A Combined Gurson-RKR Model for the Ductile to Brittle Transition in Steel

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Problem text

The problem text for the master's thesis is the same as for the specialization project delivered in December 2016, and is thus presented here.

THE NORWEGIAN UNIVERSITY
OF SCIENCE AND TECHNOLOGY
DEPARTMENT OF ENGINEERING DESIGN
AND MATERIALS

PROJECT WORK FALL 2016
FOR
STUD.TECHN. INGRID HOLTE

Modelling the transition from ductile to brittle behaviour in steel

Modellering av omslag fra duktil til sprø oppførsel hos stål

Background - For steel structures to be installed in the Arctic region, the risk of brittle fracture represents a primary concern due to the ductile to brittle usually transition taking place at sub-zero temperatures. Recent results have demonstrated that the toughness may be on the borderline for both the heat affected zone and the weld metal, indicating that required robust solutions are not yet available for the most challenging part of the Arctic region, unless some constraint loss corrections are applicable.

Objective – The overall objective of the present study is to model the transition from ductile to brittle behaviour of steels for low temperature applications.

Work tasks - The work will include the following topics:

1. Carry out literature survey of modelling the ductile to brittle transition in steel
2. Modelling of fully ductile behaviour (upper shelf)
3. Modelling of fully brittle behaviour (lower shelf)
4. Propose models with subsequent simulations applied to the transition region
5. Reporting

Formal requirements:

Students are required to submit an A3 page describing the planned work three weeks after the project start as a pdf-file via "IPM DropIT" (http://129.241.88.67:8080/Default.aspx). A template can be found on IPM's web-page (https://www.ntnu.edu/ipm/project-and-specialization).

Performing a risk assessment is mandatory for any experimental work. Known main activities must be risk assessed before they start, and the form must be handed in within 3 weeks after you receive the problem text. The form must be signed by your supervisor. Risk assessment is an ongoing activity, and must be carried out before starting any activity that might cause injuries or damage materials/equipment or the external environment. Copies of the signed risk assessments have to be put in the appendix of the project report.

No later than 1 week before the deadline of the final project report, you are required to submit an updated A3 page summarizing and illustrating the results obtained in the project work.

Official deadline for the delivery of the report is 13 December 2016 at 2 p.m. The final report has to be delivered at the Department's reception (1 paper version) and via "IPM DropIT".

When evaluating the project, we take into consideration how clearly the problem is presented, the thoroughness of the report, and to which extent the student gives an independent presentation of the topic using his/her own assessments.

The report must include the signed problem text, and be written as a scientific report with summary of important findings, conclusion, literature references, table of contents, etc. Specific problems to be addressed in the project are to be stated in the beginning of the report and briefly discussed. The report should not exceed thirty pages including illustrations and sketches.

Additional tables, drawings, detailed sketches, photographs, etc. can be included in an appendix at the end of the thirty-page report. References to the appendix must be specified. The report should be presented so that it can be fully understood without referencing the Appendix. Figures and tables must be presented with explanations. Literature references should be indicated by means of a number in brackets in the text, and each reference should be further specified at the end of the report in a reference list. References should be specified with name of author(s) and book, title and year of publication, and page number.

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Abstract

Steels exhibit a great temperature dependence in their deformation behaviour and toughness. At higher temperatures, steel is ductile and the ductile fracture mechanism with void nucleation, growth and coalescence, prevails. At lower temperatures, however, the mechanism shifts towards brittle, and the steel may fracture catastrophically and without warning. The ductile-to-brittle transition happens over a temperature range, which is of crucial importance when designing structures and components for the cold Arctic.

The goal of this work was to establish a simulation scheme that incorporates both ductile and brittle fracture modes with respect to temperature in order to describe the aforementioned toughness dependency on temperature. Whether or not changing only temperature and constraint level would be sufficient to show the ductile-to-brittle transition without incorporating ductile material softening through the Gurson model was investigated. It was found that a stress-criterion alone would not capture the transition of material behaviour.

The complete Gurson model was used to simulate softening induced ductile tearing in ABAQUS. The model was incorporated through a user subroutine, UMAT. Simulations for three different temperatures ($21°C$, $0°C$ and $−60°C$) were run. Fracture resistance curves for all temperatures were plotted from the simulations and compared to experimental data. From this the ductile-to-brittle transition as captured by the complete Gurson model could be plotted. As the model was fitted from the highest temperature, $21°C$, the fit was very good and the model predicted both CTOD and Δa-values here. However, the Gurson model is not able to capture the brittle characteristics that appear at lower temperatures, and the results clearly deviated at both $0°C$ and $−60°C$.

To account for cleavage, a brittle stress criterion, the RKR-criterion, was applied as a post-processing routine. The input parameters for the criterion were fitted from $−60°C$, and the prediction of CTOD at this temperature from simulations was very good. A parametric study of the input parameters for the RKR-criterion has been conducted. The length scale, which should be tied with microstructure, was used as a material fitting parameter.

The combined Gurson+RKR model severely overestimated brittleness at high temperatures and needed a competing criterion to determine if cleavage has occurred or not. The CTOD at the increment in the simulation corresponding to the maximum force of the characteristic experimental value was used for this. The resulting ductile-to-brittle transition curve gave accurate results at both the upper and lower shelf, and satisfactory, if somewhat conservative, results in the intermediate region. The model captured the change of fracture mechanism over the temperature range from $−60°C$ to $21°C$. The model still needs some improvement. Some of the material parameters have been detached from their physical value and used as fitting parameters. The simulated DBT-curve is not uniquely determined, but can be shifted.

Sammendrag

Stål viser stor temperaturavhengighet i sin deformasjonsadferd. Ved høyere temperaturer er stål duktilt og den duktile bruddmekanismen med nukleasjon, vekst og koalesens av porer råder. Ved lavere temperaturer skifter mekanismen seg mot sprø, og stålet kan bryte katastrofalt og uten forvarsel. Den duktile til sprø overgangen skjer over et temperaturområde som er avgjørende for utformingen av konstruksjoner og komponenter for kalde arktiske strøk.

Målet med oppgaven var å etablere et simuleringforløp som inkorporerer både duktile og sprø bruddmekanismer med hensyn til temperatur. Hvorvidt endring av bare temperatur og constraintnivå ville være tilstrekkelig til å vise den duktile til sprø overgangen uten å inkorporere materialmykning gjennom Gurson-modellen ble undersøkt. Det ble konkludert med at et stresskriterium alene ikke kunne fange overgangen i materiell atferd. Den komplette Gurson-modellen har blitt brukt til å simulere duktil riving i ABAQUS. Modellen ble innlemmet gjennom en bruker subrutine, UMAT. Simuleringer for tre forskjellige temperaturer ($21°C$, $0°C$ og $-60°C$) ble utført. Bruddmotstandskurver for alle temperaturer ble plottet fra simuleringene og sammenlignet med eksperimentelle data. Fra dette kan den duktile til sprø overgangen som fanget av den komplette Gurson-modellen bli plottet. Da modellen var tilpasset høyeste temperatur, $21°C$, var prediksjonen veldig bra, og modellen fanget både CTOD- og Δa-verdier her. Gurson-modellen er imidlertid ikke i stand til å fange de sprø egenskapene som opptrer ved lavere temperaturer, og resultatene avviker klart ved både $0°C$ og $-60°C$.

For å ta hensyn til spaltning ble et sprøtt stresskriterium, RKR-kriteriet, anvendt som en rutine etter simulering. Inputparametrene for kriteriet ble tilpasset $-60°C$, og derfor var prediksjonen av CTOD ved denne temperaturen fra simuleringer meget god. En parameterstudie av inputparametrene for RKR-kriteriet er utført. Lengdeskalaen, som skal knyttes til mikrostruktur, ble brukt som en tilpasningsparameter.

Den kombinerte Gurson + RKR modellen overvurderte sterkt sprøhet ved høye temperaturer og trengte et konkurrerende kriterium for å avgjøre om spaltning har oppstått eller ikke. CTOD ved inkrementet i simuleringene tilsvarende den maksimale kraften av den karakteristiske eksperimentelle verdien ble brukt til dette. Den resulterende duktile-til-sprø overgangskurven ga nøyaktige resultater på både øvre og nedre platå og tilfredsstillende resultater i mellomområdet. Modellen fanger mekanismeendringene i materialet over temperaturintervallet fra $-60°C$ til $21°C$. Modellen trenger imidlertid videre utvikling. Noen av materialparametrene er løsnet fra deres fysiske verdi og brukes som tilpasningsparametere. Den simulerte overgangskurven er ikke unikt bestemt, men kan tilpasses etter ønske.

Preface

This dissertation is submitted for the degree of Master of Science in Materials Science and Engineering at the Norwegian University of Science and Technology. The thesis has been written at the Department of Mechanical and Industrial Engineering in collaboration with SINTEF Materials and Chemistry. The research described herein has been conducted under the supervision of Antonio Alvaro. Guidance has been provided by Bård Nyhus, Odd Magne Akselsen, Xiaobo Ren and Vidar Osen, all from SINTEF Materials and Chemistry.

A special thanks to all my boys at SINTEF, whose combined experience and humorous approach to science have made the work both manageable and fun.

Nomenclature

A Specimen Cross-Section Area

A_0 Initial Specimen Cross-Section Area

B Depth of a SENB Specimen

C_0 Particle Diameter

E Young's Modulus of Elasticity

E' Plane Strain Dependent Young's Modulus

F Applied Force

G Shear Modulus

K_{Ic} Critical Stress Intensity Factor

L Elongation

L_0 Initial Specimen Length

R Artificial Unit Cell Dimension

R_0 Initial Artificial Unit Cell Dimension

S Distance Between Applied Loads

T_p Peak Temperature

W Width of a SENB Specimen

Δa Crack Extension

Δa_{avg} Average Crack Extension

$\Delta t_{8/5}$ Cooling Time from 800-500 ° C

Φ Gurson Yield Function

α Ferrite

δ_{ij} Kronecker Delta

ϵ True Strain

ϵ^p Plastic Strain Tensor

γ Austenite

γ_p Plastic Surface Energy

γ_s Elastic Surface Energy

γ_e Effective Surface Energy

γ_{gb} Plastic Surface Energy over a Grain Boundary

$\bar{\epsilon}^p$ Equivalent Plastic Strain

$\bar{\sigma}$ Flow Stress

$\bar{r}$ Mean Void Radius

σ True Stress

σ_{22} Opening Stress

σ_{UTS} Ultimate Tensile Stress

σ_{VM} Von Mises (equivalent) Stress

σ_{app} Applied Remote Stress

σ_c Critical Stress

σ_e Equivalent Stress

σ_f Critical Crack Tip Stress

σ_h Hydrostatic Stress

σ_{ij} Stress Tensor

σ_i Stress Resisting Dislocation Movement

σ_m Mean Normal Stress

σ_{ys} Yield Stress

σ_{yy} Opening Stress

τ_i Shear Stress Resisting Dislocation Movement

τ_s Applied Shear Stress

b   Burger's Vector

v Poisson's Ratio

a Crack Length

d Average Grain Diameter

e Engineering Strain

f Void Volume Fraction

$f(\frac{a}{W})$ Dimensionless Shape Factor

f^* Artificially Accelerated Void Growth

f_ϵ Void Nucleation Intensity

f_0 Initial Void Volume Fraction

f_F Void Volume Fraction at Final Fracture

f_c Critical Void Volume Fraction

l_c Mesh Size

n Strain Hardening Exponent

q Heat Input per Unit Length Weld

q_1 Constant Factor (=1.5)

q_2 Constant Factor (=1)

r Void Radius

r_p Rotational Factor

s Engineering Stress

x_c Characteristic Distance

BCC   Body-Centered Cubic

CGHAZ   Coarse Grained Heat Affected Zone
CMOD   Crack Mouth Opening Displacement
CTOD   Crack Tip Opening Displacement

DBTT   Ductile-to-Brittle Transition Temperature

FCC   Face-Centered Cubic

HAZ   Heat Affected Zone

M-A   Martensite-Austenite

RKR   Ritchie-Knot-Rice

SENB   Single-Edge-Notched Bend Specimen

UMAT   User-Defined Material Model

Contents

1 | Introduction

Industrial activity in arctic climates is increasing. The Arctic region is characterized by ice, harsh weather, low temperatures and large distances, which all contribute to the need of enhanced material performance and abilities. In order to fully exploit the Northern region's resources, better materials, including better comprehension of their mechanical properties under the influence of extreme weather conditions, is both a necessity and a concern.

One of the most sought after mechanical properties of steel is the ductile-to-brittle transition temperature (DBTT). This temperature range is often characterized by a more or less gradual shift from a ductile to brittle behaviour as the temperature decreases. Brittle behaviour may be catastrophic as the fracture will happen abruptly, and must therefore be avoided. Setting a scheme for determining a steels behaviour over a large temperature interval ranging from complete ductile to complete brittle, including the transition, will improve the ability to design materials for extreme weather conditions. Using computational simulations to determine the DBTT for a material requires less testing in the lab. This will lower the costs as both time and test material requirements are reduced. A simulation scheme for the ductile-to-brittle transition must be able to capture material softening at higher temperatures, brittle characteristics a low temperatures as well as a combination in the intermediate temperature region.

This thesis presents the necessary underlying theoretical principles behind the ductile-to-brittle transition phenomena, along with the material mechanics that define the material models used in simulation. The Gurson model has been used to simulate ductile rupture in ABAQUS and the RKR-criterion has been applied as a post-processing routine to account for cleavage. The underlying ideas for both models are presented and their implementation to the computational simulation scheme discussed.

The scope of the thesis is to establish whether or not a combined Gurson-RKR model is able to capture the shift in material behaviour with temperature. Each model and their respective attributions have been assessed individually before the combined model has been evaluated.

2 | Theoretical Background

This section will cover theory required for understanding and using the numerical calculations presented in the thesis. Some theoretical elements are used directly in calculations and discussion in subsequent chapters, while others are added solely to substantiate the discussion and enhance comprehension.

2.1 Heat Affected Zone

The base material investigated in this thesis is a weld simulated steel. A description is provided in Section 4.1. Weldments are considered the most dangerous part of large steel structures as the heat input changes the mechanical properties of the steel in both the weld and the adjacent areas. The welds are brittle and have a large density of impurities, which contributes to the degradation of toughness. Research on weld simulated steel and their toughness degradation is thus a large part of further material development.

Large steel structures are assembled by welding components together. There are many ways in which welding can be carried out, but all methods involve deposition of molten weld metal between the components to be joined. When the weld metal solidifies the two components are combined. The heat flow from the weld metal will cause changes in the regions of the steel structure in close proximity to the weld, which will influence the performance. The region adjacent to the weld will melt completely. This, along with the weld metal itself, is called the fusion zone and will exhibit a solidification microstructure after cooling. The region that is heat affected, but not melted, is called the heat-affected zone (HAZ), and is a region of great interest.

