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Modeling and simulation of creep in a thermal energy storage unit

Master's thesis in Applied Mechanics

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MASTER'S THESIS

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CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2020

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Cover: Bottom view of the TES unit. Temperature distribution during operation.

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Abstract

Azelio is developing a solution for storing renewable energy in the form of a Thermal Energy Storage (TES) unit. The TES unit, which holds an aluminium alloy, is made out of the heat-resistant austenitic steel alloy 253MA. Due to the high temperatures and the weight of the aluminium, it is of interest to evaluate the creep strains that develop in the TES unit over the 25 year service life.

A creep model is constructed using primary creep data from 316LN steel and three steady-state deformation mechanisms that describe the strain-generating movement of defects throughout the crystal lattice. Some model parameter values are taken from austenitic steel alloys, while some parameter values are obtained from fitting to 253MA secondary creep rate data.

A limited validation of the creep model is performed, and the model is implemented in ANSYS through a custom creep subroutine. Creep is simulated in the TES unit over 25 years at the operational temperature of $\sim 600^\circ\text{C}$. The analysis results show substantial stress relaxations, and that the largest creep strains develop in the suspension blade welds.

The limited validation of the creep model against 1% creep strength data gave strain values in the vicinity of the ideal values. However, some model parameter values from other alloys are used, whose values may not apply to 253MA. The deformation mechanism models are simplistic, and may not accurately reflect reality. In order to gain a better understanding of creep in 253MA, and to properly calibrate the creep model, more experimental data on 253MA is required.

Keywords: 253MA, Austenitic stainless steel, Thermal Energy Storage, Creep, Diffusion creep, Dislocation creep, Deformation mechanism.

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Alexander Lindvall, Gothenburg, June 2020

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1

Introduction

This introductory chapter gives a brief overview of the contents of this thesis. The motivation behind the thesis is given, as well as a short introduction to the creep phenomenon. The aim and limitations of the work are also defined.

1.1 Background

Azelio is a Swedish company headquartered in Gothenburg which is developing a Stirling engine system for electricity production. The system includes a thermal energy storage unit which heats the Stirling engine working fluid. Such a system may for example be used to provide electricity at night using the stored energy generated by a solar power system during the day.



Figure 1.1: Illustration of thermal energy storage units mounted in a container.
Source: [1]

The thermal energy storage (TES) unit (see Figure 1.1) is a pressurized steel tank which contains a phase change material (PCM). The steel used is 253MA, an austenitic stainless steel with heat-resistant properties. During operation, the PCM, an aluminium alloy, is heated to circa 600 °C by the circulation of hot liquid sodium

around the bottom of the tank. This because the PCM stores and releases energy by solidifying and melting at the phase change temperature. The service life of the system is 25 years, or 219 000 hours. The tank will thus be subjected to high temperatures, the weight of the PCM and pressurization over a long time period.

Creep is a phenomenon where inelastic deformation occurs over time in a material when it is continually subjected to stress. Creep occurs below the yield strength and becomes more severe with higher temperatures and stresses. Given long exposure to stress, a component may fail due to creep rupture. At 600 °C, the creep rupture strength for 253MA falls below the yield strength for operational times over 10 000 hours [2]. Some analyses have been performed on the tank where the risk of creep rupture has been investigated, but none where actual creep strains have been calculated. A creep model is therefore pertinent in order to evaluate the creep behaviour in the tank over the service life.

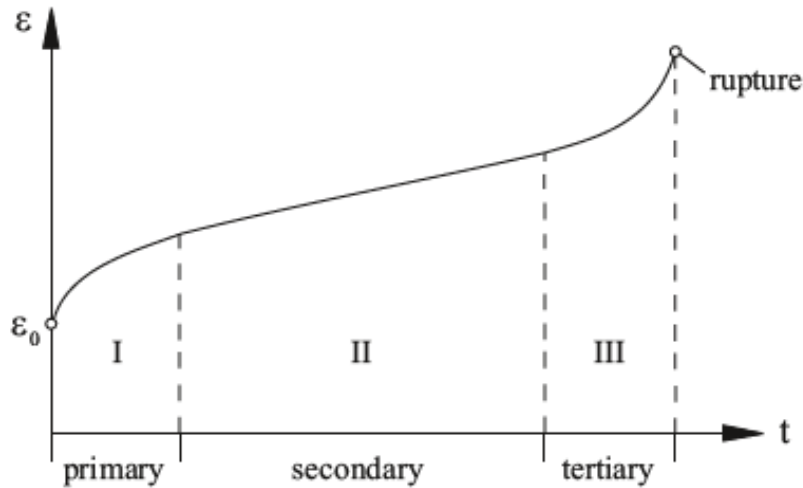


Figure 1.2: A creep curve showing the three stages of creep. Source: Adapted from [3]

The creep behaviour of a material can be represented by creep curves, see Figure 1.2. Creep curves describe the strain as a function of time and are obtained by uniaxial tensile tests at constant stress and temperature. Creep in metals and alloys can typically be divided into three stages [4]. An applied load gives an instantaneous strain and the beginning of primary creep (Stage I). During primary creep, the initially high strain rate decreases and approaches a constant value. Secondary creep (Stage II) follows, where the strain rate is constant. The strain rate during this stage is called the minimum creep rate. Eventually, the strain rate increases due to accumulated damage and necking of the test specimen. This is the tertiary stage (Stage III) of creep which eventually leads to creep rupture [5]. A good creep model should accurately reproduce the strain versus time behaviour seen in the creep curves.

1.2 Aim and outline

The aim of the thesis work is to model the creep behaviour of 253MA and perform a creep analysis of the TES unit using ANSYS Mechanical APDL (ANSYS Parametric Design Language). In order to fulfill the aim of the thesis, a literature review is performed concerning the properties of austenitic stainless steels, creep models and creep mechanisms. In the thesis the following sections are presented:

- An overview of creep modeling.
- The properties of austenitic steels and 253MA.
- The physical mechanisms of creep in austenitic steel at high temperatures.
- Modeling of such mechanisms.
- Fitting of model parameters and implementation in ANSYS.
- Results and discussion.

1.3 Limitations

The tertiary creep stage and creep rupture will not be modeled as it is deemed out of scope for the thesis.

2

Theory

This chapter presents the theoretical concepts used to build the creep model. Some fundamental concepts of creep modeling are introduced, as well as the physical phenomena behind creep deformation. Some relevant properties of austenitic steels and 253MA are described. Finally, the physical mechanisms of high-temperature creep and a set of models that describe these mechanisms are presented.

2.1 Overview of creep modeling

This section presents some fundamental concepts of creep modeling. The stress- and temperature dependence of creep is presented, as well as the forming of the full creep curve by summing of the separate creep stages. The concept of physical creep modeling is also introduced.

2.1.1 Stress and temperature dependence

Creep models express the creep strain rate as a function of the applied stress. This relationship is often non-linear, and can be represented as

$$\dot{\epsilon} \propto \sigma^n \quad (2.1)$$

where n is a positive constant. If the model should cover a range of temperatures, the temperature dependence can be described by an Arrhenius term:

$$\dot{\epsilon} \propto \exp\left(-\frac{Q}{RT}\right) \quad (2.2)$$

where Q is an activation energy, R is the ideal gas constant, and T is the temperature in Kelvin. In chemistry, the Arrhenius term describes the temperature dependence of chemical reaction rates. It is used in creep modeling to model the strain rate variation with temperature. The relations (2.1) and (2.2) can be used to form a

stress- and temperature-dependent expression for the creep strain rate. One of the most common creep models is the Norton creep law [6]:

$$\dot{\varepsilon} = A \left(\frac{\sigma}{\sigma_0} \right)^n \exp \left(-\frac{Q}{RT} \right) \quad (2.3)$$

where A and σ_0 are constants. The constant σ_0 is inserted to simplify the dimension of A , and may simply be set to 1 Pa. For a given set of strain data obtained at different stress levels and temperatures, A , n and Q can be estimated using the least-squares method.

2.1.2 Primary and secondary creep

The deceleration of the strain rate during primary creep is caused by work hardening of the material as it deforms over time. This can be modeled by introducing a time variable t to the creep expression [7]:

$$\dot{\varepsilon}_p = A \left(\frac{\sigma}{\sigma_0} \right)^n \left(\frac{t}{t_0} \right)^m \exp \left(-\frac{Q}{RT} \right) \quad (2.4)$$

where $-1 < m < 0$, and t_0 is a constant that may be set to 1 s. Thus, as t increases, Equation (2.4) will approach zero. Equation (2.4) is known as time-hardening primary creep.

As mentioned in Section 1.1, the secondary creep rate is constant with respect to time. Equation (2.3) is an example of a secondary creep equation. Most creep models found in the literature describe secondary creep, as it is often of greater interest than primary or tertiary creep [8]. For example, the majority of creep deformation in long-life applications such as power station components occurs in the secondary stage [9]. In order to obtain the total creep strain ε_{cr} at time t , the primary and secondary strain rate contributions $\dot{\varepsilon}_p$ and $\dot{\varepsilon}_s$ are integrated with respect to time and summed:

$$\varepsilon_{cr} = \int_0^t \dot{\varepsilon}_p dt + \dot{\varepsilon}_s t \quad (2.5)$$

2.1.3 Empirical and physical modeling

After fitting the unknown constants in a creep expression like Equation (2.3) to a data set, an empirical model is obtained. The constants simply describe a mathematical curve and are not grounded in any physical phenomena. Without any physical foundation, creep prediction may be poor when the model is extrapolated outside of the fitting range [10].

Crystalline solids such as metals contain microscopic defects, or interruptions in the regular crystal lattice structure. When a load is applied, strain is generated by their movement through the crystal lattice. Physical creep models describe the creep strain rate as a function of the movement and interactions of these defects.

2.2 Crystal defects

This section presents some types of defects that are present in crystal lattices. In this section, defects are presented according to their dimension; point, linear, planar or bulk.

2.2.1 Point defects

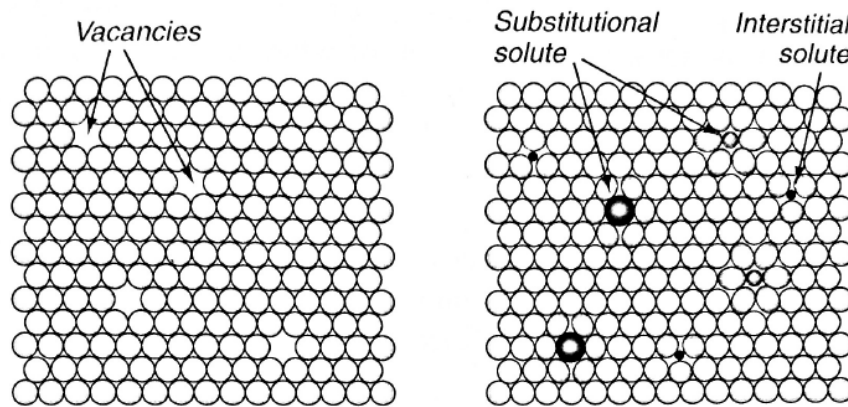


Figure 2.1: Illustration of vacancies and interstitial defects in an atomic plane.

Source: [11]

Point defects are the size of a single atom. They can take the form of vacancies, where an atom is missing from a lattice site. Other forms of point defects are substitutional and interstitial defects. In a substitutional defect, a “host” atom has been replaced by a foreign atom. In an interstitial defect, a foreign atom is present in the space between lattice sites. These defects are introduced deliberately in solid solution hardened alloys, where they improve the strength of the material.

2.2.2 Linear defects

Linear defects in crystals are called dislocations. The edge dislocation is an idealized form of a dislocation. An edge dislocation can be visualised by an extra half-plane of atoms that abruptly ends in the middle of the lattice, see Figure 2.2. The dislocation line runs along the edge of this half-plane. The symbol $\perp$ is used to represent a dislocation, where the vertical line represents the extra atomic plane, and the horizontal line represents the dislocation slip plane. Dislocations are a major contributor to creep deformation as they can glide along the slip plane. When a shear stress is applied, the dislocation line can travel by the breaking and rebonding of atomic

bonds at the edge of the half-plane. This process can repeat until the dislocation reaches the crystal surface [12].

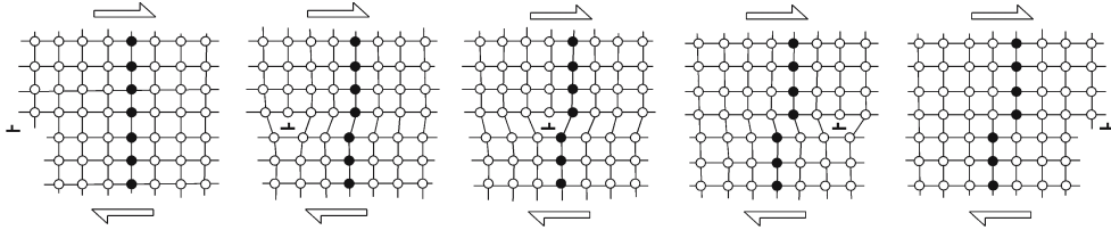


Figure 2.2: An edge dislocation moving through a lattice by gliding on a slip plane. Source: [13]

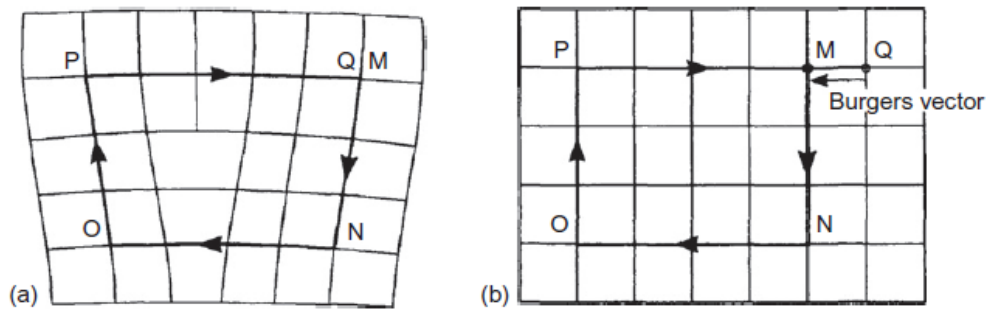


Figure 2.3: The lattice distortion caused by a dislocation. Source: [12]

The magnitude and direction of the lattice distortion caused by an edge dislocation is given by the Burgers vector. The Burgers vector can be obtained by drawing a closed atom-to-atom path MNOPQ around the dislocation, see Figure 2.3. In the right image, the same path is drawn with the dislocation removed. The closure failure QM gives the lattice distortion caused by the dislocation, and is thus the Burgers vector. As can be seen, the Burgers vector direction is parallel with the slip plane for edge dislocations.

