine the number of active slip systems, \( n_{\text{ass}} (f_{n+1} > 0) \)

if \( i > 1 \) or \( n_{\text{ass}} = 0 \)

Check convergence \( \mathbf{R} \rightarrow 0 \)

Break loop if convergence is reached or if \( n_{\text{ass}} = 0 \)

end if

Build \( \frac{\partial \mathbf{R}}{\partial \mathbf{A}} \)

Solve \( \frac{\partial \mathbf{R}}{\partial \mathbf{A}} \mathbf{\delta A} = -\mathbf{R} \)

Update increments

\[
\gamma_{n,i+1}^{\alpha} = \gamma_{n,i}^{\alpha} + \delta \gamma_{n,i+1}^{\alpha}
\]

\[
\mathbf{F}_{n+1}^{p,i+1} = \left( \mathbf{I} - \sum_{\alpha} \Delta \gamma_{n,i+1}^{\alpha} \mathbf{n}^\alpha \otimes \mathbf{n}^\alpha \right)^{-1} \mathbf{F}_{n}^{p,i}
\]

Iteration is updated \( i = i + 1 \)

end loop

Final pl. def. grad is stored in history variable \( \mathbf{F}_{n+1}^{p} = \mathbf{F}_{n+1}^{p,i+1} \)

\[
\mathbf{\sigma}_{n+1} = \frac{1}{\det \mathbf{F}_{n+1}^{p}} \mathbf{F}_{n+1}^{p} \mathbf{\sigma}_{n+1} \mathbf{F}_{n+1}^{p \text{T}} \] is calculated and returned to the FE-software

Flowchart of the critical plane model

Pre-processing: input files are defined
FE-simulations: store total shear strains in history variables
Post-processing: retrieve total shear strains from history variables as functions of time for a specified element list

\[ \text{loop, } i : \text{element list} \]
  \[ \text{loop, } \alpha : 1 \rightarrow 12 \]
  \[ \text{Determine } \Delta \gamma_{\text{tot}}^{\text{max}} \]
  \[ \text{The element number } i \text{ is stored for } \Delta \gamma_{\text{tot}}^{\text{max}} \]
  \[ \text{end loop} \]
  \[ \text{end loop} \]

The fatigue life to initiation is calculated \[ N_i = \left( \frac{\Delta \gamma_{\text{tot}}^{\text{max}}}{a} \right)^{1/b} \]

Flowchart of the critical distance model

Pre-processing: input files are defined
FE-simulations: store total shear strains in history variables
Post-processing: the maximum total shear strain range and corresponding element at the notch surface is obtained by the critical plane model

\[ \text{loop, } i : 1 \rightarrow 5 \]
  \[ \text{Determine } \text{elem}_i \text{ under notch surface} \]
  \[ \text{Determine center of } \text{elem}_i \]
  \[ \text{Determine distance } r_i \text{ from notch surface to center of } \text{elem}_i \]
  \[ \text{loop, } \alpha : 1 \rightarrow 12 \]
  \[ \text{Determine } \Delta \gamma_{\text{tot}}^{\text{max}} \text{ of } \text{elem}_i \]
  \[ \text{The critical slip plane } \alpha \text{ is stored for } \text{elem}_i \]
  \[ \text{end loop} \]
  \[ \text{end loop} \]

\[ \Delta \gamma_{\text{tot}}^{\text{max}} \text{ for each elem is plotted versus } r \]
A power-law function is determined \( \Delta \gamma^{\text{tot}} = erf \)

The fatigue life to initiation is calculated by the equation system:
\[
\begin{align*}
\Delta \gamma^{\text{tot}} &= a \left( N_i \right)^b \\
N_i &= c r^d \\
\Delta \gamma^{\text{tot}} &= e r^f
\end{align*}
\]