Diffusion of heat from the fusion zone will cause microstructural changes and, consequently, changes in the mechanical properties of the HAZ. The heat-flow gradient from the fusion zone to surrounding material is well-defined, making it beneficial to categorize the HAZ based on changes in microstructure and mechanical properties as a function of distance from the fusion zone. The transformation temperature from ferrite, α, to austenite, γ, is, although dependent on the chemical composition, roughly 950°C[12], as seen in Figure 2.1. The region closest to the fusion zone is heated well above this temperature and will not only be completely transformed to γ, but also be annealed giving rise to a coarse grained zone, the coarse-grained HAZ (CGHAZ). Further from the fusion zone, the temperature will not be sufficient to cause full annealing, and the fine-grained HAZ will occur. Beyond this zone, the heat input will not be sufficient to completely transform the microstructure to γ, and a partially transformed zone will arise called the intercritical HAZ. At a threshold distance from the fusion zone, the heat input will not be sufficient to give temperatures above 950°C, and no γ will form in the subcritical HAZ[12]. All zones are indicated in Figures 2.1

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Figure 2.1: Different regions of the HAZ. a) fusion zone, b) partially melted zone, c) CGHAZ, d) fine-grained HAZ, e) partially transformed zone, f) subcritical zone. From [29]

Figure 2.2: Regions of the HAZ in a single pass weld.

and 2.2.

Both peak temperature, T_p, and heating rate decrease with distance from the fusion zone, while the cooling rate is less dependent on distance. The cooling rate is expressed as the time, t, it takes to cool from 800°C to 500°C, Δt_{8-5}, and is central for the transformation from austenite to ferrite after heating[12]. This parameter along with T_p can be used to express the thermal cycles of the HAZ. Both parameters are proportional to the heat input, q, given per unit length of weld. Thus, T_p and Δt_{8-5} can be used to determine the thermal cycle at any point in the HAZ, and are given by Equations 2.1 and 2.2, respectively, where r is the distance from the fusion line and n equals 1 or 2 depending on the thickness ratio of the components to be welded and the weld[12].

$$T_P \propto \frac{q}{r} \tag{2.1}$$

$$\Delta t_{8-5} \propto q^n \tag{2.2}$$

2.1.1 Coarse-Grained HAZ

The CGHAZ is the zone adjacent to the fusion zone, where T_p reaches its ultimate value. This region is of particular interest due to the mechanical properties caused by the significant austenite coarsening and rapid cooling rates, resulting in brittle microstructures. During cooling, new and complex microstructures will occur, changing the properties of the steel. The final microstructure of the CGHAZ will be dependant on alloy composition and Δt_{8-5}, as well as the density of impurities in the parent metal.

During cooling, the new microstructure will often be more complex than the parent metal. This is caused by the wide variety of possible transformation products such as bainitic ferrite, pearlite, carbides and M-A constituents. Bainitic lamella and needle structure are typically nucleated at γ-boundaries, making the γ grain size affect the microstructural properties of the CGHAZ. Bainite packet boundaries influence the brittle fracture properties[2]. During rapid cooling, i.e. low Δt_{8-5}, the transformation from γ to α-bainite is incomplete, resulting in the presence of M-A constituents[2][41]. The M-A constituents are hard, brittle islands of carbon rich martensite and retained austenite enclosed in a bainitic ferrite matrix. They are further discussed in Section 2.1.2.

The CGHAZ has historically been viewed as the region in the HAZ with lowest toughness. In later studies, the intercritically reheated CGHAZ (ICCGHAZ) has shown the highest degradation in toughness because it exhibits several unfavourable microstructural features, large prior austenite grain size, bainite, M-A constituents and microalloy precipitates[63]. During mulitpass welding the CGHAZ will be reheated to the $\alpha + \gamma$-region shown in Figure 2.1. The material will experience a partial transformation to γ where γ will nucleate and grow along prior austenite grain boundaries and bainitic boundaries in the CGHAZ[63]. Upon cooling, M-A constituents will form in a bainite matrix, degrading the toughness of the steel.

2.1.2 M-A Constituents

M-A constituents are generally considered as the major contributor to deterioration of HAZ toughness [23][41][50][51][63]. The brittleness of the M-A constituents is linked to cleavage. They crack readily and promote cleavage fracture initiation. The M-A constituents are significantly harder than the matrix and will therefore promote a local stress concentration when the material is stressed. The high stresses around the M-A constituent interface might eventually lead to debonding between the M-A constituent and the matrix. This will introduce a microcrack that might propagate either in a brittle manner, as described in Section 2.5.1 or in a ductile manner, described in Section 2.5.2, by linking with other debonded regions

During the phase transformation from γ to α-bainite, the unit cells of the material change from a FCC to a BCC structure meaning that the material experiences a volume expansion. This will introduce stresses in the matrix which will be influenced by the presence of M-A constituents. Two or more M-A constituents in proximity will generate overlapping stress and strain fields that amplify the stress concentration. The effect of flaws and microcracks

on stress fields in treated in Section 2.7.1.

Several studies have concluded with M-A constituents being the dominating factor for lowered toughness in the HAZ. The degree of deterioration is linked directly to the size and volume fraction of M-A constituents[23][24][50][51]. This is further treated in Section 2.5.3

2.2   Deformation

All materials experience deformation when subjected to an external load. The deformation process may be divided into two separate stages, the elastic stage and the plastic stage. During elastic deformation, the interatomic bonds in a material will only be stretched, and the material will recover its original shape if the stresses are relieved. When the applied load exceeds the elastic limit, the mode of deformation switches to plastic. The interatomic bonds will be broken and rebuilt leaving permanent changes so that the material will not recover its original shape upon removal of the load.

Materials can generally be classified as either ductile or brittle depending on their ability to undergo plastic deformation. A brittle material will fracture at the elastic limit load, whereas a ductile material will redistribute the stresses. This means that a ductile material is able to undergo plastic deformation and experience plastic flow[25]. The main deformation mechanism in a ductile material is dislocation movement.

2.2.1   Dislocations and Slip

Using the term *dislocation* to describe a line defect at the atomic scale was first introduced by G.I. Taylor (1934)[68]. A dislocation can be perceived as a two-dimensional fault in the homogeneous atomic stacking pattern of a material. The movement of dislocations is responsible for plastic deformation of a material[16][25]. Thus, a ductile material can be viewed as a material where dislocations may move freely. When the stresses within a material reach a critical value, the dislocations move, and the adjacent atoms move from one side of a dislocation to the other. The dislocations and the atoms move one interatomic length, which corresponds to the Burgers vector, **b**. As the material is deformed through dislocation movement, new dislocations are nucleated.

The process of plastic deformation by dislocation movement is called slip. The dislocation moves along preferred crystallographic planes and directions called *slip plane*, shown in Figure 2.3 and *slip direction*, respectively. Together these two constitute the *slip system*. The preferred slip plane is the plane with the most dense atomic packing, and the slip direction is the most densely packed direction within that plane.

2.2.2   Cracking Due to Dislocations

Dislocations may pile up along their slip planes at obstacles, such as grain boundaries and M-A constituents, and cause a build up of stresses. The idea that a dislocation pile-up might

Figure 2.3: A dislocation moves through a crystal lattice along the slip plane. From [16].

cause fracture was first introduced by Zener[84]. Stroh[67] showed that if these stresses were not relieved through plastic deformation, they would nucleate microcracks in the material. Cottrell[20] expressed this mathematically through Equation 2.3 where τ_s is the applied shear stress, τ_i is a frictional stress resisting dislocation movement, n is the number of dislocations with Burgers vector $\mathbf{b}$, β is a constant related to the stress state, and γ_s is the surface energy of the crack, i.e. the energy requirement to create two new surfaces.

$$(\tau_s - \tau_i)n\mathbf{b} = \beta\gamma_s \tag{2.3}$$

Equation 2.3 is an energy balance, which relates the work done by the applied shear stress in producing a displacement, $n\mathbf{b}$, of dislocations against the frictional stress to the surface energy requirement of opening a crack. The equation shows that a material will create a crack when the surface energy requirement is lower than the stress requirement for further propagation of dislocations. The total displacement expressed by $n\mathbf{b}$ is a function of grain size [25][45], which indicates that a material's ductility is dependent on the grain size. This is shown in the Hall-Petch equation, Equation 2.4, where σ_{ys} is the yield strength, σ_i is the friction stress related to dislocation movement, k a material parameter and d is the average grain diameter[31][53].

$$\sigma_{ys} = \sigma_i + \frac{k}{\sqrt{d}} \tag{2.4}$$

2.3 Stress-Strain Curve

The elastic and plastic characteristics of a material mentioned in Section 2.2, are described by its stress-strain curve. An example of a stress-strain curve with some key material parameters indicated, is shown in Figure 2.4. The curve is found from tensile testing, described in Section 2.8.1.

The slope of the elastic part of the curve is the Young's modulus, E, which is a measure of the stiffness of a solid material. The yield strength defines the point where the stress-strain curve bends over into the plastic region, namely, the stress level at which plastic deformation of a material initiates. Beyond the yield point, the stresses continually increase with strain due to hardening of the material. The slope of the curve is described by a hardening

exponent, *n*, which ranges between 0.1 and 0.5 for most metals[16]. If *n* = 0, the material is perfectly plastic, and the plastic part of the stress-strain curve will be flat. The region between σ_{ys} adn σ_{UTS} is called the plastic flow curve. After reaching the ultimate tensile stress, σ_{UTS}, necking will initiate. Non-uniform deformation will prevail until the material eventually fractures.

Figure 2.4: Stress-strain curve.

2.3.1   Physical Interpretation

On an atomic scale, elastic strain is manifested as small changes in the interatomic spacing and the stretching of interatomic bonds. Young's modulus can be viewed as a measure of the resistance to separation of adjacent interatomic bonds[25]. In other words, the resistance to undergo plastic deformation and slip.

At the yield stress, σ_{ys}, the stress is sufficient to activate dislocations and slip and homogeneous deformation occurs. As the density of dislocations increases it becomes increasingly difficult for them to move, and more stress is required for further propagation. This is called hardening, described by the hardening exponent, and explains the rising plastic flow curve. When the stress levels reach the ultimate strength of the material, necking will start. At the onset of necking, local deformation initiates. The voids in the material will grow and coalesce to form a crack, ultimately resulting in ductile fracture. This is further treated in Section 2.5.2.

2.3.2   Mathematical Approach

A material's stress-strain curve is found through tensile testing, described in Section 2.8.1. The output from such a test is the applied force, *F*, and the elongation of the material, *L*. From the initial dimensions of the test specimen, engineering stresses and strains can be found through Equations 2.5 and 2.6, respectively. A_0 is the initial cross-section area of the specimen and L_0 the initial length.

$$s = \frac{F}{A_0} \tag{2.5}$$

$$e = \frac{L - L_0}{L_0} \tag{2.6}$$

The specimen elongation will happen in the direction of the applied load. In the direction perpendicular to the load, the material contracts giving rise to transversal strains. The axial and transversal strains are related through Poisson's ratio, v. The expression for Poisson's ratio is shown in Equation 2.7[16].

$$v = -\frac{\epsilon_{transversal}}{\epsilon_{axial}} \tag{2.7}$$

When transforming applied force and elongation to engineering stresses and strain, the initial dimensions of the specimen are used in calculation throughout the test sequence. This gives a somewhat inaccurate curve as the specimen dimension change with deformation. To account for the constant change in specimen dimensions and relate F and and L to the incremental dimensions, Equations 2.8 and 2.9 can be used to transform the engineering stresses and strains to true stresses and strains. The derivation of these equations can be found in Appendix A.1. Both curves are shown in Figure 2.4. Equations 2.8 and 2.9 are only valid until necking. After reaching σ_{UTS}, the specimen deforms locally and constantly updating the dimensions becomes impossible.

$$\sigma = s(1 + e) \tag{2.8}$$

$$\epsilon = ln(1 + e) \tag{2.9}$$

A constitutive approximation for the true stress-strain curves is the Ramberg-Osgood relation, which may be presented as Equations 2.10 and 2.11[58]. The linear elastic part of the curves may be described solely through the Young's modulus E, as shown in Equation 2.10. The plastic region, however, is approximated through the three parameter relation given in Equation 2.11, where K is a material dependent constant and n is the strain-hardening exponent. These equations have been used when creating material input for the simulation scheme, as presented in Section 4.1.1.

$$\epsilon = \frac{\sigma}{E} \tag{2.10}$$

$$\epsilon = K\left(\frac{\sigma}{E}\right)^n \tag{2.11}$$

2.4   Yield Criteria

Subjecting a specimen to uniaxial stress in tensile testing allows for determining the yield strength as a single scalar value. However, in most cases, materials are subject to complex three-dimensional loading conditions, which are best described by a stress tensor. This is called a triaxial stress state, and is shown in Figure 2.5. The stress tensor can be expressed by a 3x3-matrix as shown in Expression 2.12[25]. Due to conservation of angular momentum, the tensor is symmetric, also indicated in Expression 2.12. The strain state of a material under triaxial loading can be expressed by a tensor as well. The strain tensor is described by a symmetrical 3x3-matrix, equal to the one for stress.

Figure 2.5: Components of stress in three dimensions.

$$\begin{bmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{bmatrix} \rightarrow \begin{bmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \sigma_{yy} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \sigma_{zz} \end{bmatrix} \tag{2.12}$$

The general three-dimensional stress state consists of three unequal principal stresses acting at a point. Principal stresses are found when the stress tensor is rotated so that all shear-components, τ_{ij}, are zero. If all three principal stresses are equal, the stress state is called hydrostatic and the resulting stress in the material can be calculated from the average of the three principal stresses, i.e. $\sigma_h = (\sigma_1 + \sigma_2 + \sigma_3)/3$[25]. To incorporate this in the expression for a three-dimensional stress state, the stress tensor can be split into two components: the hydrostatic stress tensor and the deviatoric stress tensor, as seen in Equation 2.13. The hydrostatic stress tensor involves only pure tension or compression and induces volume change in the material, while the deviatoric stress tensor constitutes distortions.

$$\begin{bmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \sigma_{yy} & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \sigma_{zz} \end{bmatrix} = \overbrace{\begin{bmatrix} \sigma_h & 0 & 0 \\ 0 & \sigma_h & 0 \\ 0 & 0 & \sigma_h \end{bmatrix}}^{Hydrostatic} + \overbrace{\begin{bmatrix} \sigma_{xx} - \sigma_h & \tau_{xy} & \tau_{xz} \\ \tau_{xy} & \sigma_{yy} - \sigma_h & \tau_{yz} \\ \tau_{xz} & \tau_{yz} & \sigma_{zz} - \sigma_h \end{bmatrix}}^{Deviatoric} \tag{2.13}$$

The stress state of a material can be related to its yield strength by reducing the complex three-dimensional loading condition to a single scalar number, enabling direct comparison with the yield strength during simple tension. A mathematical relationship as such must

fulfill the following terms:

- Yielding under a situation of combined stresses can be related to some particular combination of principal stresses.

- Pure hydrostatic pressure does not cause yielding in a continuous solid, i.e. the hydrostatic stress component does not influence the yield stress. Yield strength is dependent only on the deviatoric stresses.

- The yield criterion must be independent of the choice of axes for an isotropic material, i.e. it must be an invariant function.

- The yield criterion must be a function of the invariants of the stress deviator[25].