2.2.3 Planar defects

In metals, the orientations of the microstructural grains are random. This creates lattice discontinuities where the grains meet, see Figure 2.4. These grain boundaries are a few atomic diameters thick, but can be classified as planar defects.

2.2.4 Bulk defects

Three-dimensional defects in crystals are called bulk defects. An example of bulk defects is precipitates, which are solid impurities in the crystal lattice. Some alloys are precipitation hardened by an aging treatment, where particles precipitate throughout the microstructure when heat is applied. These particles increase the strength of the material as they impede the movement of other defects such as dislocations.

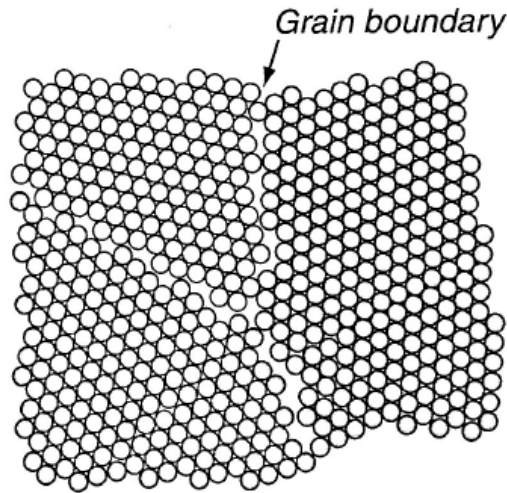


Figure 2.4: Boundaries between grains of different lattice orientation. Source: [11]

2.3 Austenitic stainless steels and 253MA

Austenitic steels are characterized by their austenitic, or face-centered cubic (FCC) crystal structure. Normally, the FCC phase of iron is stable only at temperatures above 723 °C in plain-carbon steels [11]. But through the addition of austenite stabilizers such as nickel and manganese, the FCC structure becomes stable at room temperature. The most widely used sub-group of austenitic stainless steels is the 300-series, which achieve the austenite structure by nickel alloying. In addition to stabilizing the austenite, nickel provides corrosion resistance and increased creep strength at high temperatures [14].

During the 20th century, highly alloyed austenitic steels were developed to meet the demands for use in more efficient power plants. These steels are typically high-chromium, high-nickel and low-carbon, and exhibit high creep strength and oxidation resistance at temperatures around 600 °C. The low carbon content minimizes the formation of chromium carbide precipitates at high temperatures, which could cause intergranular corrosion by chromium depletion [14].

Table 2.1: The chemical composition in wt. % of two 300-series austenitic steels and 253MA. Source: [2], [15]

Type	C	Mn	Si	Cr	Ni	Mo	N	Other
316	≤0.08	≤2.0	≤1.0	16-18	10-14	2.0-3.0	-	-
316LN	≤0.08	≤2.0	≤1.0	16-18	10-14	2.0-3.0	0.10-0.16	-
253MA	0.08	≤0.8	1.6	21	11	-	0.17	Ce 0.05

The steel used by Azelio in the TES unit is 253MA, a low-C, high Cr-Ni austenitic stainless steel that is also alloyed with nitrogen. Nitrogen has been shown to improve creep strength in austenitic steel [14]. 253MA also contains silicon and cerium. They act as deoxidizers, reducing the amount of inclusions and thus increasing the

strength of the steel [16]. The chemical composition of 253MA and some other 300-series steels can be seen in Table 2.1.

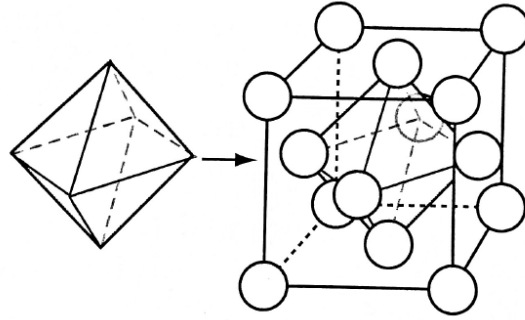


Figure 2.5: The octahedral void in the FCC unit cell. Source: [11]

An FCC unit cell can be seen in Figure 2.5. In 253MA, the atoms of alloying elements are placed in the FCC lattice sites, with the exception for carbon and nitrogen. They are interstitial solutes as their diameter is small enough to fit into the octahedral void in the FCC cell [17]. 253MA is thus a solid solution hardened alloy.

2.4 Deformation mechanisms

The mechanisms that drive creep are presented in this section. The deformation map is also presented, by which the creep mechanisms present in a material can be identified for a range of stresses and temperatures.

2.4.1 Mechanisms of creep

Creep mechanisms can roughly be divided into two groups: diffusion creep and dislocation creep. Diffusion creep is dominant at lower stresses, and is caused by the stress-activated movement of vacancies. The stress dependence (see Equation (2.1)) is usually low with the stress exponent $n \approx 1$. Dislocation creep is caused by the movement of dislocations through the lattice. Dislocation creep is dominant at higher stresses, and has a higher stress dependency with $3 < n < 7$ or higher [6].

2.4.2 Deformation maps

A deformation map for 316 austenitic stainless steel can be seen in Figure 2.6. The lower x-axis shows the temperature as a fraction of the melting temperature T/T_M and the left y-axis shows the applied shear stress normalized with the shear modulus. The creep strain rate contours are drawn for above $T/T_M \approx 0.4$. In the area marked diffusional flow where the stresses are low, the strain rate stress dependence is roughly linear. With higher stresses, the power-law creep domain is entered ($n > 1$). It can be deduced that both diffusional and dislocation creep is present in austenitic steel. With an operational temperature of 600°C , T/T_M

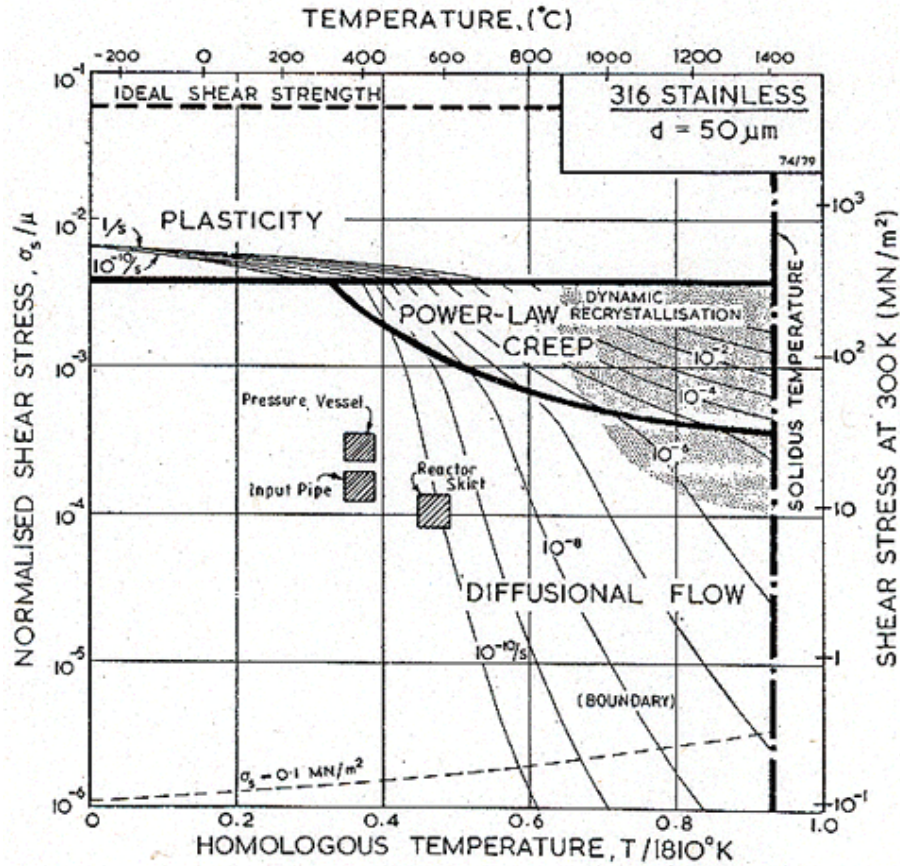


Figure 2.6: A deformation map of 316 steel, showing the strain rate at different stresses and temperatures. Source: [18]

is approximately 0.5 for the TES unit. At this temperature, both diffusion and dislocation creep take place over the stress range. Modeling of both mechanisms is thus required.

2.5 Diffusion creep

During diffusion creep, vacancies are transported through the material by changing places with neighboring atoms in the lattice. The rate at which an atom diffuses through a material can be described by a diffusion constant D :

$$D = D_0 \exp\left(-\frac{Q}{RT}\right) \quad (2.6)$$

where D_0 is a diffusion constant prefactor, and Q is the activation energy for diffusion. Different diffusion constants are used based on how the atoms diffuse through the material.

There are two main models that describe diffusion creep in metals. These are the Nabarro-Herring and Coble models [6]. Both models treat the diffusion of atoms through a single crystal, or grain. In the Nabarro-Herring model, atoms diffuse through the ordered crystal lattice in the interior of the grain. In the Coble model, the atoms instead diffuse through the grain boundaries. It has been found that the activation energy for grain boundary diffusion is lower than the activation energy for lattice diffusion in stainless steels [18]. This suggests that Coble creep is the dominant diffusive mechanism in stainless steel at lower temperatures.

2.5.1 The Coble model

The Coble model [19] is based on the proposal that the equilibrium vacancy concentration in a crystal increases with the applied stress:

$$\Delta C = \frac{C_0 \sigma \Omega}{kT} \quad (2.7)$$

where C_0 is the vacancy concentration in the stress-free crystal at temperature T , σ is the applied stress, Ω is the atomic volume, and k is the Boltzmann constant. The stress expands the lattice on boundaries perpendicular to the stress axis. For an idealized spherical grain where the stress direction defines a polar axis, the increase in vacancy concentration occurs at the poles. The difference in concentration drives the diffusion of vacancies from the poles to the equator of the grain, where they annihilate. The poles can thus be seen as a vacancy source, and the equator as a vacancy sink. The following assumptions are now made:

- The generation and annihilation rates are equal.
- The vacancy sink and source areas are equal.

The boundary between equal areas on a half-sphere lies 60° below the pole, see figure 2.7. The average concentration gradient between the pole and the equator is

$$\frac{(C_0 + \Delta C) - C_0}{(2\pi r)/4} = \frac{\Delta C}{\pi r/2} \quad (2.8)$$

where r is the grain radius. If secondary creep is assumed, the diffusion rate across the 60° boundary is constant and can thus be given by Fick's first law:

$$J = -D \frac{d\varphi}{dx} \quad (2.9)$$

where J is the diffusion flux per unit area and second, D is a diffusion constant and $d\varphi/dx$ is the concentration gradient. The flux per second through the 60° boundary

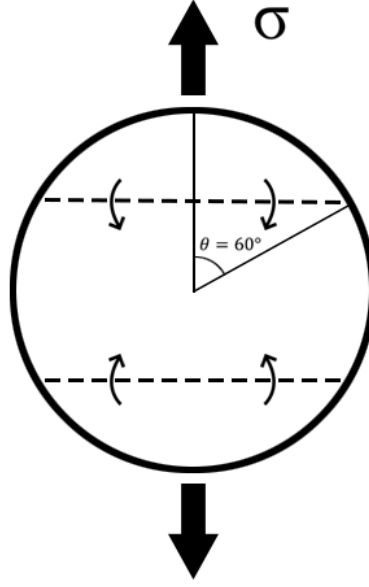


Figure 2.7: Coble model: Vacancies flow from the poles to the equator of a spherical grain under load.

can thus be written as

$$J = DN \left(\frac{\Delta C}{\pi r/2} \right) W 2\pi r \sin 60^\circ \quad (2.10)$$

where N is a proportionality constant that relates the maximum concentration gradient at the 60° boundary to the average gradient, and $W 2\pi r \sin 60^\circ$ is the cross-sectional boundary area, with W being the grain boundary width. With the assumptions listed above, the flux increases linearly with area away from the pole:

$$dJ = B dA = B 2\pi r^2 \sin \theta d\theta \quad (2.11)$$

and

$$J_\theta = B 2\pi r^2 (1 - \cos \theta) \quad (2.12)$$

for $0^\circ \leq \theta \leq 60^\circ$. B is the rate of vacancy generation per unit area. For $60^\circ \leq \theta \leq 90^\circ$ we have

$$J_\theta = B 2\pi r^2 \cos \theta \quad (2.13)$$

2. Theory

Using Equation (2.9), (2.12), (2.13) and the expression for the boundary area, the surface concentration gradient can be written as:

$$\frac{1}{r} \frac{dC}{d\theta} = \frac{B2\pi r^2(1 - \cos \theta)}{DW2\pi r \sin \theta} \quad (2.14)$$

for $0^\circ \leq \theta \leq 60^\circ$, and

$$\frac{1}{r} \frac{dC}{d\theta} = \frac{B2\pi r^2 \cos \theta}{DW2\pi r \sin \theta} \quad (2.15)$$

for $60^\circ \leq \theta \leq 90^\circ$. The average gradient is

$$\frac{\Delta C}{\pi r/2} = \frac{Br}{DW\pi/2} \left(\int_{0^\circ}^{60^\circ} \frac{(1 - \cos \theta)}{\sin \theta} d\theta + \int_{60^\circ}^{90^\circ} \frac{\cos \theta}{\sin \theta} d\theta \right) \quad (2.16)$$

and the maximum gradient is

$$\left(\frac{1}{r} \frac{dC}{d\theta} \right) \Big|_{\theta=60^\circ} \quad (2.17)$$

Dividing the maximum gradient by the average gradient gives $N = 2.15$. Inserting this into Equation (2.10), the vacancy flux over the 60° boundary is obtained:

$$J = 7.4DW\Delta C \quad (2.18)$$

At a pole, the vacancies diffuse from a uniform source of area πr^2 . The volume change is thus

$$J\Omega = \pi r^2 \frac{dr}{dt} \quad (2.19)$$

The strain rate is

$$\dot{\epsilon} = \frac{1}{r} \frac{dr}{dt} = \frac{J\Omega}{\pi r^3} = \frac{7.4DW\Delta C\Omega}{\pi r^3} \quad (2.20)$$

Substituting ΔC with Equation (2.7), the strain rate becomes a function of the applied stress. Coble adds a stress relaxation factor of $5/2$, giving the final expression for Coble creep as

$$\dot{\epsilon} = \frac{148\sigma W\Omega}{d^3 kT} D_{GB} \quad (2.21)$$

where d is the grain diameter and D_{GB} is the grain boundary diffusion coefficient:

$$D_{GB} = D_{0,GB} \exp\left(-\frac{Q_{GB}}{RT}\right) \quad (2.22)$$

where $D_{0,GB}$ is a prefactor and Q_{GB} is the activation energy for boundary diffusion.