M.T. Huber proposed a yield criteria in 1904[33], but received little attention until R. von Mises re-proposed it in 1913[77]. The von Mises yield criteria, also called the J_2 flow rule, states that yielding will occur when the second invariant of the stress deviator, J_2, exceeds some critical value, as seen in Equation 2.14. The relationship between the constant k and yield stress, σ_{ys}, was found to be $k = \sigma_{ys}/\sqrt{3}$ at the onset of yielding. The second invariant of the deviatoric stress tensor can be expressed through the terms of the stress tensor by Equation 2.15.

$$J_2 = k^2 \tag{2.14}$$

$$J_2 = \frac{1}{6}\left[(\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{yy} - \sigma_{zz})^2 + (\sigma_{zz} - \sigma_{xx})^2\right] + \sigma_{xy}^2 + \sigma_{yz}^2 + \sigma_{zx}^2 \tag{2.15}$$

Combining Equation 2.14, 2.15 and the expression for k, gives the von Mises yield criterion as expressed by Equation 2.16[25].

$$\sigma_{VM} = \frac{1}{\sqrt{2}}\left[(\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{yy} - \sigma_{zz})^2 + (\sigma_{zz} - \sigma_{xx})^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{xz}^2)\right]^{1/2} \tag{2.16}$$

The von Mises stress, also called equivalent stress, σ_e, can be used to determine whether or not a material will yield by comparing it to the material's yield strength. The onset of yielding is when $\sigma_{VM} = \sigma_{ys}$[25].

2.4.1 Yield Surface

In a three-dimensional space with the axes aligned with the principal stresses, Equation 2.16 can be represented by an open cylinder oriented at equal angles to the axes. The cylinder wraps around an axis given by the hydrostatic stress component. This is the von Mises yield surface, shown in Figure 2.6.

Figure 2.6: The von Mises yield surface in principal stress coordinates circumscribes a cylinder with radius $\sqrt{\frac{2}{3}}\sigma_{ys}$ around the hydrostatic axis.

A yield surface can be viewed as a map in a three-dimensional stress space which distinguishes non-yielding regions from flowing regions. A particularly useful yield surface is the π-plane, the projection down the line corresponding to pure hydrostatic stress. The stress at any point in the stress space can be regarded as the sum of the stress state at the corresponding point on the π-plane and the hydrostatic stress. For the von Mises criterion, the π-plane is a circle with radius $\sqrt{\frac{2}{3}}\sigma_{ys}$.

The yield surface indicates the onset of yielding under a certain state of stress. A state of stress which gives a point inside the cylinder represents elastic behaviour, while a point outside the cylinder indicates yielding. As plastic deformation occurs the yield surface expands outwards, maintaining its geometric shape[5][25].

2.4.2 Stress Triaxiality

Stress triaxiality, or the triaxiality of the stress state, is simply given by the ratio between hydrostatic stresses and the von Mises equivalent stress, as presented in Equation 2.17 where σ_1, σ_2 and σ_3 are the principal stresses. Plastic deformation of a ductile material under loading results in void growth and coalescence. The damaged region, where necking occurs and voids grow and coalesce, has stress in three directions, even if the specimen is subject to a uniaxial load.

$$T = \frac{\sigma_h}{\sigma_e} = \frac{\frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3)}{\frac{1}{\sqrt{2}}\sqrt{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2}} \qquad (2.17)$$

The triaxial stress state promotes void growth, hence constitutive equations that account for damage, such as the Gurson model, must be able to describe the effect of triaxiality[14]. The Gurson model is explained in Section 3.1. Stress triaxiality relates the stresses that are not responsible for plastic flow to the ones that are. The hydrostatic stresses do not cause

plastic deformation, while the von Mises equivalent stress expressed as the square root of the second invariant of the deviatoric stress, is responsible for plastic flow, as explained in Section 2.4.

2.5   Fracture in Metals

Fracture can generally be defined as the separation of a solid body into two or more parts under the action of a load. This load will be distributed in the solid body as stresses, which may build up and cause failure. From a phenomenological point of view, fracture may be divided in two separate stages, crack initiation and crack propagation or crack growth. The relative importance of these stages define the fracture type. Brittle fracture occurs when crack initiation is the critical stage, and ductile when propagation/growth is prominent. From a mechanistic point of view, brittle fracture is related to cleavage, while ductile fracture is linked to void nucleation, growth and coalescence[72].

2.5.1   Cleavage Fracture

Cleavage fracture is characterized by rapid, unstable crack growth. A material may only fail by cleavage if the stresses ahead of the crack front exceed the cohesive strength of the material. Materials that fail by cleavage are brittle, meaning that the plastic flow is restricted[5]; it is energetically favourable to create two new surfaces rather than undergo plastic deformation. The abrupt breaking of atomic bonds without plastic deformation leaves a sharp, smooth fracture surface with river markings in the direction of crack propagation originating from the crack initiation site.

As brittle fracture may be characterized by a stress limit, it occurs without warning, and must therefore be avoided at all costs. The tendency for brittle fracture is inversely proportional to temperature, indicated through the temperature dependant transition from ductile to brittle fracture, further discussed in Section 2.6.

2.5.1.1   Cleavage Fracture Initiation

Initiation of cleavage fracture is influenced by a number of factors, such as:

- Second phase particles

- Grain size

- Temperature dependency of yield stress

Second phase particles are suitable initiation sites for cracks. These particles can crack under the influence of high stresses or plastic strains in the surrounding matrix, initiating micro-cracks. These micro-cracks, called Griffith-cracks, may propagate through the material if the stresses ahead of the crack tip are sufficient. The presence and concentration of

brittle particles, such as M-A constituents, play a major role in the fracture characteristics of steel. If a given particle is round and produce a penny-shaped micro-crack, the fracture stress, σ_f will be given by Equation 2.18, where E is Young's modulus, γ_p is the required plastic work to create new fracture surfaces, ν is Poisson's ratio and C_0 is the particle diameter[5].

$$\sigma_f = \sqrt{\frac{\pi E \gamma_p}{(1-\nu^2)C_0}} \qquad (2.18)$$

Grain size influences the transition from ductile to brittle behaviour. Smaller grains shift the transition temperature down, as well as increase ductility and yield strength of the material. Consequently, for large grain sizes, cleavage is more readily initiated. N.J. Petch showed that the transition temperature is proportional to $ln\frac{1}{\sqrt{d}}$[54]. This is related to crack initiation at dislocation pile-ups as discussed in Section 2.2.2. Smaller grain sizes lead to fewer dislocation pile-ups, ultimately reducing the local stress concentration. Grain size refinement does not only increase the yield strength, but also σ_f. A decrease in grain size implies an increase in grain boundary area, which leads to smaller grain boundary carbides and thus higher σ_f[5]. In fine-grained steels, the critical event for cleavage initiation may be the propagation of a microcrack across the first grain boundary it encounters. In such cases, Equation 2.18 is updated to Equation 2.19, originally proposed by Griffith. In Equation 2.19, γ_{gb} is the plastic work per unit area required to propagate into adjacent grains and d is the average grain diameter[5].

$$\sigma_f = \sqrt{\frac{\pi E \gamma_{gb}}{(1-\nu^2)d}} \qquad (2.19)$$

Yield stress decreases with increasing temperature. This is due to the temperature dependency of dislocation velocity in a material. With decreasing temperature, initial dislocation propagation travel with increased velocity[12][43]. This will ultimately increase the probability dislocation coalescence, which, as discussed in Section 2.2.2, may lead to the formation of a crack nucleus.

2.5.2   Ductile Fracture

Ductile fracture is defined as failure occurring with a certain degree of measurable plastic deformation. From the micro-mechanism point of view, ductile failure in metals is often linked to ductile crack growth which is the result of nucleation, growth and coalescence of microvoids. When the voids coalesce in an unstable manner, the material will fail by tearing instability (rapid ductile crack growth) or plastic collapse (all over structural instability)[5]. Ductile fracture is also a process of breaking atomic bonds. Ductile failure always involves void or crack coalescence at some level. There are, however, situations where failure is essentially coalescence controlled and situation where macroscopic plastic instability governs. In notched or precracked specimen, failure by coalescence is dominating.

The material is said to be in a damaged state when the mechanisms of void growth, dis-

tortion and coalescence operate. This pertains to both initially crack-free specimen as well as in front of a crack tip. As the individual mechanisms proceed, damage accumulates until either a crack initiates, a pre-existing crack propagates or plastic instability occurs. An important, generally neglected aspect of ductile failure is failure without considerable void growth. It is likely that for high strength steels, failure is governed by linkage of crack-like voids. This mechanism is not picked up by computational micro-mechanical models, and poses challenges for analytic modelling[3].

The process of void nucleation, growth and coalescence is shown in Figure 2.7. For nucleation and growth, plastic deformation is homogeneous throughout the material matrix, whereas it localizes at the onset of coalescence. In the following sub chapters each individual mechanism is described in detail.

Figure 2.7: a) Void nucleation, b) strain localized between voids after growth, c) intervoid necking, d) void coalescence. Adapted from [5].

2.5.2.1   Void Nucleation

C.F. Tipper[72] established that metals fracture prematurely due to void formation at second-phase particles in the matrix. Goods and Brown[28] reviewed the phenomenon and addressed both homogeneous and heterogeneous void nucleation. Under certain conditions voids may form homogeneously in the material matrix. In regions with high dislocation density and high strain, cavities may form by vacancy condensation. This idea was challenged by Balluffi et al.[10], who showed that the vacancy concentration generated during deformation would never reach a high enough value to nucleate cavities homogeneously without the presence of a cavity nuclei of a reasonable size. Homogeneous void nucleation may happen in regions of high dislocation density in front of a growing crack. The material has lost its ability to work harden, and in conjunction with the stress triaxiality at the crack tip, localized deformation happens. As the crack grows and new surface area is formed, plastic relaxation occurs allowing dislocations running into the crack to open into cavities[28]. In locations with high dislocation density, pinned or immobile dislocations may act as barriers for gliding dislocations. The dislocations may pass these obstacles by climbing, inducing a net flow of vacancy diffusion towards itself ultimately resulting in cavity nucleation.

Under heterogeneous nucleation, second-phase particles and grain boundaries play an important role. First it is important to distinguish between the mechanism and the mode of cavitation. The mechanism defines the micromechanics of material transport resulting in a

cavity, i.e. diffusion or plasticity. The mode defines the driving force of the transport, either grain boundary sliding or growth in the bulk of the grain under remote stresses. The role of grain boundaries has been thoroughly investigated[13][18][42][59]. At intermediate temperatures and lower strain rates, the primary mode of deformation is grain boundary sliding. The nucleation of cavities is independent of temperature during sliding, indicating that it is the matrix displacement rather than the vacancy production and diffusion that determines nucleation[28]. If the grain boundary sliding meets an obstacle, this can be modelled as a dislocation pile-up. Gifkins[26] proposed a nucleation model that combined grain boundary sliding and bulk deformation. If a blocked slip band stops dislocations at a grain boundary, high tensile stresses may form due to sliding of the grain boundary. The boundary may separate enabling the dislocations within the slip band to run into the cavity nucleus, resulting in a stable cavity.

Second phase particles are viewed as the most important factor concerning ductile rupture. Lindley et.al.[69] demonstrated that it was not the magnitude of applied stress that determines the cavity initiation, but the local deformation state at the interaction between the particle and matrix. There are two mechanism for void nucleation, decohesion between the particle and the material matrix or cracking of the particle as presented in Section 2.1.2. Equiaxed particles generally suffer decohesion while irregularly shaped particles fail by internal fracture[28].

2.5.2.2   Void Growth

Rice and Tracey[61] proposed a void enlargement law of an isolated void in a perfectly plastic matrix. Equation 2.20 shows the law, where α is a numerical factor, $\overline{r}$ is the void radius given by $r_1+r_2+r_3/3$, r_0 is the initial void radius, σ_h is the hydrostatic stress, σ_e is the effective (von Mises) stress and ϵ_{eq} is the equivalent (von Mises) strain. Becker et al.[57] later studied void growth in sintered iron, motivating important choices in micro-mechanical parameters entering the Gurson model.

$$ln\left(\frac{\overline{r}}{r_0}\right) = \alpha \int_0^{\epsilon_{eq}} exp\left(\frac{1.5\sigma_h}{\sigma_e}\right) d\epsilon_{eq}^p \tag{2.20}$$

More recently, the growth of artificially inserted voids has been studied through tomography. Under uniaxial tension, voids concentrate stress and initially elongate at roughly twice the speed of the specimen. The voids also grow laterally at a speed commensurate with the increase in stress triaxiality. At a ratio of lateral void-diameter to void-spacing of about one third, the kinetics of growth change drastically due to localization of plastic flow in the ligaments. This has been further studied by Pardoen et al.[52], Koss et al.[17], and Bezerga et al.[1]. The common finding was that the onset of a macroscopic crack in a notched specimen was at a porosity level of about 0.01. This is quite large considering a typical initial void volume fraction of about 10^{-4} for structural metals and mean void enlargement ratios in excess of 4-5[3].

An important aspect for engineering alloys is to consider the possibility of coexistence of continuous void nucleation and void growth. Structural material usually contain several nucleation sites that may initiate at different times. Situations where nucleation occurs at separate scales pose serious challenges for modelling void nucleation, growth and coalescence within conventional continuum mechanics.

2.5.2.3 Void Coalescence

There are several modes of void coalescence depending on the plastic flow characteristics and microstructure of the material as well as the loading condition. The physics of coalescence has long been obscure, and while some aspects are still unclear, the phenomenon has been documented through empirical observations[3]. There are three commonly observed coalescence modes, internal necking of the void ligaments, void sheeting, and necklace coalescence.

Void impingement, described by internal necking of the void ligaments what hypothesized by Cottrell[21] and later rationalized by Thomason[70]. After an amount of void growth, the intervoid matrix will loose its load bearing capacity. Deformation will localize in these areas, ultimately resulting in necking of the matrix between voids. As the material fails, the voids link together and form a crack. Internal shearing of the void ligaments may cause distant cavities to coalesce due to localized shearing. The result is local failure by void sheeting where voids nucleate and develop in narrow bands of secondary voids[22]. Primary voids nucleate from second phase particles, and grow as the material is plastically deformed. At higher levels of stress/strain, smaller particles will nucleate secondary voids. Voids from the larger particles will link together with the smaller, secondary voids, and the material path between the two void distributions will look like sheets, hence the name void sheeting[47]. Necklace coalescence happens when voids link together along their length. This is thought to be favourable to ductility, although it could result in delamination[56].

2.5.2.4 Ductile Crack Growth

After a microcrack has been formed, a plastic zone develops at the crack tip and the tip blunts. As described in Section 2.7.1, large normal stresses develop at the crack tip favouring nucleation of voids at second phase particles. The size of the highly stressed zone, hence the opening of the crack, must be large enough to encompass void nucleation sites. A zone of high stress triaxiality concurrently develops at a distance roughly equal to the crack tip opening where plastic strains become large. This region favours void growth. When the voids get large enough and the distance from the crack tip small enough, plastic localization, i.e. necking, occurs and a coalescence mechanism joins the crack tip and the adjacent void, similar to the mechanism between two voids[3]. Depending on the initial volume fraction of voids in the material, as well as their size and the strain hardening capacity of the material in question, four different coalescence scenarios are distinguished based on experimental and

numerical studies. They are all shown in Figure 2.8.

Multiple void interaction mechanism happens at sufficiently high porosity. The voids are closely spaced and grow at roughly the same rate. The voids interact with each other, including the ones farther from the crack tip, resulting in higher growth rate for voids. Coalescence between several voids and the crack tip starts simultaneously generating multiple void coalescence[75].

Void by void coalescence mechanism is the most common mechanism for metallic alloys. These alloys tend to have initial void volume fractions smaller than 10^{-2}, meaning that the voids do not interact. The void nearest the crack tip grows alone before coalescing with the crack tip. As the crack grows, the voids are one by one absorbed[60].

Shear coalescence in the fracture process zone yield a void by void coalescence process in a zig-zag pattern at the crack tip in low hardening steels[19][44][49]. This is detrimental to the fracture toughness as shear localization involves less plastic work than a full void growth/coalescence mechanism.

Diffuse damage zone describes scenarios that do not fit with the three previous mechanisms. If the fracture process zone at the crack tip contains a large amount of very small voids, these may be viewed as a damage volume element inside a specimen, rather than adjacent to a crack tip. The first coalescence may not occur with the crack tip, but rather in the damage volume. Some metals could exhibit a diffuse damage zone mechanism at crack initiation and transition into one of the other three mechanism during crack propagation. This is associated with the change of crack tip stress and strain fields, which has important consequences for the ductile-to-brittle transition[3].

Figure 2.8: a) multiple void interaction, b) void by void coalescence, c) zig-zag void by void coalescence, d) diffuse damage zone.

2.5.3   Fracture in CGHAZ

Several studies on the fracture surface of a CGHAZ specimen have been performed in the recent years, especially concerning fracture mechanisms and the effect of temperature. J.H. Chen et al. published a paper in 1984[41] studying the fracture surface and crack appearance in a weld simulated steel at room temperature and at the temperature of liquid nitrogen

($-196°C$). They concluded that there are two different patterns of fracture induced by the M-A constituents in the CGHAZ: rupture (ductile crack growth) and cleavage (brittle fracture).

At room temperature, the studied fracture surface showed that the majority of cracks nucleated at the boundaries between the M-A constituents and the ferrite matrix. The ferrite matrix will yield easily at this temperature, but the M-A constituents are hard and unductile, and will not deform. This creates an amplification of stress in the matrix causing large amounts of strain, which will result in breaking of the M-A constituent or debonding, inducing microcracks in the matrix. The damage mechanism leading to crack initiation (shearing of the M-A particle vs decohesion) is dependent on local stress and strain rate[2]. Due to heavy strain and deformation of ferrite, the microcracks grow to voids during deformation. With further deformation, the main crack is formed and propagated by coalescence of voids due to internal necking, ultimately leading to rupture of the specimen. The studied fracture surface showed that slip bands, localized bands of plastic deformation, stopped in front of M-A constituents, and deep hole dimples formed by coalescence of several smaller holes[41].

At the temperature of liquid nitrogen, the fracture surfaces showed clear signs of cleavage, with river patterns indicating re-initiation of the crack at grain boundaries. The cleavage fracture facet at the origin of fracture showed that all streaks pointed to a M-A constituent, making it obvious that cleavage fracture was induced by the constituent. The M-A constituents have two effects on the stress distribution in the matrix: it will create a stress amplification and form a triaxial stress state ahead of itself. This is further discussed in Section 2.7.1. Since the ferrite will not deform easily at this temperature, it will not be able to relieve the stresses and will therefore cleave. When the crack is formed, it will push the stress concentration ahead, inducing new microcracks that will link to the main crack eventually resulting in a brittle cleavage fracture[41]. P. Mosheni et al.[51] found that cleavage cracks may also be initiated in the matrix between two M-A constituents due to residual phase transformation stresses and overlapping stress concentrations.

J.H. Chen et al.'s study was later supported by S. Lee et al.[63] and A. Lambert-Perlade et al.[2]. S. Lee et al. tested specimen at $-80°C$, and observed that the crack propagated as a number of microcracks connected in a zig-zag pattern, rather than by the connection of voids. As the M-A constituents are brittle, they will break and form a crack that acts as so-called Griffith crack when external stresses are applied, meaning that they will cleave at a certain threshold stress level. The paper also showed that the void nucleation strain in the CGHAZ is very low due to the premature void nucleation or brittle fracture at M-A constituents, confirming their role in the degradation of the CGHAZ[63].

The paper by A. Lambert-Perlade et al. supported the findings that the fracture surface depends on temperature. The number of cracking events before final fracture increases with test temperature. For higher temperatures, stable ductile crack propagation preceded final fracture.

Figure 2.9: Ductile to brittle transition with temperature. From [5].

2.6   The Ductile to Brittle Transition

From previous sections it is obvious that the fracture mode of a material is temperature dependent. The studies presented in Section 2.5.3 show that low temperatures correspond to cleavage fracture, whereas the material behaves in a ductile manner at higher temperatures. It has been established that steel undergoes a ductile-to-brittle transition over a temperature range, corresponding to increased material toughness with rising temperature[5][16][54]. The temperature where the transition happens is called the ductile-to-brittle transition temperature, shown in Figure 2.9. At sufficiently low temperatures, the material is brittle and will exhibit low fracture toughness values. These values gradually increase as the behaviour of steel shifts towards ductile. At high enough temperatures, the steel is completely ductile and will have a high fracture toughness. At intermediate temperatures, however, a transition regime exits. Both brittle and ductile fracture modes are present. Any factor contributing to embrittlement of the steel, such as M-A constituents, prohibited plastic flow, flaws or cracks, will raise the ductile-to-brittle transition temperature, which is problematic for service in Arctic climates.

To account for all variables in a brittle fracture, Cottrell reformulated Equation 2.3 to Equation 2.21. The derivation is shown in Appendix A.2. Equation 2.21 can be seen as as summary of the ductile-to-brittle transition where σ_i is the resistance to dislocation movement, k_y and k_s express the grain boundary condition to strength, G is the shear modulus, and β expresses the overall ratio of shear to normal stress; for a notch, $\beta \approx 1/3$. k_y and k_s are related through $k_y = mk_s$, where m expresses the average normal-to-shear stress ratio in the slip plane[25][45].

$$(\sigma_i d^{1/2} + k_y)k_s \geq G\beta\gamma_s \tag{2.21}$$

If the left side of Equation 2.21 is larger than the right side, a microcrack may form, but not grow[25], and the material will fail by cleavage when the local stresses reach a critical value. The temperature dependency of the parameters in Equation 2.21 is indicative of a transition temperature from ductile to brittle fracture. Any factor that increases σ_i, k_y or d, or decreases γ_s will increase the material's tendency for brittle failure. Hence, the transition temperature is dependent on grain size, the resistance to propagation of slip, the surface energy and the stress triaxiality, given by β[45].

As σ_i is proportional to the yield strength, shown in Equation 2.4, a high value of frictional resistance will lead to brittle fracture since high stresses must be reached before yielding occurs[25]. The transition temperature's dependency on the frictional stress may be expressed through the temperature dependency of plastic deformation and flow. As the yield strength of a material increases with decreasing temperature, the stresses required for plastic deformation are higher at lower temperatures[55]. The contribution from plastic deformation will depend on the number of available slip systems and the number of mobile dislocations at the tip of the crack [25]. Von Mises' criterion for plasticity in a metal states that at least five independent slip systems are necessary for a polycrystal to undergo a homogeneous deformation[78]. This has to some extent been applied to explain low temperature brittle characteristics when the number of slip systems is restricted. Brittleness may, however, be encountered in polycrystals that fulfill Von Mises criterion due to barriers of plastic flow, such as grain boundaries, M-A constituents and microcracks, especially when dislocation mobility is constrained[73].

Since fracture is defined as the separation of a solid, the fracture surface energy, γ, should be investigated. For cleavage fracture, where crack nucleation is the critical step, the appropriate value of γ is the true elastic surface energy, γ_s[45]. If crack propagation is the critical step, as for ductile fracture, an effective surface energy, γ_e, must be considered. Gilman[27] proposed $\gamma_e = \gamma_s \rho / a_0$, where ρ is the crack tip radius and a_0 is the equilibrium atomic spacing. If plastic deformation is restricted by low temperatures, and blunting cannot occur, ρ will be small, reducing γ_e. The right side of Equation 2.21 will decrease and the material will be more susceptible for brittle failure as the temperature declines.

Both ductile and brittle fracture mechanisms initiate through the presence of microcracks or other defects in the material, which nucleate as a result of plastically induced stress or strain concentrations. The distinction between the modes must be the manner in which the crack propagates[54]. Ductile crack growth is dependent on plastic strain in the intervoid matrix which is only possible with unrestricted plastic flow. The nature and distribution of plastic flow and slip in the material is expected to have major influence on the stress or strain at fracture. Susceptibility to cleavage fracture is generally enhanced by almost any factor that increases the yield strength, such as low temperature, strain rate and a triaxial stress state[5]. The underlying mechanism of the temperature dependence of toughness can evidently not be separated from the mechanisms of plastic flow. At the macro scale, this affects energy dissipation before fracture, i.e. the fracture toughness. At the micro scale, the flow stress de-

pendency of temperature might affect conditions for void nucleation[28] as well as the rate of growth and coalescence[47].

2.7 Fracture Mechanics

The occurrence of brittle fracture of normally ductile materials demonstrated the need for better understanding of the mechanisms of fracture. This lead to the evolution of the field fracture mechanics, which quantifies the relationship between material properties, stress levels, flaw sizes and shapes, and crack propagation mechanisms. This section is dedicated to some fundamental principles of the mechanics of fracture.

2.7.1 The Amplified Stress Field

The measured fracture strength for most materials is significantly lower than the one derived from theoretical calculations of atomic bonding energies. This inconsistency is based in the presence of microscopic flaws or cracks present in all solid materials. As mentioned in Section 2.1.2, the flaws produce an amplified or concentrated stress field at their interface with the material matrix, making them detriment to the fracture strength. This is demonstrated in Figure 2.10, which shows a stress profile over a cross section containing an internal crack of length $2a$. Figure 2.10 shows that the magnitude of the localized stresses decrease with distance from the crack. At far removed positions, the stress is the applied stress σ_{app}.

Figure 2.10: Schematic stress profile demonstrating the stress amplification at the crack tip.

The amplification of the local stress is dependent on the orientation and geometry of the crack. For some configurations it is possible to derive expressions for the local stresses in the material. Irwin [37], Sneddon [66], Westergaard [81] and Williams [82] were among the first to publish such solutions. In a polar coordinate system with the origin at the crack tip, the local stress field in any linear elastic cracked body is given by Equation 2.22, where σ_{ij} is the stress tensor, k is a constant, f_{ij} is a dimensionless function of θ for the leading term, A_m is the amplitude and g_{ij}^m is a dimension function of θ in the m-th term[5].

$$\sigma_{ij} = \left(\frac{k}{\sqrt{r}}\right) f_{ij}(\theta) + \sum_{m=0}^{\infty} A_m r^{\frac{m}{2}} g_{ij}^m(\theta) \tag{2.22}$$

Equation 2.22 shows that the solution for any given configuration contains a leading term proportional to $1/\sqrt{r}$, which approaches ∞ as r approaches zero. This is a description of the stress singularity in front of the crack tip. An issue with the local stress asymptote at $r = 0$ is that the material should in theory fracture for any applied load as the local stresses near the crack tip far exceed the critical fracture stress. This is, obviously, not the case, and needs to be treated, as described in Section 2.7.2.

2.7.2 The Stress Intensity Factor

The stress intensity factor K, often denoted with the mode of loading, i.e. K_I, K_{II} or K_{III}, is a scaling factor that relates the $1/\sqrt{r}$-singularity to the mode of loading. It is convenient to replace k in Equation 2.22 with the stress intensity factor given by Equation 2.23, which allows for updating Equation 2.22 to Equation 2.24 for all modes.

$$K_I = k\sqrt{2\pi} \tag{2.23}$$

$$\lim_{r \to 0} \sigma_{ij}^{(I)} = \frac{K_I}{\sqrt{2\pi r}} f_{ij}^{(I)}(\theta) \tag{2.24}$$

The stress intensity factor is essentially a description of the amplitude of the crack-tip singularity. In other words, the stresses and strains near the crack tip are proportional to K_I[5]. Thus, K_I can be viewed as a scaling factor. Another important characteristic of K_I is that it defines the crack tip conditions. This means that if K_I is known, it is possible to solve all components of stress, strain and displacement as functions of r and θ. This has made K_I one of the most important concepts in fracture mechanics.

K_I can be related to the applied load and specimen dimensions through Equation 2.25, where F is the load, B is the depth of the specimen and W is the width. $f\left(\frac{a}{W}\right)$ is a dimensionless constant that depends of the geometry and mode of loading. For a singe-edge notched bend test, as described in Section 2.8.2, $f\left(\frac{a}{W}\right)$ is given by Equation 2.26, where S is the distance between the applied loads[8].

$$K_I = \frac{F}{B\sqrt{W}} f\left(\frac{a}{W}\right) \tag{2.25}$$

$$f\left(\frac{a}{W}\right) = \frac{3\frac{S}{W}\sqrt{\frac{a}{W}}}{2\left(1 + 2\frac{a}{W}\right)\left(1 - \frac{a}{W}\right)^{3/2}} \left[1.99 - \frac{a}{W}\left(1 - \frac{a}{W}\right)\left\{2.15 - 3.93\left(\frac{a}{W}\right) + 2.7\left(\frac{a}{W}\right)^2\right\}\right] \tag{2.26}$$

The effect of cracks and flaws is more extensive in brittle than in ductile materials. Plastic deformation will ensue when the maximum stress exceeds the yield strength in a ductile

material. Consequently, the stress distribution will be more uniform in the vicinity of the crack or flaw, and the fracture strength goes down. Yielding and stress redistribution does not happen in brittle materials.

Using principles of fracture mechanics, it is possible to show that the critical stress, σ_c, required for crack propagation in a brittle material is described by Equation 2.27, where E is the Young's Modulus, γ_s is the specific surface energy and a is one-half the length of an internal crack[16]. This equation is similar to Equations 2.18 and 2.19.

$$\sigma_c = \sqrt{\frac{2E\gamma_s}{\pi a}} \tag{2.27}$$

To relate the critical fracture stress the fracture toughness of the material, the critical stress intensity factor can be used. K_{Ic} shows the material's resistance to brittle fracture when a crack is present[5][16]. K_{Ic} is given by Equation 2.28 where a_c is the critical crack length and σ_c is the critical remote stress[5].

$$K_{Ic} = \sigma_c \sqrt{\pi a_c} \tag{2.28}$$

The fracture toughness of a material describes the ability to resist brittle fracture. Brittle materials do not have appreciable plastic deformation in front of an advancing crack, and are thus vulnerable to cleavage. These material have low K_{Ic}-values, while ductile materials have high fracture toughness values[32]. The basis for the derivation of K_{Ic} is Equation 2.22 which accounts for stresses in a linear elastic material. Consequently, K_{Ic} is not a valid fracture toughness parameter for materials that exhibit ductile behaviour. They are in the range of elastic-plastic fracture mechanics, and need other parameters to the describe fracture toughness.

2.7.3   CTOD and CMOD

The crack-tip opening displacement, CTOD, was first defined by Wells[79][80]. Wells discovered that the fracture surfaces of a fracture test specimen moved apart prior to fracture as a result of plastic deformation and blunting at the crack tip. This is shown in Figure 2.11. The degree of blunting is proportional to the fracture toughness of the material, and can thus be used as a fracture toughness parameter. Since the CTOD accounts for plastic crack-tip conditions, it is a valid elastic-plastic fracture mechanics parameter.