2.6 Dislocation creep

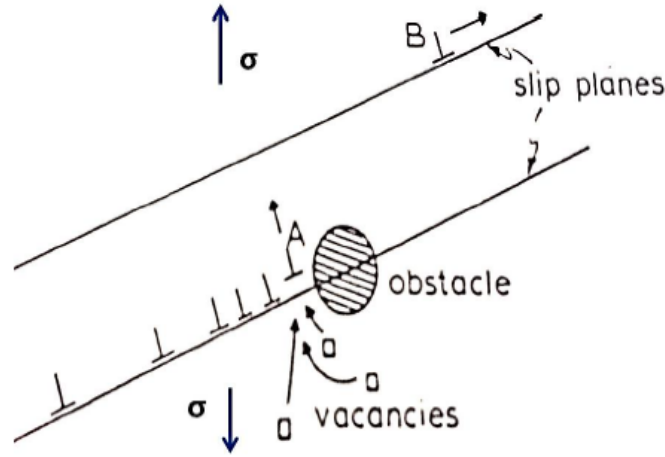


Figure 2.8: A blocked dislocation climbing over an obstacle. Source: [20]

At higher stresses, creep in steel is dominated by dislocation movement. Dislocation creep can be divided into two mechanisms: climb and glide. As a dislocation moves along the slip plane, it encounters other defects that act as obstacles. Depending on the stress level, the dislocation can pass the obstacle in two ways. At intermediate stresses, the dislocation is stopped by the obstacle. In order to pass the obstacle, the dislocation can then climb in a direction perpendicular to the slip plane [6] through the diffusion of vacancies, see Figure 2.8. At higher stresses, the dislocation can glide through obstacles, but experiences a resistance based on the obstacle type and density [21]. Before presenting models for these mechanisms at the end of this section, some concepts of dislocation slip and mechanisms of dislocation generation and annihilation are introduced.

2.6.1 FCC slip

Dislocation slip occurs on slip planes with the highest planar density. The FCC crystal lattice structure of austenitic steels is made up of close-packed atomic planes

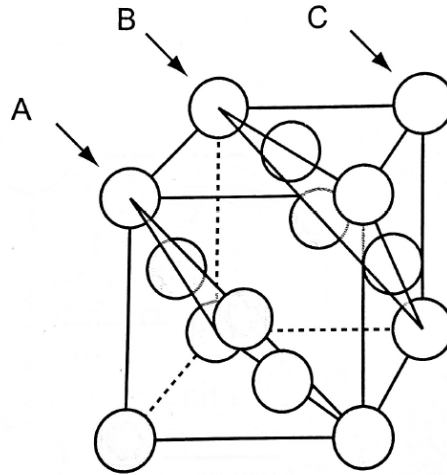


Figure 2.9: The close-packed atomic planes of the FCC unit cell. Source: [11]

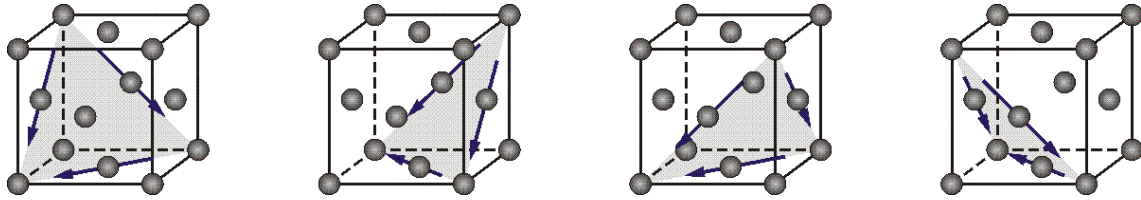


Figure 2.10: The 12 slip systems in the FCC crystal. Source: [22]

stacked in a repeating ABC configuration, see Figure 2.9. Using Miller indices, the unique close-packed planes correspond to the $\{111\}$ family, which contains four planes. In the close-packed planes, slip occurs in the $\langle 110 \rangle$ directions, as these vectors give the shortest atom-to-atom path. This gives a total of 12 combinations of slip plane and slip direction, or 12 possible slip systems in FCC crystals [23], see Figure 2.10.

2.6.2 The Taylor factor

The movement of dislocations on a slip plane is driven by the shear stress acting on the plane. An applied uniaxial stress σ on a crystal is related to the shear stress component τ on a given slip plane by:

$$\tau = \sigma \cos \phi \cos \lambda \quad (2.23)$$

where ϕ is the angle between the stress axis and the normal to the slip plane, and λ is the angle between the stress axis and the slip direction. $\cos \phi \cos \lambda$ is called the Schmid factor. In a polycrystalline FCC material there are 12 possible slip planes, and the grains in the microstructure are randomly oriented. The Taylor factor M is an averaged inverse Schmid factor for polycrystalline materials that relates σ to the average plane shear stress τ_{avg} :

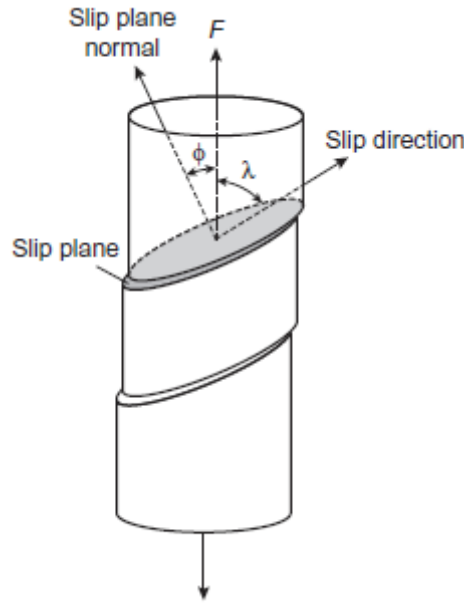


Figure 2.11: Slip in a cylindrical crystal. Source: [12]

$$\tau_{avg} = \frac{\sigma}{M} \quad (2.24)$$

The Taylor factor takes the value $M = 3.06$ for FCC materials [24]. Consider an incremental macroscopic strain $d\varepsilon$ in a polycrystal generated by an uniaxial stress σ by the total slip $d\gamma$ on the slip planes. The virtual work principle gives [25]:

$$\sigma d\varepsilon = \tau_{avg} d\gamma_{avg} \quad (2.25)$$

where $d\gamma_{avg}$ is the average plane slip. The average Taylor factor thus also gives a relation between the average microscopic slip and the macroscopic strain:

$$M = \frac{\gamma_{avg}}{\varepsilon} \quad (2.26)$$

2.6.3 The Orowan equation

The Orowan equation is a fundamental equation in dislocation creep modeling that gives the shear strain rate as a function of dislocation density and dislocation velocity. Consider a crystal with dimensions hld that contains edge dislocations. When a shear stress is applied, the dislocations start to glide in the d direction. If a dislocation reaches the edge of the crystal, it contributes one Burgers vector length b to the total displacement D . The contribution made by a dislocation that moves some distance x_i through the crystal can be taken as the fraction x_i/d of b . If the number of dislocations in the crystal is N , the total displacement is

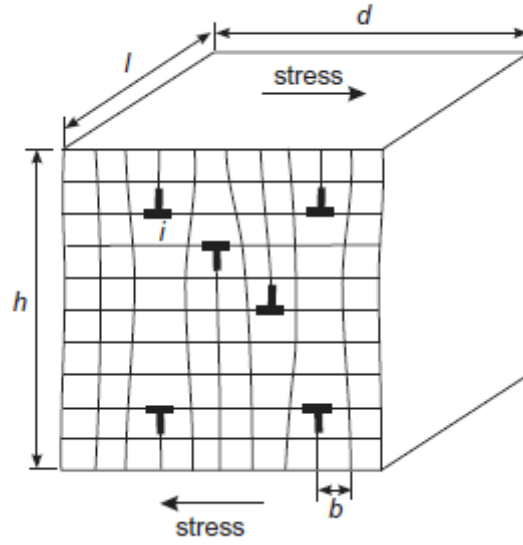


Figure 2.12: Edge dislocations in a crystal. Source: [12]

$$D = \frac{b}{d} \sum_{i=1}^N x_i \quad (2.27)$$

and the macroscopic shear strain γ is

$$\gamma = \frac{D}{h} = \frac{b}{hd} \sum_{i=1}^N x_i \quad (2.28)$$

The average distance $\bar{x}$ moved by one dislocation is

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i \quad (2.29)$$

and the mobile dislocation density ρ_m (dislocation line length per volume) is

$$\rho_m = \frac{Nl}{hld} \quad (2.30)$$

Combining Equation (2.28), (2.29) and (2.30) and taking the time derivative, the Orowan equation is obtained:

$$\dot{\gamma} = \rho_m b \bar{v} \quad (2.31)$$

where $\dot{\gamma}$ is the shear strain rate and $\bar{v}$ is the average dislocation velocity [12].

2.6.4 Generation and annihilation

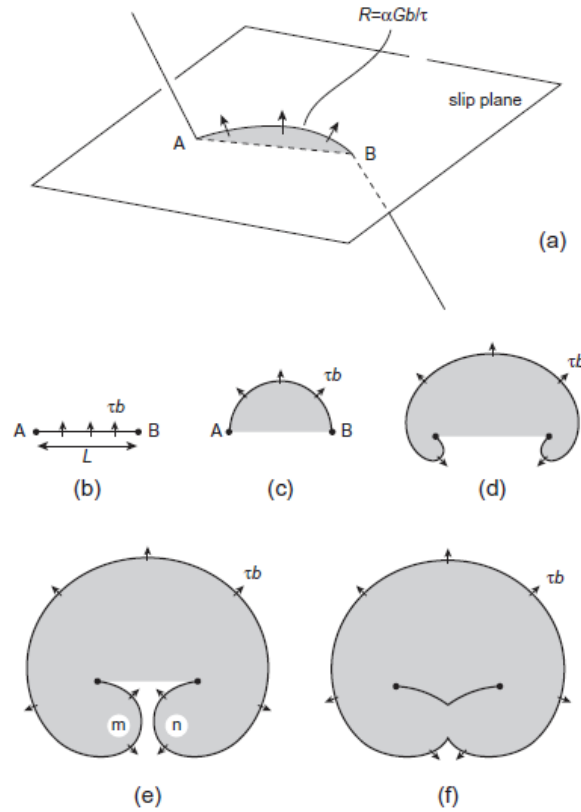


Figure 2.13: The operation of a Frank-Read source under an applied shear stress. Source: [12]

A dislocation creep model can include sources and sinks to model steady-state creep. An example of a dislocation generator is a Frank-Read source. A non-ideal dislocation line may be only partly located in its slip plane, see Figure 2.13(a). When a shear force per unit length τb is applied on the dislocation, the dislocation line will bow outwards as it is pinned at points A and B. The line will continue to expand until the two line segments meet (Figure 2.13(e)). The dislocation line splits off into a dislocation loop that continues to expand in the slip plane, and a dislocation between A and B that repeats the process.

Due to the extra half-plane, the lattice above and below a dislocation are in compression and tension respectively, see Figure 2.14. The dislocations A and B will attract each other as their stress fields are polar opposites. The two dislocations can glide towards each other on the slip planes and join together to form a full atomic plane, annihilating in the process [12]. This is an example of a dislocation sink.

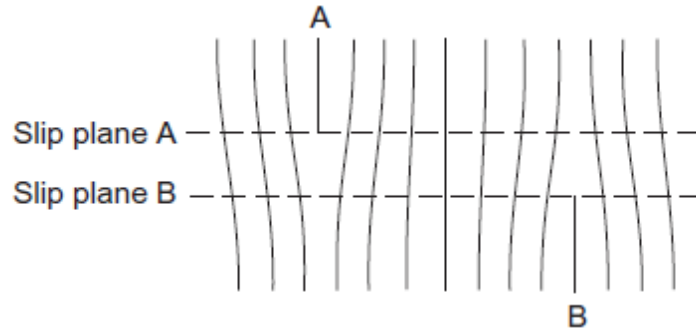


Figure 2.14: Two opposite dislocations on parallel slip planes. Source: [12]

2.6.5 The Weertman model

The Weertman model [26] is a creep model based on the generation, movement, and annihilation of dislocations in an array of parallel slip planes, see Figure 2.15. The head dislocations on parallel planes separated by a distance d block each other and start to climb at the length L from the Frank-Read sources. At the end of the climbing process, they annihilate as shown in Section 2.6.4. As the head dislocation annihilates, dislocations previously trapped behind the head dislocation can glide an average length of $L/2$ before the climb and annihilation process repeats.