The CTOD relates to the stress intensity factor, K_I, through Equation 2.29, where m is a dimensionless constant equal to 1 for plane stress and 2 for plane strain, σ_{ys} is the yield stress and E' is the plane stress or plane strain-dependent Young's Modulus of the material. For plane stress conditions, $E' = E$, but for plane strain, E' is given by Equation 2.30, where v is the Poisson's ratio, which relates axial and transversal strains in the material.

$$CTOD = \frac{K_I^2}{m\sigma_{ys}E'} \tag{2.29}$$

Figure 2.11: Displacement and blunting of the crack tip.

Figure 2.12: Hinge model for notched three-point bend specimen.

$$E' = \frac{E}{1 - v^2} \tag{2.30}$$

For macro-sized specimen it is common practice to determine CTOD from measurements of the crack-mouth opening displacement, CMOD. The calculation of CTOD is based on a hinge model of a three-point bend specimen. The specimen is assumed to be divided into two parts, divided by the notch, and rotate about a hinge point, shown in Figure 2.12. This method is known from both literature and standards[5][36].

CTOD can be calculated from Equation 2.31, where the two components are displayed in Equation 2.32. The first term of Equation 2.32 is the elastic part and relates to elastic fracture toughness K_I. The second term is the plastic term, and uses specimen dimensions presented in Figure 2.12, where z is the distance of knife edge measurement point from the notched edge on the specimen, in this thesis equal to 0, and r_p is a rotational factor assumed to be 0.4.

$$CTOD = CTOD_{elastic} + CTOD_{plastic} \tag{2.31}$$

$$CTOD = \frac{K_I^2 (1 - v^2)}{2\sigma_{ys}E} + \frac{r_p (W - a_0) CMOD}{r_p W + 0.6a_0 + z} \tag{2.32}$$

2.7.4   Crack-Tip Constraint

Constraint may be viewed as a material's inhibition to plastic flow. As explained in Section 2.7.1, stresses and strains are increased in the presence of a crack tip. This causes high strain gradients to develop in the local region. The highly strained region is constrained by the surrounding material, which causes triaxial stress states that in turn complicates stress analyses, as well as influences crack growth and fracture behaviour. The triaxiality of stresses at the crack tip will to a lesser extent be dissipated through plastic flow, and therefore be available to enhance material degradation. This elevates local stress, making it easier for the material to reach its critical fracture stress[4][39][40]. To quantify this restrain on plastic flow in a flawed material, the ratio of the actual load at plastic collapse for a flawed structure over the ideal plastic load limit of an unflawed material body, is frequently used.

Constraint level is greatly dependent on factors such as specimen geometry, crack location relative to external boundaries, material thickness, type and magnitude of applied load and stress-strain properties of the material[40]. Deeper notched specimen have more crack tip constraint than specimen with longer ligaments. Growing cracks, which is a result of plasticity, influence constraint by shortening the crack ligament. The plastic zone at the crack-tip will at higher deformation levels merge with the global plasticity in the specimen, ultimately causing a significant loss of constraint. The stress-strain properties influence constraint through the plastic zone at the crack tip. For a given applied stress, this zone will be larger for a lower strength material, which will result in constraint relaxation[4][39].

Constraint is obviously not a material parameter, but greatly dependent on many outside factors. The purpose of studying this is to find appropriate methods to characterize crack-tip stress-strain fields in a specimen so that the fracture toughness results can be transferred between geometries, crack sizes and types, and loading conditions[38]. The transferability of material toughness is a key issue in the field of fracture mechanics when it comes to assess structural integrity of components.

2.8   Testing

In order to determine characteristic material parameters as well as fracture mechanics parameters, material testing is necessary. In the following section two important test methods and their applications are described: the tensile test and the stress-strain curve, and the fracture toughness test and the R-curve.

2.8.1   Tensile Testing

Tensile tests are designed to obtain specific material parameters, such as σ_{ys}, σ_{UTS} and E. This is done by subjecting a tensile specimen, as shown in Figure 2.13, to controlled uniaxial tension until failure. During testing, the specimen is fastened in the shoulders and slowly extended until fracture. An extensometer is fastened to the gage to measure its elongation. The

stress-strain curve can be obtained from the applied tensile force and the increase in gage length, both normalized with respect to the specimen dimensions, as descibed by equations in Section 2.3.2. The benefit of plotting stress and strain rather than load and elongation is that the curve will give material characteristics independent of specimen dimensions.

A typical tensile test specimen is shown in Figure 2.13. The shoulders are enlarged for gripping, and the gage section is reduced relative to the remainder of the specimen in order to ensure that deformation and failure will be localized in this region. The size limit given to the transformation area, x, is to ensure that this section does not constrain the deformation in the gage area.

The stress-strain curve is discussed in Section 2.3.

Figure 2.13: A tensile test specimen

2.8.2 Fracture Toughness Testing

A fracture toughness test is designed to measure the crack growth resistance in a material. There are five types of specimens permitted in the ASTM E-1820 standard[8], one of which is the single-edge-notched bend (SENB) specimen used in this thesis and shown in Figure 2.14. The specimen is made from a rolled plate. As engineering steels seldom are homogeneous, the rolling direction has influence on the result. Some directions may for instance require less energy for crack propagation than others, and keeping track of this is important for accurate fracture toughness testing. When the specimen has been cut with the right dimensions from the rolled plate, a notch is machined in the specimen edge. From the notch a fatigue precrack has to be made. These cracks are produced through cyclic loading of the specimen. The cyclic loading produces a crack with a small crack tip radius and a small plastic zone at the tip. The crack will thus not influence the material properties and the fracture toughness test will be accurate.

Figure 2.14: A single-edge-notched bend specimen. From [5]

The data extracted from the SENB tests for this thesis is the force-CMOD curves. The force is relatively easy to extract as most set-ups are equipped with load cells. The elongation, CMOD, is measured through a clip. The clip attaches to the mouth of the crack through its cantilever beams which are equipped with strain gages that measure an applied voltage. Deflection of the beams results in change in the voltages which can be related to the opening of the crack mouth. The output is the force-CMOD curve for the material in question, from which material toughness parameters, such as K_I or CTOD, can be calculated. Determining the crack extension can be done by cracking open the specimen and examining the fracture surface in an optical microscope. From these values, the material's fracture resistance curve can be plotted.

2.8.2.1   R-curves

A method to illustrate stable and unstable crack growth is through a fracture resistance curve, also called R-curve. These are made with crack extension after initiation Δa on the x-axis and a fracture toughness parameter such as K_I, $CTOD$ or J on the y-axis. The R-curve illustrates the manner of crack growth as well as the materials resistance to further crack growth, and implies that a material's fracture toughness may change with crack extension.

The shape of the R-curve is dependent on material behaviour. A brittle material will have a flat R-curve, the materials resistance is constant with crack growth. When the stresses in the material reach a critical value corresponding to a critical value of K_I, $CTOD$ or J, rapid, unstable crack growth will initiate, ultimately resulting in fracture.

When ductile behaviour is involved, however, the shape of the R-curve differs. Growth and coalescence of microvoids, which accounts for ductile crack growth, is associated with a rising R-curve[5]. This is due to the change in size of the plastic zone at the crack tip. It increases as the crack extends, making each successive increment of crack extension require more energy than the preceding increment in order to drive the crack farther. The result is that the fracture resistance curve of a ductile material increases with increasing crack growth[5][65]. An example of an R-curve is shown in Figure 2.15.

As shown in Figure 2.15, the fracture resistance curve gives a complete description of the fracture behaviour of a material. The material will start with a small amount of crack growth due to blunting. In this region the R-curve is nearly vertical. At the onset of stable crack growth, indicated through the initiation toughness, $CTOD_C$, in Figure 2.15, the material at the crack tip will fail locally and the crack will grow. Finally, a steady-state is reached. The fields around the crack tip will move congruently along the crack ligament at constant remote loading. This is denoted $CTOD_C^{SS}$ in Figure 2.15. The slope of the R-curve at a given amount of crack growth after initiation indicates the stability of the growth. A steep R-curve is indicative of stable crack growth in the material as energy is increasingly required in order to maintain crack growth[5][65]. Another configuration that may occur is when the crack growth resistance decreases locally. The load does not follow the decreasing $CTOD_R$ and the crack propagates in this range until it arrests again. This is according to ASTM E-1290

Figure 2.15: An example of an R-curve. Adapted from [34].

termed as a pop-in[9].

The R-curve of a material is greatly dependent on the geometry of the tested specimen. As mentioned in Section 2.7.4, different configurations give different constraint levels. The crack-tip process zone, which affects the fracture toughness, is reliant on the state of constraint that prevails in different geometries. Crack growth resistance decrease with increasing crack depth, i.e. shallow notched specimen that have low constraint levels will exhibit a steep R-curve after crack initiation[39].

For single-edge notched bend specimen, as described in Section 2.8.2, the region below the hinge point will have a compressive stress field. This tends to produce additional constraint, flattening the R-curve. For deep notched specimen, the hinge point is closer to the crack-tip, and the effect from the compressive field will be more prominent. As the crack grows and the ligament decreases, the compressive field approaches the crack-tip, increasing the constraint in the process zone[4]. SENB specimen will yield conservative fracture toughness values for the tested material.

3 | Material Models

This section describes the material models that constitute the basis for the simulations in the thesis work. There are two models used, the Gurson model which accounts for ductile crack growth through void nucleation, growth and coalescence, and the RKR-criterion which is a stress criterion for brittle fracture. The background and theory of both models are described here, while the implementation to the modelling scheme is given in Chapter 4.

3.1 The Gurson Model

Gurson attempted to develop a constitutive theory to describe the whole ductile fracture process[30]. He did, however, only manage to describe the first deformation phase of ductile fracture, the homogeneous deformation phase with void nucleation and growth. The proposed constitutive theory contains a yield criteria and a flow rule to incorporate the role of hydrostatic stress in yield and void growth. The theory also contains elements as void nucleation, hardening behaviour and a ductile fracture criterion.

The Gurson model builds on the work of Rice and Tracey(1969), who related the change in the shape of a void to stress triaxiality and plastic strain [61]. The Rice and Tracey model is based on a single spherical void in an infinite perfectly plastic medium, and is thus not able to take into account interaction between voids, nor predict ultimate failure. A separate failure criterion must be applied to characterize void coalescence. The Rice and Tracey model predicts failure when the void growth ratio has reached a critical value assumed to be a material parameter[5]. Since the Rice and Tracey model is applied as a post-processing calculation, there is no coupling between plasticity and damage.

Gurson's model accounts for the coupling between plasticity and damage. This was done through the analysis of plastic flow in a porous medium assuming continuum behavior. The effect of the voids is averaged throughout the material, and their presence is accounted for through their influence on the global flow behavior. Gurson presented a yield function that reflected the softening effect of the voids[30].

The original Gurson yield surface had the issue of only being able to predict complete loss of load carrying capacity when the void volume fraction had reached 100%. This ultimate value corresponds to the complete disappearance of material, which is impossible. The yield function was later modified by Tvergaard [74] to avoid the issue of complete material loss. The modified yield function is presented in Equation 3.1.

$$\Phi(q, \overline{\sigma}, f) = \frac{\sigma_{VM}^2}{\overline{\sigma}^2} + 2 \cdot q_1 \cdot f \cdot cosh\left(\frac{3q_2\sigma_m}{2\overline{\sigma}}\right) - 1 - (q_1 \cdot f)^2 = 0 \tag{3.1}$$

In Equation 3.1, f is the current void volume fraction, q_1 and q_2 are constants introduced

Figure 3.1: The cluster nucleation model and the characteristic parameter f_0. From [89]

by Tvergaard, with values of 1.5 and 1, respectively [74], σ_m is the mean normal stress, σ_{VM} is the von Mises stress, and $\overline{\sigma}$ is the flow stress of the matrix material. Setting the void volume fraction, f, to zero, gives the conventional von Mises yield model. The term $\frac{\sigma_m}{\sigma_{VM}}$ accounts for the stress triaxiality as discussed in Section 2.4.2

Since the Gurson model uses a yield function dependent on the void volume fraction in the material, both void nucleation and growth are essential parameters. Void nucleation may be stress or strain controlled. Of these two, strain controlled is preferred as it is easier to handle in the finite element implementation of the Gurson model. The mathematical presentation of strain controlled nucleation is shown in Equation 3.2, where f_ϵ is the void nucleation intensity, and $\overline{\epsilon}^p$ is the equivalent plastic strain.

$$\mathrm{d}f_{nucleation} = f_\epsilon \cdot (\overline{\epsilon}^p)\, \mathrm{d}\overline{\epsilon}^p \tag{3.2}$$

Three different models for nucleation exist. In this thesis, the cluster nucleation model has been used and is thus the only one described. For further reading on the other nucleation models see e.g. [86] or [89]. For the cluster nucleation model, the assumption is that all voids are nucleated at the beginning of plastic deformation. The corresponding parameter is called initial void volume fraction, f_0, and is shown in Figure 3.1.

For void growth in the Gurson model, a homogenization process is used [5][86]. This means that the volume fraction of voids for each load increment will be summed and homogenized as one single void before the next load increment, as shown in Figure 3.2. Because of incompressibility of the matrix material and the requirement of a volume preserving plastic flow of the matrix material, the growth rate of existing voids can be described through Equation 3.3 where ϵ^p is the plastic strain tensor and **I** is the second-order unit tensor, otherwise known as the Kronecker delta, δ_{ij}.

$$\mathrm{d}f_{growth} = (1 - f)\, \mathrm{d}\epsilon^p : \mathbf{I} \tag{3.3}$$

The Gurson model cannot in itself predict void coalescence. However, Tvergaard and Needleman[76] introduced a modification to the yield function in Equation 3.1 that accounts for final material failure. This modification is in Equation 3.4, where f_F is the void volume fraction at final fracture and $f_u^* = 1/q_1$.

Figure 3.2: Homogenization of voids.

$$f^* = \begin{cases} f & \text{for } f \leq f_c \\ f_c - \frac{f_u^* - f_c}{f_F - f_c} & \text{for } f > f_c \end{cases} \tag{3.4}$$

Equation 3.4 implies that before coalescence, both the void volume fraction and the decrease of load carrying capacity follow the Gurson model without adjustment. However, when a critical void volume fraction, f_c, has been reached, the Gurson model assumes coalescence through an artificially accelerated void growth, f^*, after which the load carrying capacity drops rapidly. The void volume fraction at final failure, f_F implies that the load carrying capacity has vanished, and can be calculated from $f_F = 0.15 + 2 f_0$[89].

3.1.1   Thomason's Plastic Limit Load Model

The Gurson model is able to simulate void nucleation and growth as well as the post-coalescence response of the material. It is, however, not able to predict the coalescence itself. As discussed in Section 2.5.2, ductile crack growth and fracture consists of two distinct phases, the homogeneous phase with void nucleation and growth and the localized phase with void coalescence. Thomason argued that the two deformation modes are in competition, and that the shift from the homogeneous deformation phase to the localized deformation phase could be described by a plastic limit load model[71]. The base of this model is that both deformation modes are dilatational, meaning that the plastic deformation results in change of the material volume. The prevailing deformation mode will be the one that at the moment requires less energy. The condition for shift of deformation mode is thus given by Equation 3.5.

$$\sigma_1^{homogeneous} = \sigma_1^{localized} \tag{3.5}$$

In Equation 3.5, $\sigma_1^{homogenous}$ corresponds to the applied maximum principal stress at the current yield surface. This value is independent of the void volume fraction. It is, however, important to note that the plastic limit load itself is dependent on the void geometry. For a material without voids, the plastic limit load is infinite [86]. When the void volume fraction is small $\sigma_1^{localized}$, which characterizes the localized deformation, is high, as shown in Figure 3.3. This means that the material will deform homogeneously throughout the matrix. As the voids grow, the capacity of the material to resist intervoid necking decreases until it reaches the plastic limit load where deformation localizes through intervoid necking, i.e. coalescence[71]. The deformation modes are shown in Figure 3.4.

Figure 3.3: Competiton of the two deformation models.

Figure 3.4: Homogeneous and localized deformation. From [88]

To define the plastic limit load stress, Thomason proposed an equation incorporating stress and strain dependent void evolution. For a 2D plane strain problem, the limit is given by Equation 3.6, where r is the void radius and R is the dimension of the artificial unit cell. These are given by Equations 3.7 and 3.8, respectively, and shown in Figure 3.4

$$\frac{\sigma_1}{\bar{\sigma}} < \frac{0.3}{r/R-r} + 0.6, \quad \text{no coalescence}$$

$$\frac{\sigma_1}{\bar{\sigma}} = \frac{0.3}{r/R-r} + 0.6, \quad \text{coalescence starts}$$

(3.6)

$$r = \sqrt{\frac{f}{\pi}} e^{\epsilon_{xx}+\epsilon_{zz}}$$

(3.7)

$$R = R_0 e^{\epsilon_{xx}}$$

(3.8)

In Equations 3.7 and 3.8, ϵ_{xx} and ϵ_{zz} are components of the strain tensor, R_0 is the initial value of R and f is the current void volume fraction. The equations are based on the coordinate system in Figure 3.4.

3.1.2   The Complete Gurson Model

The plastic limit-load model from Thomason's completed the Gurson model. The new failure criterion makes the Gurson model capture the complete ductile fracture process of void nucleation, growth and coalescence. An overview of the complete Gurson model, that contains both the adjustments from Tvergaard and the plastic limit load model by Thomason is presented below.

The homogeneous yield function by the Gurson model from which the maximum principal stress at a material point can be calculated.

$$\Phi(q, \overline{\sigma}, f) = \frac{\sigma_e^2}{\overline{\sigma}^2} + 2 q_1 f \cosh\left(\frac{3 q_2 \sigma_m}{2 \overline{\sigma}}\right) - 1 - (q_1 f)^2 = 0$$

Nucleation and growth of voids for the cluster nucleation model with parameter f_0.

$$\mathrm{d}f_{nucleation} = f_\epsilon\left(\overline{\epsilon}^p\right) \mathrm{d}\overline{\epsilon}^p$$

$$\mathrm{d}f_{growth} = (1 - f) \, \mathrm{d}\epsilon^p : \mathbf{I}$$

Void coalescence criterion from Thomason's limit load model for a 2D plane strain case.

$$\frac{\sigma_1}{\overline{\sigma}} < \frac{0.3}{r/R - r} + 0.6, \quad \text{no coalescence}$$

$$\frac{\sigma_1}{\overline{\sigma}} = \frac{0.3}{r/R - r} + 0.6, \quad \text{coalescence starts}$$

where $r = \sqrt{\frac{f}{\pi} e^{\epsilon_{xx} + \epsilon_{zz}}}$ and $R = R_0 e^{\epsilon_{xx}}$.

After coalescence, the material response is given by Tvergaard and Needleman's modification, where f_c is the material response at coalesence.

$$f^* = \begin{cases} f & \text{for} f \le f_c \\ f_c - \frac{f_u^* - f_c}{f_F - f_c} & \text{for} f > f_c \end{cases}$$

3.2   The RKR-Criterion

Ritchie, Knott and Rice(1973) introduced a simple model for cleavage failure by relating fracture stress to fracture toughness. In doing so, they also solved the singularity problem discussed in Section 2.5.1 and explained why steels do not spontaneously fracture upon the application of a minimal load. Their model is referred to as the RKR-criterion and suggests that cleavage failure will occur when the stresses ahead of the crack tip exceed a critical value, σ_f, over a characteristic distance, x_c.[5][62]

Since cleavage cracks propagate in an unstable manner when the local stresses ahead of the crack tip, σ_{yy}, exceeds the critical value, σ_f, using this as a failure criterion seems natural.

Figure 3.5: Fracture stress over a characteristic distance. Adapted from [5]

Ritchie, Knott and Rice related the macroscopic fracture toughness of a body containing a sharp pre-crack to the local fracture criterion. This was done by examining the temperature dependency of K_{Ic} in specimen where σ_f is known. The $\frac{1}{\sqrt{r}}$ dependency of K ensures that the cleavage stress level is exceeded locally at the crack tip before fracturing, making a size-scale criterion in addition to the value of σ_f crucial, as shown in Figure 3.5.

Ritchie, Knott and Rice found that for unstable crack growth to happen, the applied tensile stress must be sufficient to initiate a crack at a grain boundary as well as propagating it to the next grain boundary. In other words, σ_{yy} must exceed σ_f over at least one grain diameter[62].

Stresses ahead of a sharp crack intensify very close to the crack tip, and hence, crack initiation can occur at the first grain boundary that is roughly one grain diameter from the crack tip. For unstable fracture, σ_{yy} must exceed σ_f over at least another grain diameter. This makes the total characteristic distance approximately equal to two grain diameters. The characteristic distance can be regarded as the limiting value of x necessary for unstable crack growth.

4 | Computational Implementation

This chapter outlines the work conducted in the thesis. The material is presented along with the methods for implementing its properties into the finite element model, also presented here. The work flow along with the incorporation and determination of material model parameters are discussed.

4.1 Material

The material investigated in this work is a weld simulated CGHAZ $420MPa$ steel. SINTEF performed tensile tests of the steel to obtain the mechanical characteristics presented in Table 4.1 along with the chemical composition. The steel was weld simulated with a cooling rate of $\Delta t_{8/5} = 5$ seconds to achieve a coarse grained heat affected zone and tensile tests were performed at three temperatures: room temperature (21°C), 0°C and $-$60°C. The yield stress and ultimate tensile stress for these tests are shown in Table 4.2.

Table 4.1: Material characteristics and chemical composition.

Mechanical characteristics

Young's Modulus	Yield stress	UTS	Poisson's ratio
[GPa]	[MPa]	[MPa]	
208	450	549	0.3

Chemical composition $\left[\%wt\right]$

C	Si	Mn	Cu	Ni	CE
0.09	0.19	1.54	0.28	0.72	0.42

Table 4.2: Yield stress and UTS at different temperatures for the weld simulated steel.

Temperature	Yield stress	UTS	$\frac{\sigma_{ys}}{\sigma_{UTS}}$
	[MPa]	[MPa]	
21°C	667	889	0.7503
0°C	676	901	0.7503
$-$60°C	697	961	0.7253

4.1.1 Determining the Flow Curves

The plastic flow curves for the weld simulated steel was needed in the simulation. To obtain this, nominal stress-strain curves ($s = f(e)$) for all temperatures were found through tensile testing. These are presented in Figure 4.1. This data was implemented in Microsoft Excel and used to determine the input data for the simulations. Equations 2.8 and 2.9 were used to find

Figure 4.1: Engineering stress-strain for three temperatures.

Figure 4.2: True stress-strain for three temperatures.

true stress (σ) and true strain (ϵ), respectively. The true stress-strain curves are presented in Figure 4.2.

The finite element implementation of the Gurson model uses the true plastic flow curve as material input. However, the number of data points from a tensile test far exceeds the necessary number for a computational implementation. A constitutive approximation for the true plastic flow curves was needed to obtain true stresses for desired true strains. The Ramberg-Osgood equations, Equations 2.8 and 2.9, was used for this. To determine the constants K and n, an optimization scheme in Microsoft Excel was used. A linear ln-ln-plot of the true plastic flow curve was plotted, to which least-squares was used to find the closest fit from the Ramberg-Osgood equation. The value for n was found to be 0.082. The input data was later updated to achieve a hardening exponent of 0.1. The fit from the optimization scheme for all temperatures is shown in Figure 4.3. The curves marked *Output* show the data points implemented in ABAQUS. The *Output*-curves deviate from the experimental curves at higher strains due to the updated hardening exponent value of 0.1.

(a) Room temperature, 21 °C

(b) 0 °C

(c) −60 °C

Figure 4.3: Material fitting by optimizing the Ramberg-Osgood equation.

4.2   The Finite Element Model

The finite element model used in this thesis was made in ABAQUS CAE. Due to the symmetry of a hinged three-point bend specimen, only one half of the specimen needed to be modeled. This was made as a two-dimensional, deformable shell with unit thickness. The half-model's dimensions are presented in Table 4.3 and shown in Figure 4.4a. For bending specimen, the distance between the applied loads should be equal to $4W$, which gives the length of S[8].

Table 4.3: CAE-model dimensions.

W	a	$\frac{a}{W}$	S	Length	Crack-tip mesh size
[mm]	[mm]		[mm]	[mm]	[mm^2]
10	5	0.5	20	40	0.05x0.1

Figures 4.4a and 4.4b show the boundary conditions of the model. The arrow corresponds to the applied load, which was modeled as displacement at the arrow tip. On the bottom right side, the model is constrained making it unable to follow the displacement, forcing it to bend. The crack ligament in the model is also constrained, which is equivalent

(a) Dimensions.

(b) Material section.

(c) Mesh.

Figure 4.4: Dimensions, material selection, boundary conditions and mesh of the model.

Figure 4.5: Mesh in the crack region.

to applying a symmetry condition to the cracked face of the model. These boundary conditions give the desired bending during simulation.

The Gurson model simulation results are strongly affected by the material's plastic strain distribution, and boundary conditions need to be set in the way so that the model deforms without energy loss due to deformation of the regions where the boundary conditions are applied. Figure 4.4b shows material sections of the model. The blank region is the weld simulated 420MPa steel described in Section 4.1, and the coloured region indicates elastic material. These elastic regions were applied to avoid excessive deformation and consequently energy loss in the regions. The finite element mesh is shown in Figure 4.4c. The strain sensitivity of the Gurson model indicates that the correct mesh size must be used. This is further discussed in Section 4.4.3.2. At the crack tip, where the strain gradient is strong, this is especially important. For this thesis, a mesh size of $0.05x0.1mm^2$ at the crack tip was chosen based on values from literature[86]. The mesh in the crack tip region is shown in Figure 4.5. All elements are four-node plain strain elements (CPE4).

4.3   The Modeling Work Flow

From the ABAQUS CAE model, an input-file (.inp) for the ABAQUS solver was made. This was updated with the temperature dependent true plastic flow curves, described in Section 4.1.1 and the Gurson parameters, f_0 and f_c. The Gurson model itself was implemented through a user subroutine, UMAT. This is further described in Section 4.4. The input file and the UMAT was then fed into the ABAQUS solver and the simulation run. From this, force-CMOD curves from the simulations could be plotted and compared to the ones from the fracture toughness testing done by SINTEF. The Gurson parameters were fitted by trial and error from the fit of the force-CMOD curves at $21°C$. When the force-CMOD-curves from the simulations were satisfactory, a Python-script developed by SINTEF could be run on the output file (.dat) from ABAQUS. From this, values for ductile crack growth and CTOD were extracted and R-curves were plotted in Microsoft Excel. A linear fit to the R-curves for the three different temperatures ($21°C$, $0°C$ and $−60°C$) was found in Excel, which gave an equation for CTOD as a function of Δa. This enabled the possibility of plotting CTOD for different Δa-values over the temperature range to show the ductile-to-brittle transition captured by the complete Gurson model. The results are presented in Section 5.3.1.

To implement brittle failure, the RKR-criterion was used. This was applied as a post-processing calculation on the results from the Gurson simulations with the fitted Gurson parameters. In the ABAQUS .odb-file, a path was defined along the crack ligament. The stresses perpendicular to this path, the opening stresses, were found and plotted as a function of distance from the crack tip in Microsoft Excel. The simulation from $−60°C$ was used as a basis for the RKR-criterion. A critical distance, x_c, was estimated from which the critical stress, σ_c, was found from the increment of highest force in the simulation. The same fracture criterion was used for all temperatures. The first increment where the opening stress

field at the crack-tip med the RKR-criterion was found for 0°C and 21°C. From the Python-script, the ductile crack growth and CTOD values for these increments could be found, and incorporated in the ductile-to-brittle transition curves. This is further described in Section 4.5.

Figure 4.6: The work flow

4.4 Implementing the Gurson Model

The Gurson model is derived from a local approach to fracture, which allows for a physically-based description of fracture incorporating the three stages of ductile rupture used to describe the damaged process zone. The model consists of constitutive equations coupling plasticity and damage, referred to as continuum damage mechanics. The damage is considered as an internal state variable in the continuum mechanics model, it evolves with and is coupled to the stress and strain field. The essential feature of accumulated damage in the continuum is the strain-softening. Increased damage leads to a strong decrease in the load bearing capacity in the material. When it reaches a critical value, the material point looses its load bearing capacity, mathematically representing a crack[46]. With finite element tools,

deformation and failure can be predicted with high accuracy by means of material dam-age constitutive models. The models are, however, prone to strain and damage localization, making them strongly mesh size dependent[11]. This is further discussed in Section 4.4.3.2.

The Gurson model was implemented in ABAQUS as a material user subroutine, UMAT. A UMAT defines a constitutive material model that is not part of the ABAQUS library. The UMAT requires input material data and state-dependent variables. In this thesis, these are the true plastic flow curves and the Gurson parameters.

This following subsections are dedicated to the computer implementation of the Gurson model. First, the general algorithm for plasticity simulation is explained. Further, the section discusses difficulties with the Gurson model implementation and how these have been over-come. Lastly, the scheme for determining the input parameters required in the constitutive equations is presented.

4.4.1   Return Mapping Algorithms

The basis for plasticity algorithms is that the underlying material models predict a marked change in material behaviour once the stress reaches a critical value, the yield stress. In simulations involving plasticity, return mapping algorithms are central. All such algorithms work in the same way. A trial stress is computed by assuming an entire time step is elas-tic, and compared to the yield surface of the material. If the trial stress falls inside the yield surface, the assumption is correct and the equilibrium equations are trivially solved by per-forming elastic calculations to find the final stress. If the predicted trial stress falls outside the yield surface, implying that plastic deformation occurred, the algorithm recognizes that the tentative assumption of elasticity is incorrect. The algorithm returns the correct updated stress by projecting the trial stress back to the yield surface.

For typical numerical applications, the incremental stress (and internal parameters, such as the Gurson parameters), and strain rate are presumed to be known at the beginning of each time step. The desired output of the calculation is the rate at which the stress (and the internal parameters) change in response to the applied strain. An increment is elastic if the strain would return to its initial state at the beginning of the increment if the stresses were also to be released back to their initial state. Alternatively, the interval of deformation is plastic and associated with irreversible structural changes in the material.