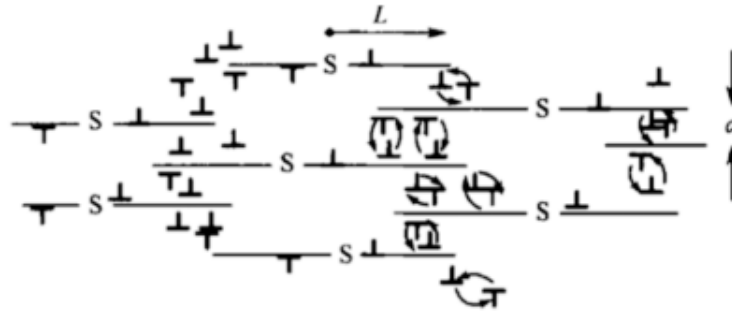


Figure 2.15: The dislocation array in the Weertman model. Source: [26]

The Weertman model is based on the Orowan equation (Equation (2.31)). The average velocity of a dislocation is

$$\bar{v} = \frac{L/2}{t_g + t_c} \quad (2.32)$$

where t_g is the time it takes for the dislocation to glide over the distance $L/2$, and t_c is the time it takes for the dislocation to climb over an obstacle. Here, $t_c \gg t_g$. The time for climb is

$$t_c = \frac{d}{2v_c} \quad (2.33)$$

where v_c is the climb velocity. Combining Equation (2.32) and (2.33), the average velocity can be written as

$$\bar{v} = \frac{L}{d} v_c \quad (2.34)$$

Dislocation loops are generated by the Frank-Read sources and expand to a maximum radius L before climbing. The average loop length is thus $2\pi L/2 = \pi L$. The number of climbing dislocation pairs per source is $L/(\beta d)$ where β is a constant. Thus, the mobile dislocation density is

$$\rho_m = \rho_{FR} \frac{L}{\beta d} \pi L = \frac{\pi \rho_{FR} L^2}{\beta d} \quad (2.35)$$

where ρ_{FR} is the Frank-Read source density. Looking at the array in Figure 2.15, the source density in a cylinder with the radius L and height d is unity:

$$\rho_{FR} \pi L^2 d = 1 \quad (2.36)$$

Inserting (2.36) into (2.35), the dislocation density can be rewritten as

$$\rho_m = \frac{1}{\beta d^2} \quad (2.37)$$

Inserting (2.34), (2.36) and (2.37) into the Orowan equation, we obtain

$$\dot{\gamma} = \frac{b v_c}{d^3 \beta \sqrt{\pi \rho_{FR} d}} \quad (2.38)$$

The driving force for climb in a dislocation pair is the attractive stress σ_d between the areas of compression and tension as seen in Section 2.6.4. This is proportional to the shear modulus and the distortion caused by a dislocation, and inversely proportional to the distance between the parallel slip planes:

$$\sigma_d \propto \frac{Gb}{d} \quad (2.39)$$

giving d as

$$d \propto \frac{Gb}{\sigma_d} \quad (2.40)$$

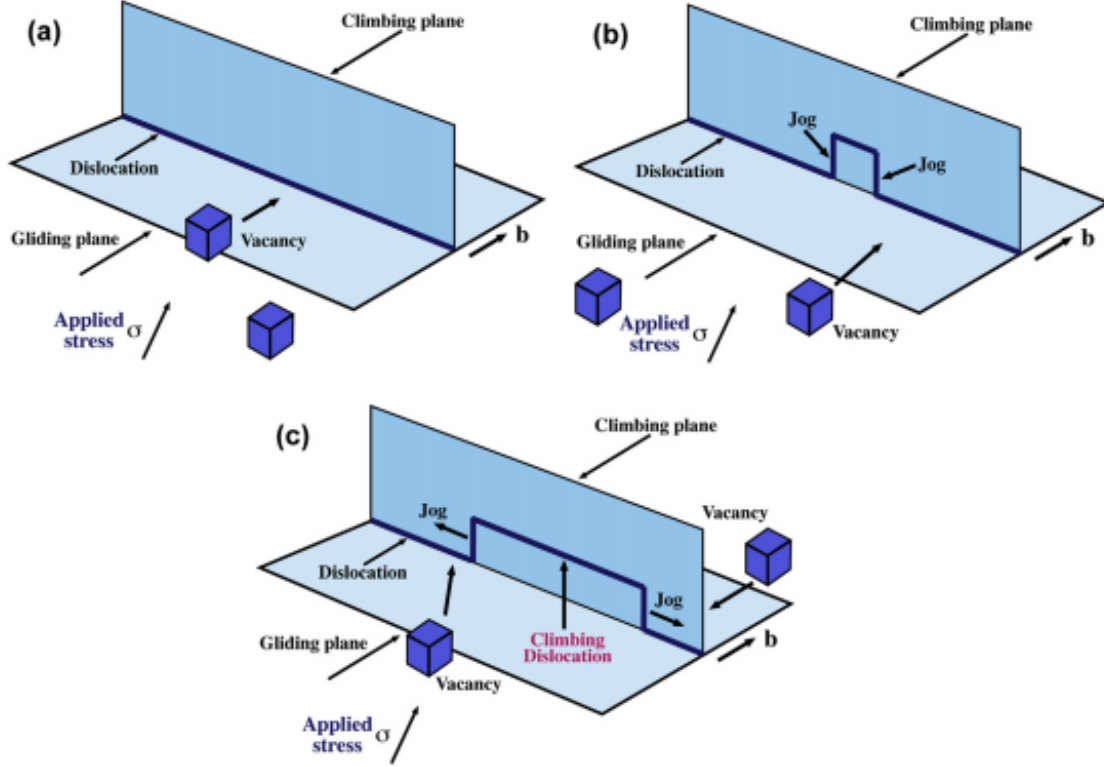


Figure 2.16: A dislocation line in the process of climb. Source: [27]

Dislocation climb is a diffusive process where the dislocation line is shifted by the diffusion of vacancies, see Figure 2.16. A vacancy diffusing into the edge of the half-plane creates a jog, which is a dislocation line step outside of the glide plane. The velocity of a diffusing defect is described by the Einstein mobility relation [28]:

$$v_c = F \frac{D}{kT} \quad (2.41)$$

where F is a force acting on the defect, D is a diffusion coefficient, k is the Boltzmann constant and T is the temperature. The driving force can be taken as the force acting on a dislocation jog when a shear stress τ is applied. The force per unit length acting on a dislocation is τb . If the dislocation jog is of height b , then the force is

$$F = \tau b^2 \quad (2.42)$$

Inserting Equation (2.40), (2.41) and (2.42) into (2.38), assuming $\sigma_d \propto \tau$ and choosing D as the lattice diffusion coefficient D_L , the expression for Weertman creep is

obtained:

$$\dot{\gamma} = \frac{\tau^{4.5}}{\beta k T \sqrt{\pi b \rho_{FR} G^7}} D_L \quad (2.43)$$

where

$$D_L = D_{0,L} \exp\left(-\frac{Q_L}{RT}\right) \quad (2.44)$$

where $D_{0,L}$ is a prefactor and Q_L is the activation energy for lattice diffusion. Rieth et al. provides an expression for Weertman creep without the unknown constant β [29]:

$$\dot{\gamma} = \frac{\pi^2 \tau^{4.5}}{4 k T \sqrt{b \rho_{FR} G^7}} D_L \quad (2.45)$$

2.6.6 The glide model

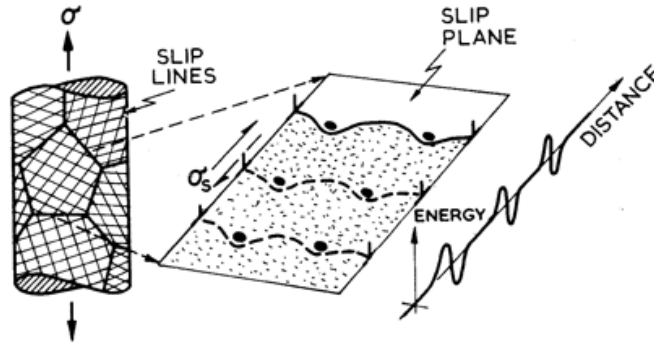


Figure 2.17: Dislocations gliding through an array of obstacles. Source: [18]

At high stresses, dislocations will start to glide through obstacles, see Figure 2.17. The passing of an obstacle requires a certain energy which is provided by the applied stress as well as the thermal vibrations of the crystal atoms [12]. The average velocity of a dislocation gliding through obstacles can thus be described by an Arrhenius term [30]:

$$\bar{v} = \kappa \omega \exp\left(-\frac{\Delta G}{kT}\right) \quad (2.46)$$

where κ is the distance traveled by the dislocation while passing an obstacle, ω is the Debye frequency, and ΔG is the activation energy for passing an obstacle. The

Debye frequency is a characteristic frequency for crystals that describes the vibration of the crystal atoms. Its value is based on the interatomic spacing and the speed of sound in the crystal. Inserting (2.46) into the Orowan equation, we get

$$\dot{\gamma} = \rho_m b \kappa \omega \exp \left(- \frac{\Delta G}{kT} \right) \quad (2.47)$$

Frost and Ashby simplify (2.47) to

$$\dot{\gamma} = \dot{\gamma}_0 \exp \left(- \frac{\Delta G}{kT} \right) \quad (2.48)$$

where $\dot{\gamma}_0 = 10^6$ 1/s to fit with experimental data [18]. ΔG depends on the applied stress and the obstacle characteristics. A array of uniformly spaced obstacles gives

$$\Delta G = \Delta F \left(1 - \frac{\tau}{\hat{\tau}} \right) \quad (2.49)$$

where ΔF is the activation energy required to pass an obstacle with no external stress applied, τ is the applied shear stress and $\hat{\tau}$ is the obstacle parameter. ΔF and $\hat{\tau}$ take on different values depending on the obstacle strength and the spacing between the obstacles, see Figure 2.18. ΔF and $\hat{\tau}$ take on higher values when obstacles are strong, such as in precipitation hardened metals. $\hat{\tau}$ also grows with denser obstacle arrays, as the obstacle spacing l is in the denominator. Medium strength obstacles are other dislocations, and low strength obstacles are solute atoms. The crystal structure thus needs to be considered when applying the model.

<i>Obstacle strength</i>	ΔF	$\hat{\tau}$	<i>Example</i>
Strong	$2 \mu b^3$	$> \frac{\mu b}{\ell}$	Dispersions; large or strong precipitates (spacing ℓ)
Medium	$0.2-1.0 \mu b^3$	$\approx \frac{\mu b}{\ell}$	Forest dislocations, radiation damage; small or weak precipitates (spacing ℓ)
Weak	$< 0.2 \mu b^3$	$\ll \frac{\mu b}{\ell}$	Lattice resistance; solution hardening (solute spacing ℓ)

Figure 2.18: Values for ΔF and $\hat{\tau}$ (μ is the shear modulus). Source: [18]

3

Model and simulation setup

This chapter describes the setup of the creep model and ANSYS analysis. The selection of model constant values and fitting of model parameters is described, as well as a limited validation against 253MA creep data. The implementation of the creep model in ANSYS and the ANSYS TES unit analysis setup is described.

3.1 Creep model setup

The full creep model should cover both primary and secondary creep. Therefore, the time-hardening primary equation (Equation (2.4)) is combined with the contributions from the three creep mechanisms (Equations (2.21), (2.45), and (2.48)) described in the Theory chapter:

$$\dot{\epsilon}_{cr} = A \left(\frac{\sigma}{\sigma_0} \right)^n \left(\frac{t}{t_0} \right)^m \exp \left(- \frac{Q}{RT} \right) + \dot{\epsilon}_{Coble} + \dot{\epsilon}_{Weertman} + \dot{\epsilon}_{Glide} \quad (3.1)$$

where

$$\dot{\epsilon}_{Coble} = \frac{148\sigma W\Omega}{d^3 kT} D_{GB} \quad (3.2)$$

$$\dot{\epsilon}_{Weertman} = \frac{\pi^2 \tau_{avg}^{4.5}}{4MkT \sqrt{b\rho_{FR}} G^7} D_L \quad (3.3)$$

$$\dot{\epsilon}_{Glide} = \frac{10^6}{M} \exp \left(- \frac{\Delta F}{kT} \left(1 - \frac{\tau_{avg}}{\hat{\tau}} \right) \right) \quad (3.4)$$

where the average FCC Taylor factor has been applied to the dislocation creep models to convert from applied stress σ to average slip plane shear stress τ_{avg} , and from average planar shear strain rate $\dot{\gamma}_{avg}$ to macroscopic strain rate $\dot{\epsilon}$.

3.1.1 Constant values

The values chosen for the model constants will now be presented, beginning with secondary creep. The shear modulus G is calculated as

$$G = \frac{E}{2(1 + \nu)} \quad (3.5)$$

where E is the Young's modulus and ν is the Poisson's ratio. The temperature-dependent Young's modulus is taken from the Sandvik 253MA datasheet [2], and the Poisson's ratio is assumed to be $\nu = 0.3$. As slip occurs in the close-packed planes in FCC crystals, the Burgers vector b is taken as twice the radius 140 pm of an Fe atom [31]. The atomic volume Ω is taken as the volume of a sphere with the radius of an Fe atom.

Rolled Alloys gives the grain size range ASTM3-6 for 253MA [32], which corresponds to between 45 and 127 μm . The average of this range, 86 μm , is taken as the grain size d . The grain boundary width W is assumed to be 1 nm. The Frank-Read source density ρ_{FR} is taken as 100/ μm^2 , which is a typical value found in the dislocation dynamics literature [33].