4.4.2   Numerical Gurson-based model

The challenge with the Gurson model is that it accounts for microscopic void growth, which leads to macroscopic dilatational flow. Correspondingly, the yield surface changes with dam-age as it does not depend on the von Mises stress, σ_e, alone, but also the hydrostatic stress, σ_h. This makes computer implementation complicated. For all numerical schemes used for analysis of elasto-plastic problems, implementing constitutive equations governing material behaviour is inevitable. For elasto-plastic material models, there exists no one-to-one rela-

tionship between stress and strain after yielding. In the elastic region, stresses and strains are related through the Young's modulus, but in the plastic, hardening range, the use of an elasto-plastic stiffness matrix (tangent moduli) with an integration scheme for determining the stresses at integration points, is imperative to ensure convergence of numerical methods.

In 1985, J.C. Simo et al.[64] proposed the use of a consistent tangent moduli for the J_2 model with a closest-point projection algorithm for the yield surface. The consistent tangent moduli is consistent with the numerical integration algorithm, and may also be called linearization moduli. The paper showed that the choice of consistent tangent moduli is dependent on the iteration scheme adopted, and that it governs the convergence rate of the iterative scheme.

Before 1985, the continuum tangent moduli was frequently used with an Euler forward integration algorithm. This moduli is derived from continuum rate equations that enforce the consistency condition that the stress point upon yielding must remain on the yield surface if no unloading occurs. The implication of this is that the stress increment can be calculated explicitly from any given increment of strain by using the continuum tangent moduli. The continuum moduli for J_2 models can be found in [64]. This requires an explicit integration algorithm, such as the Euler forward algorithm.

Porous material models, such as the Gurson model, deviate from the J_2 model by exhibiting dependence on hydrostatic pressure upon yielding. Finite element methods for modeling the behaviour of such materials is not straightforward. The task of formulating a return mapping algorithm and obtaining linearization moduli consistent with the algorithm for pressure-dependent models is laborious. Thus, Euler forward integration algorithms based on continuum elasto-plastic moduli may still be used. This, however, requires very small time steps to avoid numerical instability[83]. ABAQUS[35] presented an Euler backward integration scheme for generalized plasticity models together with an expression for the linearization tangent moduli consistent with the algorithm. According to this scheme, two matrix inversion, where at least one matrix is asymmetrical, must be performed to obtain the consistent tangent moduli. Aravas[6][7] presented a better and more generalized Euler backward integration scheme with an equation for calculating the consistent tangent moduli. The equation still requires a matrix inversion.

Z. Zhang[85] published a paper in 1995 studying the possibility of computer implementation of the Gurson-based model with all three mentioned algorithms in mind:

- Euler forward integration algorithm based on the continuum elasto-plastic moduli

- ABAQUS' Euler backward integration scheme with an expression for the consistent tangent moduli

- Aravas' Euler backward integration scheme with an equation for calculating the consistent tangent moduli

The study showed that the convergence behaviour of the first integration scheme using

the continuum elasto-plastic moduli was unacceptably poor at relatively large strain incre-
ments. For the two other integration schemes, numerical problems appeared during matrix
inversion as it was not possible. Z. Zhang presented a method for deriving an explicit expres-
sion for the consistent tangent moduli by decomposing stress increments into hydrostatic
and deviatoric components to account for the pressure-dependency of the material upon
yielding. The general consistent tangent moduli forms in [6] and [35] were derived used cou-
pled stress-strain relations. Decomposing the return mapping process, enabled the possibil-
ity of deriving the consistent tangent moduli for general pressure-dependent constitutive
models for the hydrostatic and deviatoric stress components separately. The great advan-
tage of this is that no matrix inversions are needed to obtain the consistent tangent moduli.
The complete Gurson model was implemented into ABAQUS through an Euler backward al-
gorithm with an equation for the consistent tangent moduli as proposed by Z. Zhang in [85].

4.4.3   Determining the Gurson Parameters

The input material data and state-dependent variables required for the Gurson-simulation
are the true plastic flow curves and the Gurson parameters, the initial void volume fraction,
f_0 and the critical void volume fraction, f_c. A non-uniqueness problem arises when fitting
two parameters, there exits a good fit for the force-CMOD curves for an infinite amount of
pairs[86][87]. However, as the Gurson model itself does not constitute any failure criterion
for void coalescence, it cannot determine the value of f_c itself. The new failure model by
Thomason partly solves this issue. As the void coalescence in the plastic limit-load model is
determined by a physical mechanism, and not by a single value, f_c becomes a by-product of
the coalescence prediction. Thus, the critical void volume fraction can be seen a material's
response at coalescence[87]. The material failure is solely controlled by the initial parameter,
and f_0 can be uniquely determined by comparing numerical and experimental results.

4.4.3.1   Parametric Study of the Gurson Parameters

The true plastic flow curves were incorporated as explained in Section 4.1.1. The Gurson pa-
rameters were found by fitting the force-CMOD curves from simulation to the experimental
ones for room temperature. This temperature was chosen as the Gurson model predicts duc-
tile crack growth and failure, and the material is expected to behave in a ductile manner at
room temperature. The Gurson parameters were studied individually. First f_c was kept con-
stant at 0.2, while f_0 was varied. An initial value for f_0 was chosen from literature at 0.0013.
This gave an adequate fit for the curves at room temperature, and the chosen f_0 value was
0.0014.

For the lower temperatures, the simulated curves with f_0 = 0.0014 did not fit well with
the experimental data. At 0°C, the material is expected to have some ductile crack growth
before failing in a brittle manner. The Gurson model is not able to predict brittle failure, and
will therefore not capture this. The simulation overpredicts the loss of load bearing capacity

of the material after the onset of plasticity. The material is expected to have lower rates of void growth and coalescence due to restricted plastic flow. The Gurson model, however, forces void induced ductile crack growth and will thus predict a rapid decline of load bearing capacity.

At $-60°C$, the material is completely brittle, and the Gurson model will not capture correct material behaviour. The material will cleave before plastic flow is initiated, and, consequently, before void growth and coalescence has started. The Gurson model will not capture the cleavage fractures and therefore simulate void ductile crack growth even at this temperature.

The study of the critical void volume fraction, f_c, was executed in the same manner, f_0 was kept constant at 0.0014 and f_c varied. As expected, different f_c values did not change the force-CMOD curve, confirming that material failure is solely controlled by f_0, enabling this parameter to be uniquely determined. The initial void volume fraction was kept temperature independent, so that the only temperature dependency of the simulation came from the plastic flow curves.

By fitting only one value, another problem arises. Since the Gurson model can simulate different void nucleation models with different initial parameters, each one of them can be fitted to the experimental force-CMOD curve. The problem lies in determining the correct void nucleation model. A ductility diagram, which related fracture strain and stress triaxiality (different depth notches) is proposed for this purpose[86][87][89]. The curvature of these curves differ between the nucleation modes, and the correct nucleation mode can thus be determined. This has not been done in the thesis. Only one nucleation mode, as mentioned in Section 3.1, has been studied and fitted to the experimental data.

4.4.3.2 Mesh Sensitivity

The strain sensitivity of the Gurson model, mentioned in Section 4.2, is not surprising as strain is directly related to the material softening from the damage growth. The void volume fraction controls the material softening, and is calculated at the integration points of the elements in the model. Void coalescence at the crack tip is a discontinuous process and the length of each crack growth step determines the material's resistance to crack extension. The implication is that a minimum volume of material must be involved for crack initiation to be reached. The constitutive equations in the Gurson model is formulated for individual crack points, making it difficult to incorporate the length scale necessary to account for softening. The pragmatic solution to this is to specify the size in the analysis directly, by incorporating the mesh size, l_c, as a material parameter, as done by Tvergaard and Needleman[48]. As the length scale is related to crack resistance, it will influence the R-curves obtained from simulation. The mesh size used in this thesis, $0.1 mm$ in the crack growth direction, is chosen based on values from literature and gave a satisfactory fit. Additionally, the void volume fraction is localized in only one layer of integration points due to localization. Damage happens in only one element layer, meaning that if the damage zone is wider, in the case of a coarse

Figure 4.7: Brittle fracture criterion.

mesh, the results will differ from the ones obtained with a narrower mesh. In this thesis, the damage zone width is $0.05mm$. The mesh size dependency can be solved by using non-local fracture models, but that is out of the scope of this thesis.

4.5   Implementing the RKR-Criterion

The RKR-criterion was implemented as a post-processing routine. A Gurson analysis of the two-dimensional half single-edge notched bending specimen at $-60°C$ was run and the increment corresponding to the highest force from the force-CMOD curve of the specimen with the second lowest CTOD at cleavage was found. This specimen was chosen based on the BS 7910 standard[15], which dictates that the characteristic value is the equivalent to the lowest of three cleaved specimen. The experimental data presented in Section 5.1, show that specimen number 4, has the characteristic value. The force-CMOD curve for this specimen is presented in Figure 5.2, which shows that the highest force-value is $9kN$. This corresponds to a material reaction force of $450^{N}/_{mm}$ in the ABAQUS simulation. From this force increment, the opening stress at the crack tip as a function of distance along the crack ligament was extracted. This served as the basis for fitting the RKR-criterion. As the criterion predicts cleavage, $-60°C$ was chosen as a basis due to the brittle characteristics of the material at this temperature.

4.5.1   Determining the RKR Parameters

The RKR parameters that needed to be determined were the critical stress, σ_c, and the critical distance, x_c. Ideally, the critical distance should be determined from the microstructure. It is supposed to correspond to roughly two grain diameters, as discussed in Section 3.2. However, in this thesis, the critical distance has been viewed as a material fitting parameter from which the critical stress can be found. Once the critical distance was chosen, the critical stress was estimated to be the lowest value of stress that worked over the entire characteristic distance at the increment. This is shown in Figure 4.7. The opening stress, denoted σ_{22} in Figure 4.7 corresponds to the second principal stress, as described in Section 2.4.

A parametric study of x_c was executed as this value predicts the entire fracture criterion. The results are presented in Section 5.4.2. Since the criterion was fitted from the same increment, the critical stress increases with decreasing critical distance. The criterion was kept constant over the temperature range from $-60°C$ to room temperature. For $0°C$ and room temperature, the first increment with an opening stress at the crack tip that fit the fracture criterion fitted at $-60°C$ was found. Brittle fracture was predicted to occur at this increment. From the Python script developed by SINTEF, the CTOD values from the increment could be found and used to plot the ductile-to-brittle transition for the steel.

5 | Results and Discussion

5.1 Experimental data

SINTEF performed fracture toughness tests to be used as a basis for the simulation scheme. Single-edge-notched specimen with cross section $10x10mm^2$ of the material described in Section 4.1 was used. Electrical discharge machining (EDM) was used to acquire the desired crack depth, making the crack-to-width ratio 0.5. Liquid nitrogen was used to perform tests at $0°C$ and $-60°C$.

Figure 5.1: Measuring ductile crack growth.

During bending, the applied force and CMOD of the specimen was monitored. The test was stopped either after cleavage occurred or after the specimen reached a desired CMOD value. After this, the specimen was cracked open and studied in an optical microscope. Ductile crack growth was measured through the following procedure, shown in Figure 5.1 picturing the cross-section of a test specimen. At nine points along the initial crack, the EDM crack length, denoted a_0 in Figure 5.1, was measured. From the same nine points, the total crack growth, $a_0 + \Delta a$, was measured from which the ductile crack growth, Δa could be found. The ductile crack growth was averaged through Equation 5.1, where the numbers 1 to 9 refer to the placement along the initial crack as indicated in Figure 5.1.

$$\Delta a_{avg} = \frac{\frac{\Delta a_1 + \Delta a_9}{2} + \Delta a_2 + \Delta a_3 + \Delta a_4 + \Delta a_5 + \Delta a_6 + \Delta a_7 + \Delta a_8}{8} \tag{5.1}$$

The monitored CMOD was used to calculate the corresponding CTOD through the equations presented in Section 2.7.3. For each test temperature, six parallels were run to different CMOD values, yielding different values of average ductile crack growth and CTOD that could

be plotted as a fracture resistance curve (R-curve) for the material at the given temperature. The experimental R-curves are shown in Figure 5.3. The force-CMOD curves for all temperatures are shown in Appendix B.

Figure 5.2: Experimental force-CMOD curve for specimen 4 at −60°C. The arrow indicates the point where Δa-values for caluclation has been found.

The experimental data needed to be analyzed. For some specimen, brittle fracture or a pop-in occurred before unloading. Ductile crack growth was measured after the fracture toughness test was finished, which means that the crack growth at the ultimate force value is unobtainable. An example is shown in Figure 5.2 where the legend *Calculations* implies the force- and CMOD-values used for calculating CTOD. The crack growth, which is also used in calculations, has been measured from the point in Figure 5.2 indicated by the arrow. This means that the wrong Δa-value is used in calculations of CTOD, which affects the R-curves.

For the lower temperatures, such as −60°C, the measured ductile crack growth is very small. Specimen 4 corresponds to a CTOD-value $0.076 mm$ and Δa-value $0.07 mm$, shown in Table 5.1. This is a small amount of ductile crack growth, and the difference in the calculated CTOD-values will not be greatly affected. At room temperature, all the specimens are unloaded and thus not affected by this. At the intermediate temperature, $0°C$, the material is expected to have significant ductile crack growth before possibly a brittle fracture might occur. The underlying idea for the model is to capture the change from ductile crack growth to brittle failure, and especially in the intermediate regions capture ductile crack growth before a brittle failure occurs. Taking this into account when analyzing results is important. The specimen expected to overestimate CTOD based on wrong Δa-values are marked with arrows in Figure 5.3. These are the specimen that have cleaved.

The calculated CTOD from experiments was used to create a ductile-to-brittle transition curve for the material. This is shown in Figure 5.4, where empty squared markers indicate that the specimens fractured, while the cross markers indicate that the specimens have been

Figure 5.3: Experimental CTOD-Δa-curves for all temperatures. The arrows show the specimens whose fracture toughness is not calculated with the correct Δa-value.

unloaded. This clearly shows the embrittlement of the material at lower temperatures and the change of fracture toughness, as discussed throughout Section 2.6. At room temperature all specimen have been unloaded, indicating ductile behaviour. At $0°C$, three specimen have been unloaded and three have undergone cleavage. Some of the cleaved specimen show relatively high CTOD-values which indicates that there has been ductile crack growth prior to the cleavage fracture. Other specimen have cleaved at an early stage in the testing process. The scatter in this region may be due the heterogeneous distribution of second phase particles or orientation of the cleavage grains with respect to the crack tip, which will make some of the specimen more susceptible to cleavage fracture. The large specimen size makes it impossible to achieve equal material characteristics at the machined crack tip, and the heterogeneous nature of steel, especially in the CGHAZ, will result in scattered results. However, the trend shows that the material is more brittle at $0°C$ than at room temperature. For $-60°C$ the scatter is small. The material is expected to be completely brittle at this temperature and will suffer cleavage at low CTOD values. Some of the specimen have been unloaded at this temperature in order to obtain the fracture resistance curve.

Figure 5.4: Experimental ductile-to-brittle transition curve. Empty squared markers indicate that the specimens fractured, while the cross markers indicate that the specimens have been unloaded.

Table 5.1: Experimental CTOD and Δa-values. F=fracture, U=unloading.