Diffusion constant values for 253MA have not been found in the literature. Therefore, constant values that have been found for similar austenitic steel alloys are used (see Table 2.1). The boundary diffusion prefactor is given for 316LN by Rieth et al. as $D_{0,GB} = 6.0 \cdot 10^{-6} \text{ m}^2/\text{s}$. An experiment by Sritharan on a 316 steel with the grain size 9 μm gave an approximate value for the strain rate change with applied stress $d\dot{\epsilon}/d\sigma$ at 600 °C for stresses below 10 MPa [34]. Assuming that 316 and 253MA have the same shear modulus at 600 °C, and that Coble creep is the dominant mechanism at these stresses ($\dot{\epsilon}_{Coble} \gg \dot{\epsilon}_{Weertman}$ and $\dot{\epsilon}_{Coble} \gg \dot{\epsilon}_{glide}$), a value for the boundary diffusion activation energy $Q_{GB} = 189 \text{ kJ/mol}$ is obtained.

The lattice diffusion prefactor $D_{0,L}$ and the glide model activation energy term ΔF is given by Frost and Ashby for 316 steel as $3.7 \cdot 10^{-5} \text{ m}^2/\text{s}$ and $0.5Gb^3$ respectively. In accordance with Figure 2.18, $\hat{\tau}$ is then chosen as Gb/l . This leaves the lattice diffusion activation energy Q_L in the Weertman model and the obstacle distance l in the glide model to be fitted to experimental secondary creep data.

Sandvik provides the secondary creep rate for 253MA at 600 °C for stresses above roughly 120 MPa. Secondary creep data for 316LN at 600 °C from Rieth et al. shows that the stress exponent is roughly 4 in the 60-100 MPa range, which suggests that dislocation climb is a dominant creep mechanism for austenitic stainless steels in this range. The fitting range is thus chosen as 60 to 140 MPa, where 140 MPa is the yield strength for 253MA at 600 °C [2]. The 253MA data is extrapolated down to 60 MPa, and the fitting is done using the MATLAB function `nlinfit`, giving $Q_L = 322 \text{ kJ/mole}$ and $l = 125 \text{ nm}$. The fitted secondary creep model can be seen in Figure 3.1.

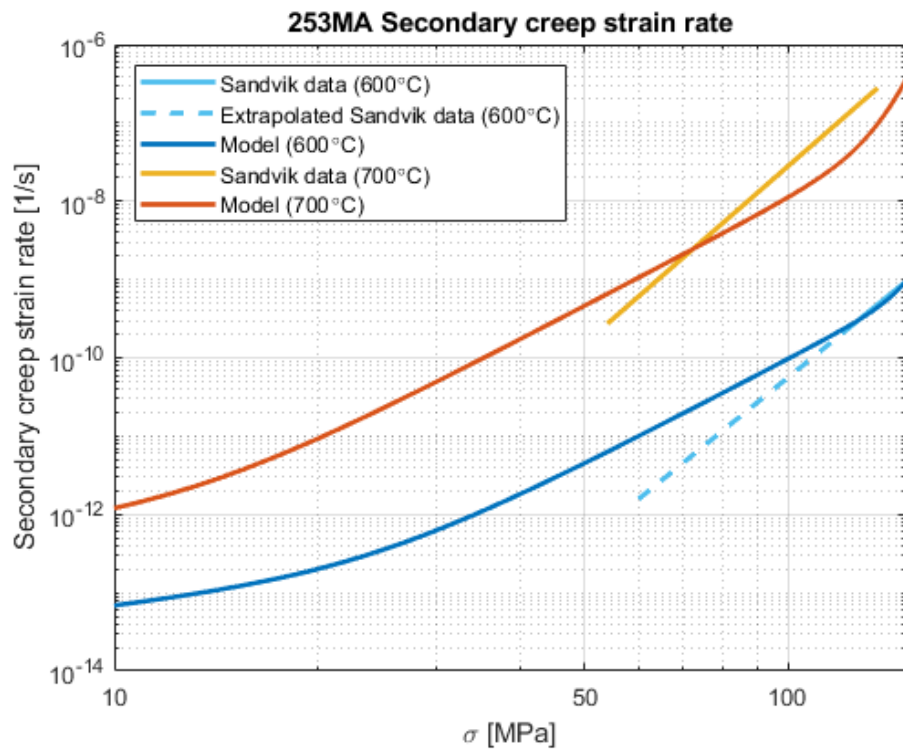


Figure 3.1: The secondary creep model at 600 °C and 700 °C versus Sandvik 253MA data.

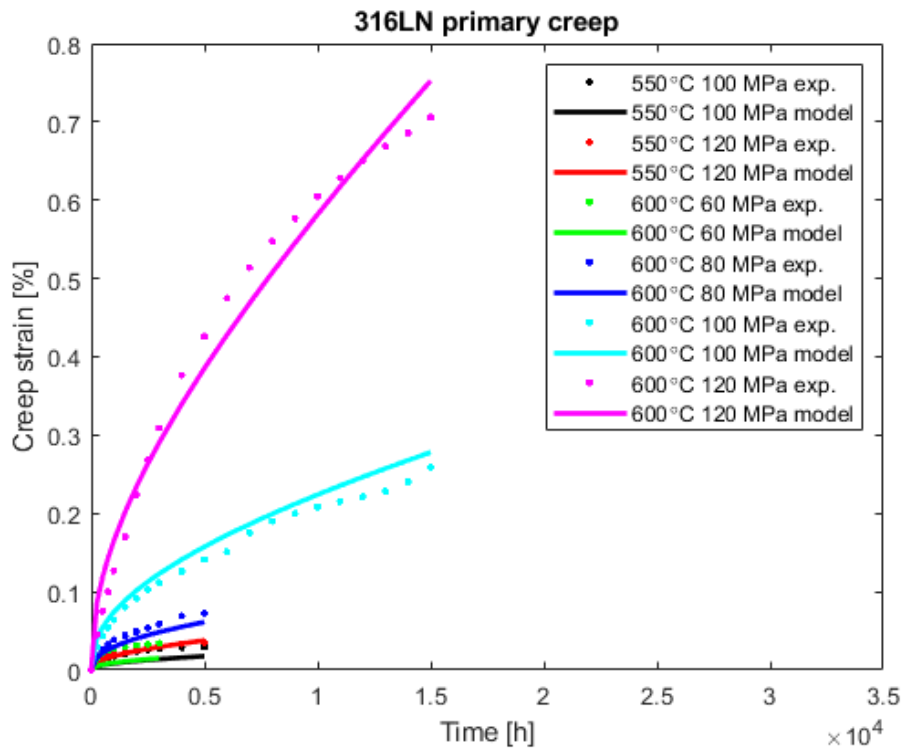


Figure 3.2: The fitted primary creep vs. experimental 316LN data.

Primary creep data for 253MA has not been found in the literature. However, Rieth et al. provide full creep curve data for 316LN at various temperatures and stresses. Equation (2.5) is globally fitted to a set of primary stage curves obtained between 60 MPa and 120 MPa as shown in Figure 3.2 using the time-hardening primary creep equation ($\sigma_0 = 1$ Pa, $t_0 = 1$ s) and the secondary creep rate values determined by Rieth et al. This gives the optimal parameter values $A = 1.375 \cdot 10^{-23}$ 1/s, $n = 4.006$, $m = -0.580$ and $Q/R = 31107$. The constants used in the creep model and their values are presented in list format in Table 3.1.

Table 3.1: The constants used in the creep model.

Constant	Value	Description
A	$1.375 \cdot 10^{-23}$ 1/s	Primary creep constant
n	4.006	Primary creep stress exponent
m	-0.580	Primary creep time exponent
Q/R	31107	Primary creep constant
W	1 nm	Grain boundary width
Ω	$1.149 \cdot 10^{-29}$ m ³	Fe atomic volume
d	86 μ m	Grain diameter
$D_{0,GB}$	$6.0 \cdot 10^{-6}$ m ² /s	Boundary diffusion constant prefactor
Q_{GB}	189 kJ/mole	Boundary diffusion activation energy
M	3.06	Average Taylor factor for FCC polycrystallines
b	280 pm	Burgers vector magnitude
ρ_{FR}	100/ μ m ²	Frank-Read source density
$D_{0,L}$	$3.7 \cdot 10^{-5}$ m ² /s	Lattice diffusion constant prefactor
Q_L	322 kJ/mole	Lattice diffusion activation energy
l	125 nm	Obstacle distance

3.1.2 ANSYS creep subroutine

In order to implement the creep model in ANSYS, a Fortran subroutine **Usercreep** is written, compiled and linked to ANSYS. **Usercreep** uses the custom creep subroutine template provided by ANSYS, where the creep model is extended to three dimensions by using a calculated equivalent stress to calculate an equivalent creep strain. The procedure ANSYS uses [35] for calculating the creep strain in an integration point will now be presented.

A modified total strain (also denoted elastic strain) tensor for the current timestep n is computed:

$$\epsilon'_n = \epsilon_n - \epsilon_n^{pl} - \epsilon_n^{th} - \epsilon_{n-1}^{cr} \quad (3.6)$$

where the plastic and thermal contributions of the current timestep and the creep contribution of the previous timestep are subtracted from the total strain. An equivalent modified total strain is defined as:

$$\varepsilon_{et} = \frac{1}{\sqrt{2}(1+\nu)} \left[(\varepsilon'_x - \varepsilon'_y)^2 + (\varepsilon'_y - \varepsilon'_z)^2 + (\varepsilon'_z - \varepsilon'_x)^2 + \frac{3}{2}(\gamma'_{xy})^2 + \frac{3}{2}(\gamma'_{yz})^2 + \frac{3}{2}(\gamma'_{zx})^2 \right]^{1/2} \quad (3.7)$$

An equivalent von Mises stress σ_e is obtained as:

$$\sigma_e = E\varepsilon_{et} \quad (3.8)$$

An equivalent creep strain increment $\Delta\varepsilon^{cr}$ is now calculated by **Usercreep** by integrating the creep expression over the current time increment using σ_e in place of σ . The **Usercreep** code can be found in Appendix A.1. A creep ratio C_s (a measurement of creep strain increment) is now calculated for the integration point:

$$C_s = \frac{\Delta\varepsilon^{cr}}{\varepsilon_{et}} \quad (3.9)$$

and the scalar equivalent creep strain increment is converted to a tensor:

$$\Delta\varepsilon_x^{cr} = C_s \frac{(2\varepsilon'_x - \varepsilon'_y - \varepsilon'_z)}{2(1+\nu)} \quad (3.10)$$

$$\Delta\varepsilon_y^{cr} = C_s \frac{(2\varepsilon'_y - \varepsilon'_x - \varepsilon'_z)}{2(1+\nu)} \quad (3.11)$$

$$\Delta\varepsilon_z^{cr} = -\Delta\varepsilon_x^{cr} - \Delta\varepsilon_y^{cr} \quad (3.12)$$

$$\Delta\varepsilon_{xy}^{cr} = C_s \frac{3}{2(1+\nu)} \gamma'_{xy} \quad (3.13)$$

$$\Delta\varepsilon_{yz}^{cr} = C_s \frac{3}{2(1+\nu)} \gamma'_{yz} \quad (3.14)$$

$$\Delta\varepsilon_{xz}^{cr} = C_s \frac{3}{2(1+\nu)} \gamma'_{xz} \quad (3.15)$$

The total creep strains for the current timestep can now be calculated (only showing the x -component here):

$$(\varepsilon_x^{cr})_n = (\varepsilon_x^{cr})_{n-1} + \Delta\varepsilon_x^{cr} \quad (3.16)$$

3.1.3 Verification and validation

Temperature	Creep strength 1%	
°C	10 000 h	100 000 h
	MPa	MPa
525	-	-
550	-	-
575	-	-
600	117	70
625	93	55
650	75	42
675	59	32
700	46	25

Figure 3.3: 1% creep strength data for 253MA. Source: [2]

As full experimental creep curves for 253MA are not available, the model can not be properly validated. For a limited validation, the MATLAB creep model is compared to 1% creep data given in the Sandvik 253MA data sheet, see Figure 3.3, where for some given temperature, the stresses that generate a 1% creep strain after 10 000 h and 100 000 h respectively are given. A comparison is made with the 600 °C and 625 °C data, see Table 3.2.

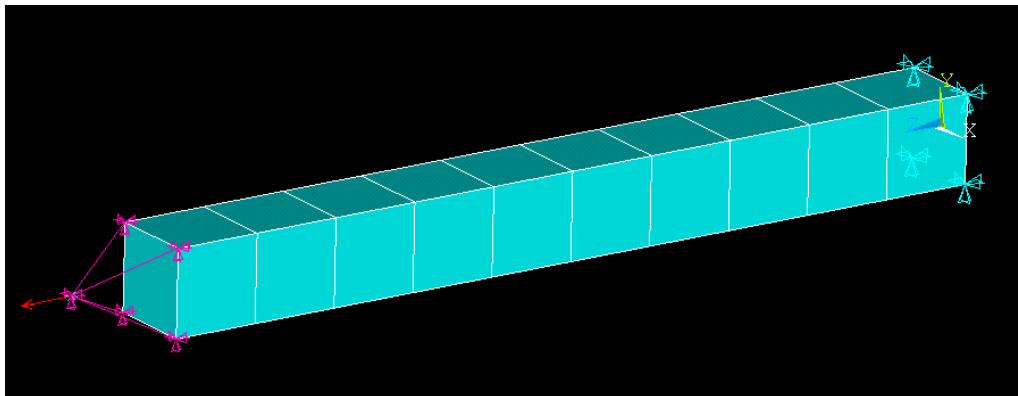


Figure 3.4: The virtual tensile test specimen.

In order to verify `Usercreep`, a tensile test specimen is modeled in Mechanical APDL, see Figure 3.4. A rectangular bar is meshed with 10 elements in the z-direction. The nodes in one end are fixed, and a tensile force is applied on a massless node connected to the four nodes on the other end by rigid links. This prevents

boundary effects that would otherwise occur if applying the force directly on the end nodes, thus giving a more accurate strain measurement. **Usercreep** was tested using the virtual tensile test with the 1% creep strength data as input, and was found to give the same output as the MATLAB model, see Table 3.2.

Table 3.2: Resulting creep strains from the 1% creep strength comparison.

	MATLAB model	Tensile test with Usercreep
600 °C, 117 MPa, 10 000 h	1.060%	1.060%
600 °C, 70 MPa, 100 000 h	0.822%	0.822%
625 °C, 93 MPa, 10 000 h	1.256%	1.256%
625 °C, 55 MPa, 100 000 h	0.971%	0.971%

3.1.4 Norton model

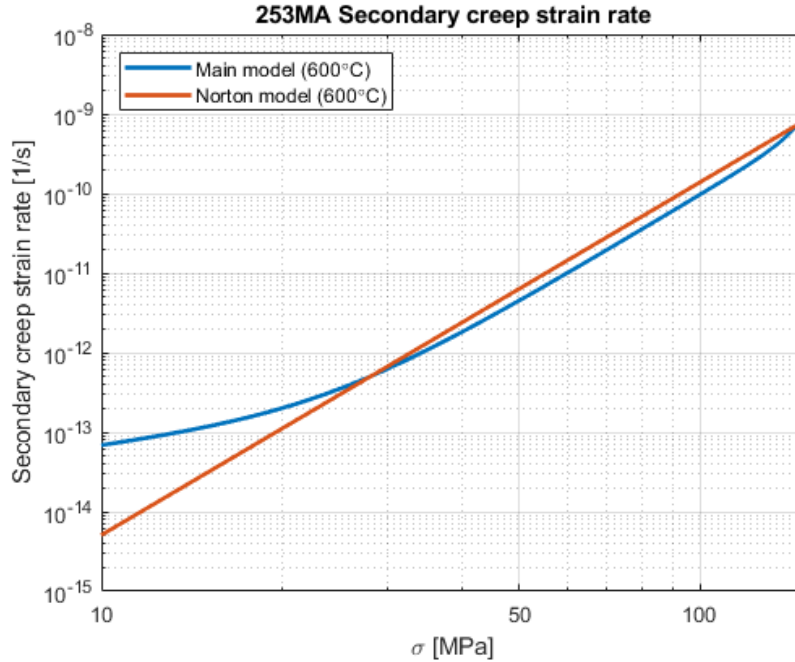


Figure 3.5: A comparison of the main model secondary creep rates and the fitted Norton model.

For comparison purposes, the Norton secondary creep model is implemented in a separate TES unit analysis. Equation (2.3) with $\sigma_0 = 1$ Pa is fitted to the 600 °C and

625 °C 1% creep strength data points by logarithmizing the equation and performing a linear regression. The following constants are obtained: $A = 8.973 \cdot 10^{-30}$, $n = 4.432$, and $Q/R = 32711$. The secondary creep strain rates of the main model (Equation (3.1)) and the fitted Norton model at 600 °C are plotted together in Figure 3.5. The Norton model is available as a predefined creep function in ANSYS. A custom ANSYS subroutine is thus not required for implementation.

3.2 TES unit analysis setup

The TES unit model includes the 253MA tank suspended from a fixed octagonal frame by four suspension blades. A cross-section of the tank can be seen in Figure 3.6. The interior of the tank holds the PCM material. Hot liquid sodium that melts the PCM circulates in a bottom compartment. This bottom compartment along with a pump & heater system on the side of the tank is called the Charge system. The stored energy in the PCM heats the liquid sodium in the Discharge compartment that in turn heats the Stirling engine working gas. A bottom view of the tank showing the suspension blades and the Charge surface temperature distribution can be seen in Figure 3.7.

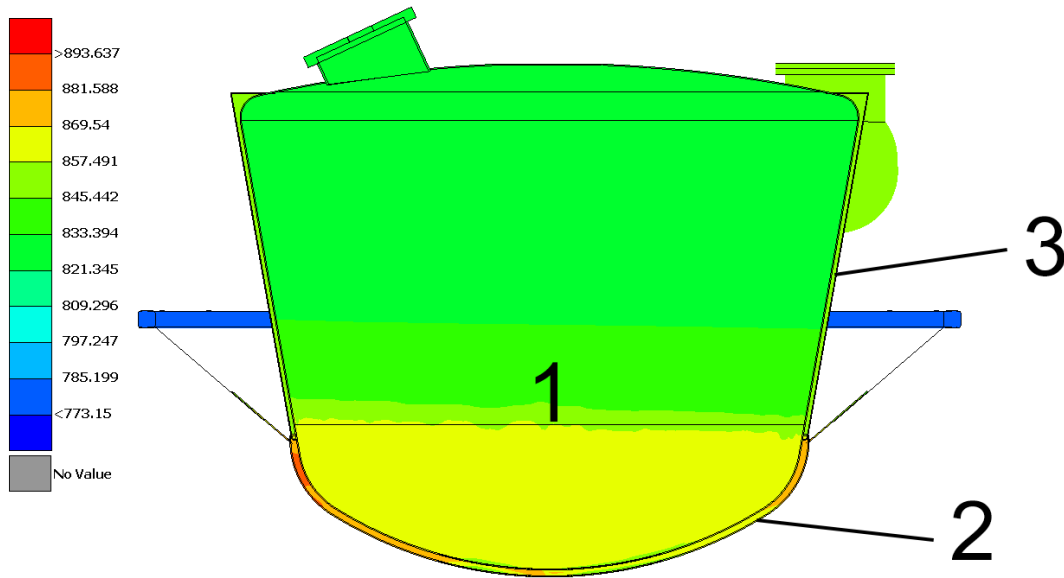


Figure 3.6: Cross-section of the tank at operational temperature (scale in Kelvin). 1. PCM. 2. Charge. 3. Discharge.

The TES unit model contains contact conditions on the suspension blades and a support bracket for the Charge system. The ANSYS option for nonlinear analysis NLGEOM is therefore enabled. The analysis consists of several steps. Initially, temperatures from CFD analysis are mapped onto the tank surfaces to simulate operational conditions. In the first load step, a thermal analysis is performed, solving for the thermal expansion.

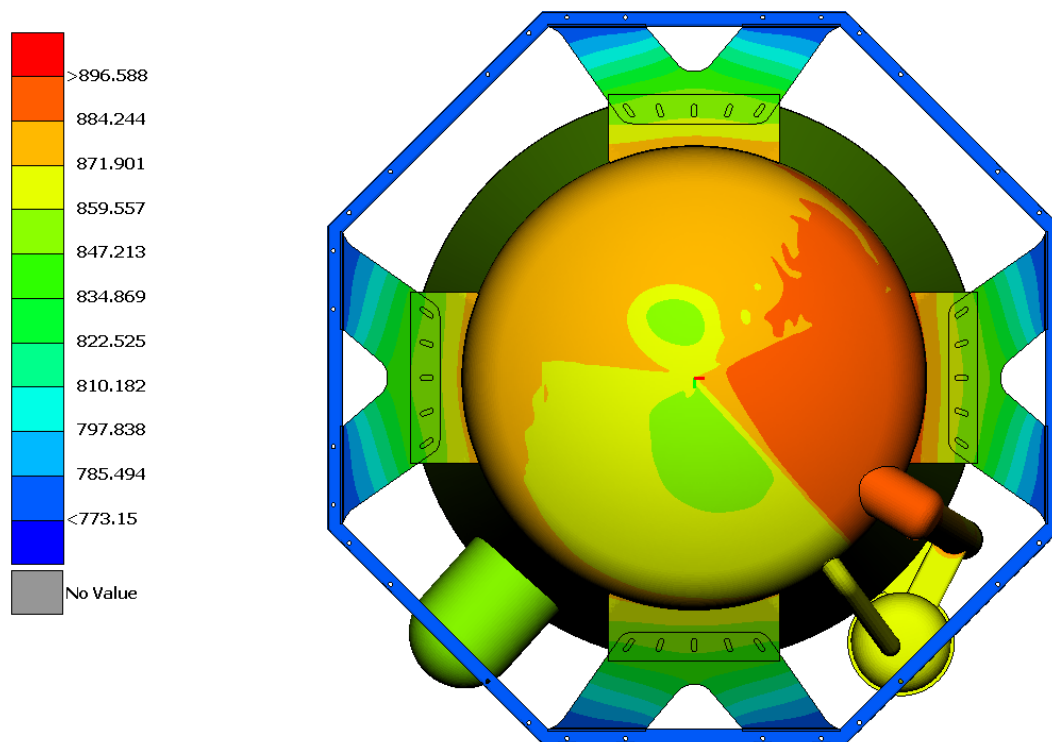


Figure 3.7: A bottom view of the tank at operational temperature. The Charge inlet and outlet and the pump system can be seen in the bottom right.

3. Model and simulation setup

In the second step, a pressure of 0.1 bar above ambient pressure is applied in the PCM, Charge and Discharge compartments, and the weight of the PCM and the liquid sodium is applied as hydrostatic pressures on the inside surfaces of the tank. The PCM, Charge and Discharge systems contain nitrogen which is inert. They are kept above ambient pressure in order to prevent air from leaking into the system and reacting with the contents. The elastic strains are now solved for.

In the third step, the plastic strains are solved for, using multilinear isotropic hardening with yield stress values taken from the Sandvik data sheet [2]. For example, at 600 °C the yield strength is 140 MPa at 0% plastic strain, 165 MPa at 0.8% plastic strain, and 340 MPa at 40% plastic strain, where 340 MPa is the ultimate tensile strength at 600 °C and 40% is the elongation at failure. ANSYS linearly interpolates the yield stress values between temperature levels. A sequence of timesteps follows where creep is enabled and the equivalent creep strains are solved for over the 25 year service life.

As the tank starts to creep, the added strains in the tank will cause stresses to relax. In order to obtain an accurate solution with resolved stress relaxation while saving computational resources, the load step size successively increases according to Table 3.3.

Table 3.3: The load steps of the ANSYS TES unit analysis.

Load step	Time
1. Thermal	instant
2. Elastic	instant
3. Plastic	instant
4. Creep	100 h
5. Creep	250 h
6. Creep	500 h
7. Creep	1 000 h
8. Creep	2 500 h
9. Creep	5 000 h
10. Creep	10 000 h
11. Creep	25 000 h
12. Creep	50 000 h
13. Creep	100 000 h
14. Creep	150 000 h
15. Creep	219 000 h

4

Results and Discussion

In this chapter, the results of the ANSYS creep analysis are presented. The model setup and the results are then discussed.

4.1 Analysis results

In order to visualise the results, a set of nodes are chosen for which the von Mises stress and creep strain history is plotted. These are a selection of nodes located in areas that experience the highest stresses and temperatures, and thus develop the largest creep strains. Looking at the results from the plastic analysis, some points of interest can be identified, see Figure 4.1. Four of these are welds or in close proximity to a weld, one is located in the Charge inlet and one is located on the upper rim of Discharge. Their stress and strain histories are plotted in Figures 4.2-4.7, and their initial and final stress values are given in Tables 4.1 and 4.2.

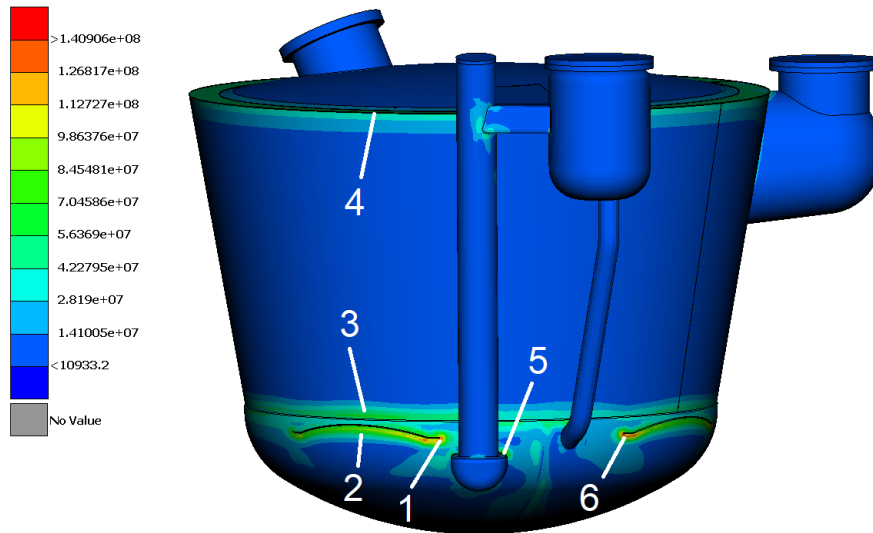


Figure 4.1: Points of interests: (1) Charge inlet suspension weld. (2) Area below Charge inlet suspension weld. (3) Charge-Discharge weld. (4) Upper rim of Discharge. (5) Charge inlet. (6) Charge outlet suspension weld. Scale shows σ_{vM} .

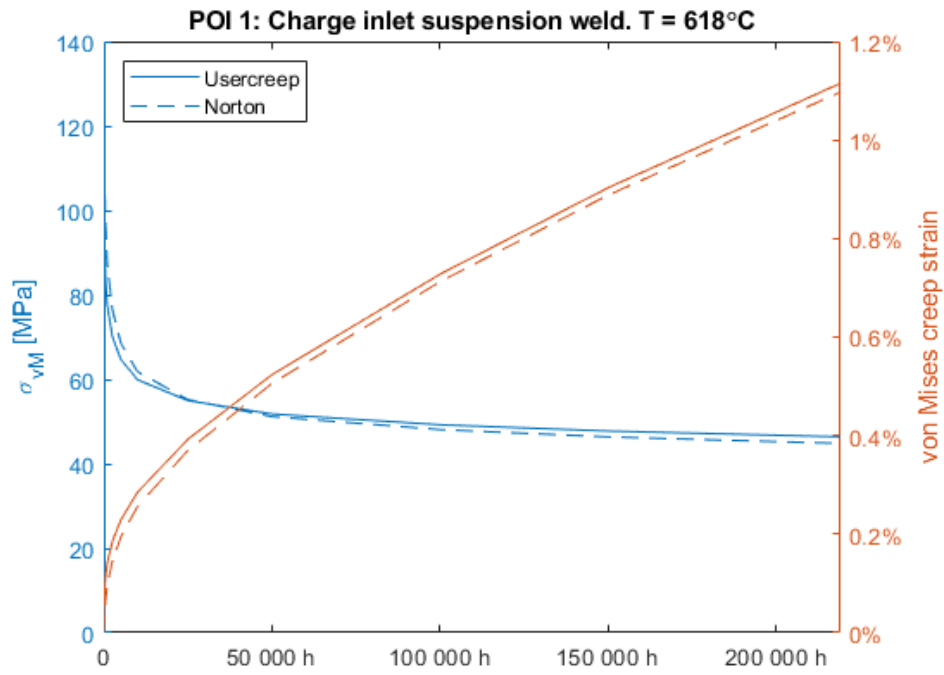


Figure 4.2: The stress and creep strain history in the suspension weld near the Charge inlet.

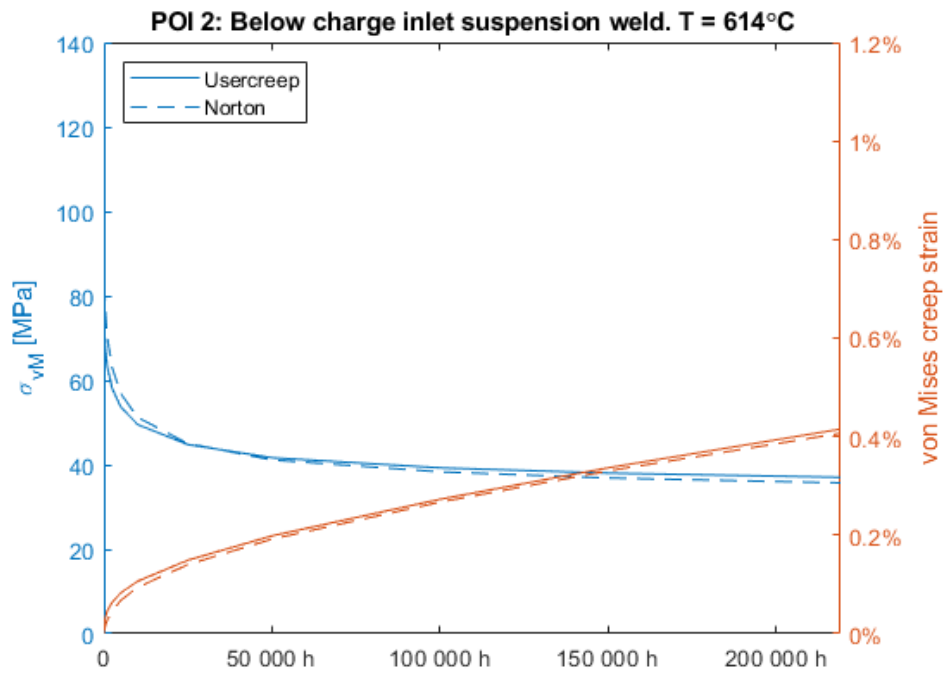


Figure 4.3: The stress and creep strain history in the area below the Charge inlet suspension weld.

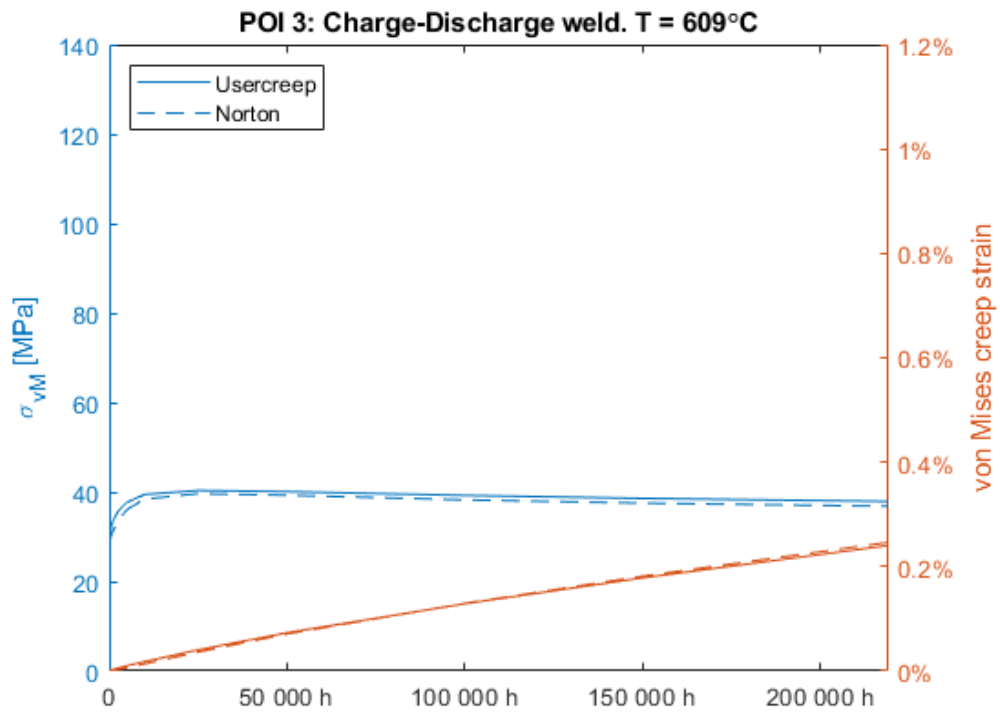


Figure 4.4: The stress and creep strain history in the Charge-Discharge weld.

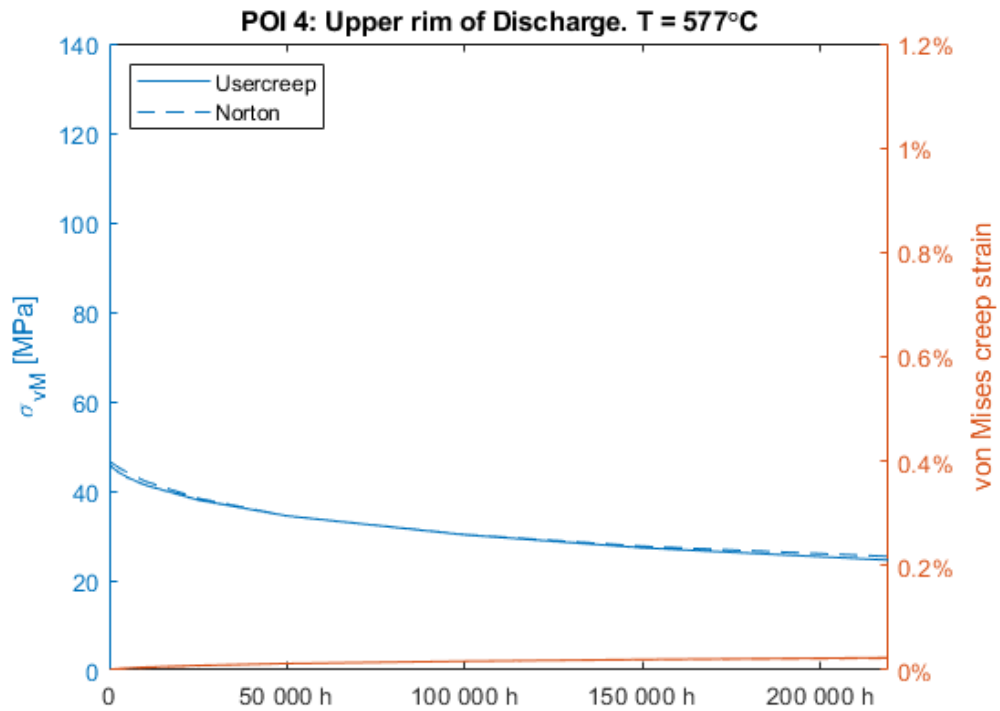


Figure 4.5: The stress and creep strain history at the upper rim of Discharge.

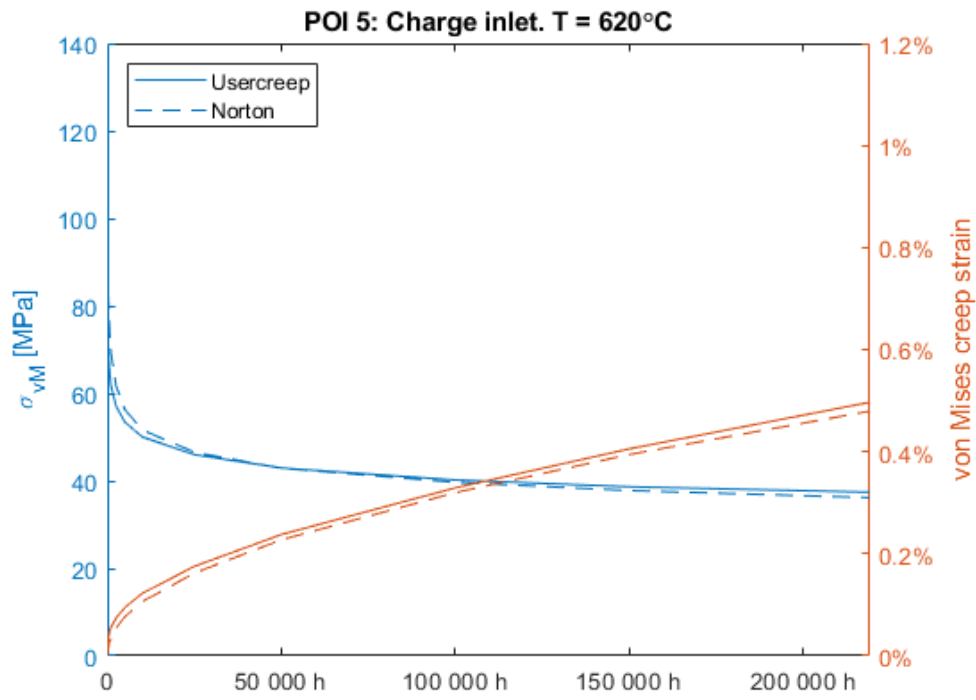


Figure 4.6: The stress and creep strain history in the Charge inlet.

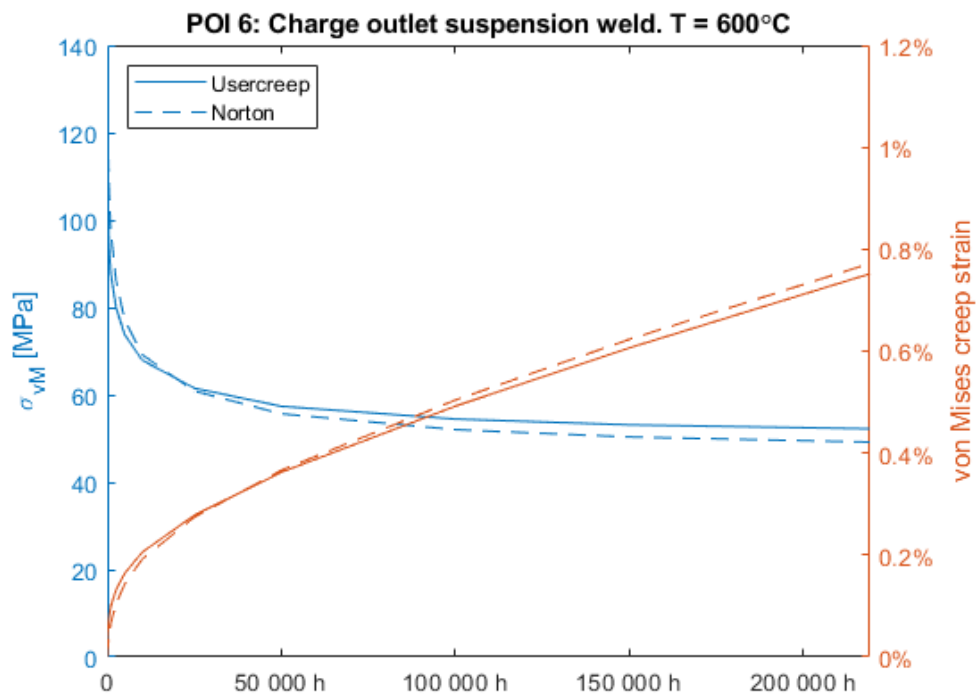


Figure 4.7: The stress and creep strain history in the suspension weld near the Charge outlet.

Table 4.1: Usercreep: Temperatures, initial and ending von Mises stress values, and final von Mises creep strains for the points of interest.

Point of interest	T [°C]	$\sigma_{vM,init}$ [MPa]	$\sigma_{vM,end}$ [MPa]	$\varepsilon_{vM,end}^{cr}$
1	618	136.3	46.4	1.11%
2	614	89.5	37.0	0.42%
3	609	29.9	37.9	0.24%
4	577	46.7	24.6	0.02%
5	620	109.5	37.4	0.50%
6	600	134.8	52.2	0.75%

Table 4.2: Norton model: Temperatures, initial and ending von Mises stress values, and final von Mises creep strains for the points of interest.

Point of interest	T [°C]	$\sigma_{vM,init}$ [MPa]	$\sigma_{vM,end}$ [MPa]	$\varepsilon_{vM,end}^{cr}$
1	618	136.3	44.8	1.10%
2	614	89.5	35.7	0.41%
3	609	29.9	36.8	0.25%
4	577	46.7	25.4	0.02%
5	620	109.5	36.2	0.48%
6	600	134.8	49.2	0.77%

4.1.1 Discussion of the analysis

The highest creep strain 1.11% after 25 years (from the **Usercreep** analysis) is found in the suspension weld near the hot Charge inlet. Overall, the resulting creep strains from the two different models are very similar. What is noticeable in the history figures is the stress relaxation that occurs due to the generated creep strain. At time zero, the stresses in the sampled suspension weld nodes are close to the 600 °C yield limit, but rapidly decrease over the first timesteps. After around 10 000 hours, the stresses in both welds are in the 60-70 MPa range. This drastically lowers the creep strain rate from an initially high value. Looking at the higher stress primary creep curves in Figure 3.2, one can see that the high stress primary creep contribution is cut short by the stress relaxation. It should be noted that the tank FE model is a global model where e.g. the welds are not modeled in detail. This may affect the accuracy of the results. In order to properly resolve the stresses and creep strains in these areas, further analyses should be performed using submodels with finer meshes.

Figure 4.8 shows areas of up to 0.1% plastic von Mises strain around one of the suspension welds. Due to the hardening rule used in the model, stresses in this region that drive creep may rise above the 600 °C yield limit. Due to the small size of the plastic strains and the substantial stress relaxation that quickly happens in the welds during creep, this is deemed to have a negligible effect on the total creep strain over the service life.

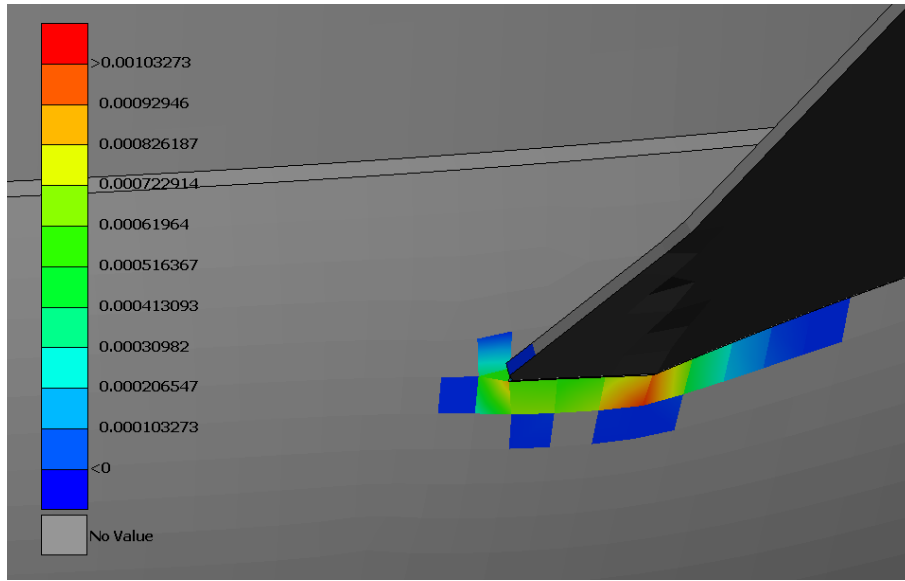


Figure 4.8: von Mises plastic strains around the Charge outlet suspension weld seen after the plastic load step.

4.1.2 Discussion of the creep models

Usercreep and the Norton model gave very similar results in the TES unit analysis. Looking at Figure 3.5, the secondary creep rates at 600 °C are similar in most of the stress range. The exception is for stresses below roughly 25 MPa, where the Coble model predicts higher strain rates than the fitted Norton model. These strain rates are however not of great practical interest, as generating a creep strain on the order of 1% in this stress range would take hundreds or thousands of years. In an application such as the TES unit where stresses are able to relax, the primary creep stage will not play as much of a role compared to a situation where high stresses are sustained over time. The simpler Norton model is therefore deemed to be a good substitute for **Usercreep** in this application.

The model parameters that were fitted to 253MA secondary creep data were the lattice diffusion activation energy $Q_L = 322$ kJ/mole and the obstacle distance $l = 125$ nm. Abe gives $Q_L \approx 300$ kJ/mole for austenitic iron [14]. Garofalo et al. found $Q_L = 314$ kJ/mole for 316 steel [36]. The fitted value for the lattice diffusion activation energy thus appears to be in accordance with similar alloy data in the literature.

Following Frost and Ashby, the activation energy $0.5Gb^3$ for a dislocation passing an obstacle in 316 steel corresponds to obstacles in the form of dislocations or small precipitates. 253MA is solid solution hardened with carbon and nitrogen, but the impact of these solute atoms on dislocation movement in austenitic stainless steel has been shown to be weak [37]. Assuming that the precipitation of chromium carbides is negligible due to the low carbon content of 253MA, other dislocations are thus the main obstacle for gliding dislocations. Assuming a uniform obstacle array of straight dislocations, $l = 125$ nm corresponds to a dislocation density of

$1/l^2 = 6.4 \cdot 10^{13}/\text{m}^2$. Pesicka et al. report a dislocation density between 10^{12} and 10^{14} in 12% Cr steel during creep at 650°C [38], which is in agreement with the optimized value of l . A uniform array of dislocations is a significant simplification however, as dislocation structures are much more complex in reality. The obstacle distance being a constant is also a simplification, as it is known that the dislocation density is dependent on the applied stress [39].

The limited validation of the model (Table 3.2) gave strain outputs in the vicinity of the ideal 1% value. This may be good enough to give an indication of creep behaviour in a full analysis, but should not be trusted completely. The models of the creep mechanisms are fairly simplistic, and experimental constants from other similar alloys have been used. The secondary creep model was fitted to extrapolated 253MA data, which may not represent the physical strain rate behavior. A proper validation against full creep curves needs to be done to see if the model truly represents 253MA creep behaviour.

5

Conclusion

The aim of this thesis work was to build a 253MA creep model and perform a 25-year service life analysis of the Azelio TES unit. A model was built consisting of 316LN primary creep, as well as three physical deformation mechanisms that cover diffusion-based and dislocation-based secondary stage creep. Due to the lack of 253MA data in the literature, model parameter values of other similar austenitic stainless steel alloys were used in the model. A limited validation against 253MA 1% creep strength data was performed, and the model was successfully implemented in a TES unit ANSYS simulation with the custom subroutine **Usercreep**.

While the aim of the thesis was fulfilled, the model may be flawed due to parameter values that do not physically represent the behavior of 253MA, simplistic modeling of the deformation mechanisms, or insufficient validation. In order to gain a better understanding of creep in 253MA, and to build a better creep model, more experimental data is needed.

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A

Appendix 1

A.1 Usercreep.F

```
*deck,usercreep  USERDISTRIB parallel gal
  SUBROUTINE usercreep (impflg, ldstep, isubst, matId , elemId,
    &                    kDInPt, kLayer, kSecPt, nstatv, nprop,
    &                    prop , time , dtime , temp , dtemp ,
    &                    tofst, Ustatev, creqv , pres , seqv ,
    &                    delcr , dcrda)
C*****
C  *** primary function ***
C    Define creep laws when creep table options are
C    TB,CREEP with TBOPT=100.
C    Demonstrate how to implement usercreep subroutine
C
C    Creep equation is
C      dotcreq := k0 * seqv ^ n * creqv ^ m * exp (-b/T)
C
C    seqv is equivalent effective stress (Von-Mises stress)
C    creqv is equivalent effective creep strain
C    T is the temperature
C    k0, m, n, b are materials constants,
C
C    This model corresponds to primary creep function TBOPT = 1
C
C gal 10.01.1998
C*****
C Copyright ANSYS. All Rights Reserved.
C
C  input arguments
C
C    impflg (in ,sc ,i)      Explicit/implicit integration
C                             flag (currently not used)
```

A. Appendix 1

c	ldstep	(in ,sc ,i)	Current load step
c	isubst	(in ,sc ,i)	Current sub step
c	matId	(in ,sc ,i)	number of material index
c	elemId	(in ,sc ,i)	Element number
c	kDInPt	(in ,sc ,i)	Material integration point
c	kLayer	(in ,sc ,i)	Layer number
c	kSecPt	(in ,sc ,i)	Section point
c	nstatv	(in ,sc ,i)	Number of state variables
c	nprop	(in ,sc ,i)	size of mat properties array
c			
c	prop	(dp ,ar(*),i)	mat properties array
c			This array is passed all the creep
c			constants defined by command
c			TBDATA associated with TB,CREEP
c			(do not use prop(13), as it is used
c			elsewhere)
c			at temperature temp.
c	time		Current time
c	dtime		Current time increment
c	temp		Current temperature
c	dtemp		Current temperature increment
c	toffst	(dp, sc, i)	temperature offset from absolute zero
c	seqv	(dp ,sc , i)	equivalent effective stress
c	creqv	(dp ,sc , i)	equivalent effective creep strain
c	pres	(dp ,sc , i)	hydrostatic pressure stress, $-(S_{xx}+S_{yy}+S_{zz})/3$
c			note that: constitutive consistency is not
	accounted for		
c			if creep strains are function of pressure
c			
c	input output arguments		input desc / output desc
c	<u> </u>		<u> </u>
c	Ustatev (dp,ar(*), i/o)		user defined internal state variables at
c			time 't' / 't+dt'.
c			This array will be passed in containing the
c			values of these variables at start of the
c			time increment. They must be updated in this
c			subroutine to their values at the end of
c			time increment, if any of these internal
c			state variables are associated with the
c			creep behavior.
c			
c	output arguments		
c	<u> </u>		
c	delcr (dp ,sc , o)		incremental creep strain
c	dcrda (dp,ar(*), o)		output array
c			dcrda(1) - derivative of incremental creep

```

c                                     strain to effective stress
c                                     dcrda(2) - derivitive of incremental creep
c                                     strain to creep strain
c
c    local variables
c    =====
c    Emod      Young's modulus (temp. dependent)
c    Gmod      Shear modulus (temp. dependent)
c    primcr    Time hardening primary creep rate
c    coblcr    Coble creep rate
c    weercr    Weertman creep rate
c    glidcr    Glide creep rate
c
c
c*****
c
c --- parameters
c
#include "impcom.inc"

      DOUBLE PRECISION ZERO
      PARAMETER      (ZERO = 0.0d0)
c
c --- argument list
c
      INTEGER      ldstep, isubst, matId , elemId,
&                 kDInPt, kLayer, kSecPt, nstatv,
&                 impflg, nprop
      DOUBLE PRECISION dtime , time , temp , dtemp , toffst,
&                 creqv , seqv , pres
      DOUBLE PRECISION prop(*), dcrda(*), Ustatev(nstatv)
c
c --- local variables
c
      DOUBLE PRECISION Emod , Gmod , dseqv , delcr , delcr2 ,
&                 primcr , coblcr , weercr , glidcr , pi
c
c*****
c
c *** skip when stress and creep strain are all zero
c
      if (seqv.LE.ZERO.AND.creqv.LE.ZERO) GO TO 990
c
c *** Young's modulus interpolation & shear modulus calculation
c
      if (temp.gt.673.15d0 .and. temp.le.873.15d0) Emod = 170.0d9 -

```

A. Appendix 1

```
& (170.0d9-155.0d9)*(temp-673.15d0)/(873.15d0-673.15d0)
c
    if (temp.gt.873.15d0 .and. temp.le.1073.15d0) Emod = 155.0d9 -
& (155.0d9-135.0d9)*(temp-873.15d0)/(1073.15d0-873.15d0)
c
    Gmod = Emod/(2.0d0*(1.0d0+0.3d0))
c
c *** Stress increment for numerical differentiation
c
    dseqv = 1.0d-5
c
c *** Define pi, calculate creep rates
c
    pi = 4.0d0*atan(1.0d0)
c
    primcr = 1.37522722422862d-23 * seqv**4.006d0 *
& time**(-0.580d0+1.0d0)/(-0.580d0+1.0d0)*exp(-31107.0d0/temp) -
& 1.37522722422862d-23 * seqv**4.006d0 *
& (time-dtime)**(-0.580d0+1.0d0)/(-0.580d0+1.0d0)*exp(-31107.0d0/temp)
c
    coblcr = 148.0d0 * 1.0d-9 * seqv * 1.149404032193386d-29
& / (8.6d-5**3 * 1.381d-23 * temp) * 6.0d-6 *
& exp(-189.0d3/(8.314d0*temp))
c
    weercr = 1.0d0/(3.06d0) * 0.25d0 * pi**2.0d0
& * (seqv/(3.06d0))**4.5d0 * 3.7d-5 * exp(-322457.976515788d0/(8.314d0*temp))
& / ((2.8d-10*1.0d14*Gmod**7.0d0)**0.5d0 * 1.381d-23 * temp)
c
    glidcr = (1.0d0/3.06d0) * 1.0d6 *
& exp(-(0.5d0*Gmod*2.8d-10**3.0d0 / (1.381d-23 * temp))
& * (1.0d0-seqv/(3.06d0*Gmod*2.8d-10/1.24572533822601d-7)))
c
    delcr = primcr + (coblcr + weercr + glidcr) * dtime
c
c *** Calculate delcr(seqv+dseqv) for the stress derivative
c
    primcr = 1.37522722422862d-23 * (seqv+dseqv)**4.006d0 *
& time**(-0.580d0+1.0d0)/(-0.580d0+1.0d0)*exp(-31107.0d0/temp) -
& 1.37522722422862d-23 * (seqv+dseqv)**4.006d0 *
& (time-dtime)**(-0.580d0+1.0d0)/(-0.580d0+1.0d0)*exp(-31107.0d0/temp)
c
    coblcr = 148.0d0 * 1.0d-9 * (seqv+dseqv) *
& 1.149404032193386d-29 / (8.6d-5**3 * 1.381d-23 * temp) * 6.0d-6
& * exp(-189.0d3/(8.314d0*temp))
c
    weercr = 1.0d0/(3.06d0) * 0.25d0 * pi**2.0d0 *
```

```
& ((seqv+dseqv)/(3.06d0))**4.5d0 * 3.7d-5 *
& exp(-322457.976515788d0/(8.314d0*temp))
& / ((2.8d-10*1.0d14*Gmod**7.0d0)**0.5d0 * 1.381d-23 * temp)
c
glidcr = (1.0d0/3.06d0) * 1.0d6 *
& exp(-(0.5d0*Gmod*2.8d-10**3.0d0
& / (1.381d-23 * temp)) *
& (1.0d0-(seqv+dseqv)/(3.06d0*Gmod*2.8d-10/1.24572533822601d-7)))
c
delcr2 = primcr + (coblcr + weercr + glidcr) * dtime
c
c *** derivative of incremental creep strain to effective stress
c
dcrda(1)= (delcr2 - delcr) / dseqv
c
c *** derivative of incremental creep strain to effective creep strain
c
dcrda(2)= 0
c
c *** write the effective creep strain to last state variable for verification
c
if (nstatv .gt. 0) then
    Ustatev(nstatv) = creqv
end if
990 continue
return
end
```