	RT				$0°C$				$-60°C$		
#	CTOD [mm]	Δa [mm]	Mode	#	CTOD [mm]	Δa [mm]	Mode	#	CTOD [mm]	Δa [mm]	Mode
17	0,259	0,22	U	9	0,205	0,23	U	1	0,111	0,07	F
19	0,538	0,89	U	10	0,318	0,39	F	2	0,094	0,08	U
20	0,368	0,51	U	11	0,353	0,47	U	3	0,052	0,05	F
21	0,458	0,77	U	12	0,101	0,08	F	4	0,076	0,07	F
22	0,134	0,09	U	13	0,133	0,11	U	5	0,042	0,03	U
23	0,190	0,19	U	14	0,175	0,17	F	6	0,110	0,06	U

5.2   Evaluation of Model Requirements

To investigate if the ductile-to-brittle transition could be captured solely by changing temperature and constraint, and not simulating material softening, CAE-models with crack-to-width ratios of 0.51 and 0.52 were made. This corresponds to Δa values of $0.1mm$ and $0.2mm$, respectively. The simulations were run without the Gurson model, thus not accounting for void growth and coalescence induced ductile crack growth. The simulations were dependent only on the temperature dependent flow curves of the material and the change in constraint due to the set crack growth values of $0.1mm$ and $0.2mm$. The opening stresses for each temperature and crack growth were found from simulation and normalized with the temperature dependent yield stress. The result is shown in Figure 5.5. The crack growth pushes the normalized stresses upwards. This is in line with theory as crack growth will increase triaxiality and constraint, pushing the stress field upwards.

Figure 5.5: Opening stress normalized by temperature dependent yield stress.

For the same value of Δa the normalized stress falls on roughly the same line for each temperature, indicating that the opening stress can be related to the yield stress through only one parameter, K, as shown in Equation 5.2. K will be dependent on crack growth.

$$\frac{\sigma_{22}}{\sigma_{ys}} = K\,\big|_{\Delta a} \tag{5.2}$$

K is proportional to Δa, which means that higher amounts of crack growth will give higher values of σ_{22}. The increased constraint should give increased stress-values. This, however, also means that for a high temperature, e.g. $21°C$, where the material should be ductile and exhibit large amounts of crack growth, the opening stress will be very large as it is proportional to Δa. This is not correct as the material will soften due to plasticity at higher

temperatures, which in turn will relax the stress field. A single stress-based fracture criterion will capture constraint effects from the set crack propagation, but not material softening effects. To accurately show the ductile-to-brittle transition, the model must capture both. Hence, the brittle stress criterion must be used in combination with a material softening model, such as the complete Gurson model.

The experimental line in Figure 5.5 has been extrapolated from experimental crack growth values. At −60°*C,* there is a negligible amount of ductile crack growth, and the Δa value has been set to zero. At 0°*C* there is roughly 0.1*mm* ductile crack growth. The crack growth at 21°*C* has been set to 0.5*mm.* The last point has been extrapolated from the simulations for 0.1*mm* and 0.2*mm.* Although the experimental line accounts for both crack growth and temperature, the difference in the normalized opening stress is still small. An issue is that the opening stress at 21°*C* is higher than for the other temperatures, which, as previously discussed, contradicts theory. This proves that accounting for material softening is crucial when showing the ductile-to-brittle transition.

5.3 Ductile Tearing: The Gurson Model

The Gurson model simulates the material's loss of load bearing capacity as voids grow in the matrix. As this constitutes damage and possibly ductile tearing, the Gurson parameters have been fitted from the temperature where the material is expected to exhibit most ductile characteristics. In this thesis, the highest temperature is room temperature, thus used for fitting. A parametric study of the Gurson parameters, f_0 and f_c, and the hardening exponent, n, was conducted by the author prior to this thesis. This is discussed in Section 4.4.3. The initial void volume fraction, f_0, was found to be 0.0014. The critical void volume fraction, f_c was found to not influence results. The hardening exponent was found to be 0.1. The mesh size, l_c was chosen from literature, and not changed as the results were satisfactory. All input parameters were kept constant throughout the temperature range from 21°*C* to −60°*C.* The temperature was only incorporated through the plastic flow curves, as described in Section 4.1.1.

5.3.1 R-curves

From the Gurson simulation R-curves for all three temperatures (21°*C,* 0°*C,* −60°*C*) were plotted as described in Section 4.3. The results are presented in Figures 5.6. At room temperature, Figure 5.6a, the simulated R-curves fits well with the experimental results. As the Gurson model constitutes ductile crack growth and the steel is expected to be ductile at this temperature, a good fit was expected. Also the Gurson parameters were fitted at this temperature. The Gurson model is able to capture both the correct CTOD value and corresponding Δa values at room temperature.

The f_0-value was kept constant for the whole simulated temperature range. Tempera-

ture was only incorporated through the plastic flow curves. The yield strength of a material increases with decreasing temperature, and according to Section 2.6, all factors increasing yield strength will embrittle the material. The Gurson model was not expected to capture the brittle characteristics of the material, making the fit from simulations worse at lowered temperatures. Figure 5.6b shows the fracture resistance curve from the Gurson simulations along with the experimental data points for 0°C. The model clearly deviates from the experimental values, as expected.

For −60°C, the results from simulation do not fit the experimental data points, as shown in Figure 5.6c. The material is expected to be completely brittle at this temperature, and the Gurson model will therefore not be valid at this point.

The Gurson model is not able to predict ductile crack growth of less than 0.1mm and CTOD of less than ≈ 0.2mm. All simulated curves in Figures 5.6 origin at these values. In the model, void growth starts at the crack tip, but the first complete failure occurs at a distance equal to the mesh size to the initial crack tip. Rupture of a material point corresponds to full loss of load-bearing capacity. The stresses are zero regardless of deformation and the consistent tangent matrix is also null. As the loss of load bearing capacity is manifested as softening in a volume element, the first crack growth will be equal to the element size. In this thesis, a mesh size of 0.1mm has been used in the crack ligament in the direction of crack growth, which explains why the model is unable to predict Δa-values below this. Before the first element is recognized as crack growth, the crack tip has blunted and the CTOD has reach a value of ≈ 0.2mm.

When comparing the simulated curves, the temperature dependency incorporated through the plastic flow curves yield lower CTOD-values for all Δa-values at lower temperatures. The R-curve becomes less steep as the temperature is lowered. This is in line with theory. A brittle material will have a flat R-curve as the materials resistance is constant with crack growth. For −60°C, where the material is brittle, the R-curve should be flat as discussed in Section 2.8.2.1. This is impossible to achieve with the Gurson model as it forces plasticity and cannot detect brittle characteristics.

5.3.2   Ductile-to-Brittle Transition

From the simulated R-curves, the ductile-to-brittle transition predicted by the Gurson model could be plotted. A linear trend line fitted to the simulated R-curves in Microsoft Excel was used to obtain equations with CTOD as a function of Δa for all three temperatures. This was used to obtain CTOD-values for the same Δa-values at all temperatures, which could be plotted as a ductile-to-brittle transition curve. The results of this are shown in Figure 5.7.

The Gurson model clearly overpredicts CTOD-vales at both 0°C and −60°C. This is expected, as the R-curves for these temperatures are also overpredicted. In addition, the lowest value of ductile crack growth used for the Gurson model is 0.1mm, and non of the specimen at −60°C have undergone such an amount of ductile crack growth. It is therefore impossible for the Gurson model to fit at this temperature. At room temperature (21°C), however,

(a) Room temperature, 21 °C

(b) 0 °C

(c) −60 °C

Figure 5.6: Gurson model fit for all three temperatures.

Figure 5.7: The ductile to brittle transition captured by the Complete Gurson model. Empty squared markers indicate that the specimens fractured, while the cross markers indicate that the specimens have been unloaded.

where the Gurson model has been fitted, the CTOD- and corresponding Δa-values should fit the experimental ones shown in Table 5.1. The Gurson-line for $1mm$ ductile crack growth predicts a CTOD at room temperature of $0.591mm$. The closest experimental data point is from specimen 19, which has a CTOD of $0.538mm$ and Δa of $0.89mm$. The specimen numbers and corresponding CTOD and Δa-values are shown in Table 5.1. It is not unlikely that a specimen with $1mm$ ductile crack growth will have CTOD of approximately $0.591mm$. For $0.5mm$ ductile crack growth, the Gurson model predicts a CTOD of $0.373mm$. The line hits the experimental data point for specimen 20, which has CTOD and Δa of $0.368mm$ and $0.51mm$, respectively. This is a very good fit.

At lower Δa-values, however, the Gurson model struggles. The line for $0.1mm$ ductile crack growth predicts a CTOD of $0.199mm$. This hits just above the data point for specimen 23, which has a CTOD-value of $0.190mm$ and $0.19mm$ ductile crack growth. The ductile crack growth from experiments at this point is double the amount from the Gurson model. The Gurson model predicts crack growth as complete loss of load bearing capacity of an element, making he first increment of Δa correspond to the mesh size, which is $0.1mm$. The crack tip has blunted sufficiently before the first increment has lost its stress bearing capacity for the model to predict a CTOD of $0.199mm$ with the first crack growth. The R-curve for $21°C$ in Figure 5.6a shows that the Gurson model does not fit for low values of Δa, which corresponds with deviation in the ductile-to-brittle transition for low crack growth values.

A prediction for the DBT for $\Delta a = 0mm$ is also shown in Figure 5.7. The Gurson model simulates ductile rupture, and at $\Delta a = 0mm$, the CTOD value predicted is solely from blunting. The model predicts $0.155mm$ blunting at $21°C$, which is an overestimation of the experimental blunting value at $0.09mm$. The onset of coalescence induced ductile crack growth

is delayed in the simulation, which might indicate that other coalescence mechanisms that void by void coalescence happen in the material, for instance sheeting coalescence as described in Section 2.5.2.4. The CGHAZ contains many second-phase particles that might nucleate voids continuously during deformation, resulting in accelerated crack growth. These problems have not been investigated in this thesis work, and are known problems in all continuum material models. The Gurson model predicts the correct fracture toughness at higher Δa-values. The void nucleation and coalescence mechanisms in the model should be further investigated. The DBT for $\Delta a = 0mm$ goes down for higher temperatures. This is solely a consequence of the linear approximation of the simulated R-curves at different temperatures.

5.4 Brittle Failure: The RKR-Criterion

The RKR-criterion is a simple stress-based criterion for cleavage fracture. According to Section 2.5.1, cleavage fracture occurs when some stress threshold is reached, which is what the RKR-criterion captures. The stress needs to work over some limit distance in order for the RKR-criterion to predict cleavage. This solves the singularity-issue presented in Section 2.7.1. According to Section 2.6, the steel is expected to be brittle at lower temperatures, thus $-60°C$ has been used for fitting the RKR-criterion. The BS 7910 standard dictates that the second lowest cleaved specimen should be used as the characteristic value[15]. This corresponds to specimen 4, which has a CTOD of $0.076mm$.

5.4.1 Effect of the Gurson Model

The RKR-criterion is applied as a post-processing routine, enabling the possibility to study the effect of the Gurson model on the brittle fracture criterion. The criterion was applied to simulations run both with and without an underlying Gurson model. To capture the difference, a large x_c value of 240µm was required for the criterion to be met at 21°C. This corresponds to a low critical stress value, $2225MPa$. For the simulations run without the Gurson model, ductile crack growth was not allowed to happen. The stress field at the crack tip was solely dictated by the difference in the plastic flow curve at the different temperatures, and not by changing constraint due to a growing crack. For 0°C and room temperature, the stress field at the crack tip was relaxed through bulk plasticity. For low values of x_c, which corresponds to high values of σ_c, the RKR-criterion was not met for higher temperatures. The simulation for 0°C would meet the cleavage criterion for lower values of x_c than room temperature. This corresponds with theory, as the material should gradually exhibit more ductile behaviour as temperature is raised and thus require crack propagation to achieve constraint sufficient to push the crack-tip stress field to meet the fracture stress criterion.

The comparison between the RKR-criterion alone and the combined model is shown in Figure 5.8. Both the RKR-criterion alone and the combined RKR-Gurson model have been

Figure 5.8: The ductile to brittle transition captured by the RKR-criterion alone and in combination with the Gurson model.

fitted from the same point at $-60°C$, thus showing the same CTOD value for this temperature. At $0°C$, the yield strength is relatively high and ductile crack growth is to some degree prohibited by the material's restriction to flow. The crack tip constraint will push the stress field upwards, and it will be energetically favourable for the material to cleave rather than release the stresses through deformation. Both models will thus predict the same value of CTOD for this temperature. The low critical stress value obtained from the large x_c-value will not require change in constraint for the stress based criterion to be met at $0°C$.

For room temperature, the Gurson model changes the predicted CTOD value. The ductile characteristics of the material at this temperature mean that the stresses at the crack tip will more readily be released through plastic deformation, resulting in ductile crack growth. As the crack grows, the constraint changes and the stress field at the crack tip will be elevated, ultimately reaching the brittle fracture criterion. Ductile crack growth will open the original crack tip and give higher CTOD-values than for a model incorporating only fracture stress as a criterion. However, the fracture criterion should ideally never be met at this temperature, as the material is not brittle. Constraint should be relaxed as the plastic zone at the crack tip merges with global plasticity, resulting in plastic collapse. The RKR-criterion, being a brittle fracture criterion, will not predict this, and cleavage will be predicted when the criterion is met. Ideally the CTOD at room temperature obtained from the combined model should be above all unloading points in Figure 5.4. This would correspond to the absence of cleavage found in all fracture mechanical tests performed at this temperature.

5.4.2 Parametric Study of the Critical Distance

It was found that the stress based RKR-criterion had to be coupled with the Gurson model to obtain CTOD values from the combined model at higher temperatures. Determining a correct x_c and corresponding σ_c was necessary, as well as performing a parametric study to investigate their effect on the ductile-to-brittle transition curve. The critical distance should ideally be determined from microstructure, but has in this thesis been implemented as a fitting parameter. As a first estimate, a critical distance of $60\mu m$ was used. This was based on the underlying theory of the RKR-criterion presented in Section 3.2, where x_c is estimated to be about two grain diameters. In CGHAZ, an average grain diameter of $30\mu m$ is often found, which gave the starting point for x_c at 60μm.

As described in Section 4.5.1, the critical distance gives the critical stress. The different stresses obtained from different distances are shown in Table 5.2, which show that smaller distances give higher stresses. As all fracture criterion are fitted from the same stress field at the same increment from simulation, this is expected. The stress peak becomes narrower towards its top, thus the distance between equal stresses is smaller for higher values of stress.

Table 5.2: RKR-criterion for different values of x_c.

x_c [μm]	240	120	60	50	40	30
σ_c [MPa]	2225	2365	2400	2404	2408	2411

The parametric study of the critical distance, x_c, is shown in Figure 5.9. As the fracture criterion is fitted from $-60°C$, all criteria hit the same point for this temperature. The effect of the variation of critical distance becomes more prominent as the temperature increases. At $0°C$, all CTOD values are in the range of $0.08 - 0.12mm$. As discussed in previous section, crack growth will change the crack tip constraint and the triaxiality of stresses. The peak opening stress will increase with crack depth, generating higher values of equivalent plastic strain. The distribution of stress triaxiality will be lowered, ultimately resulting in higher fracture toughness values for larger crack sizes. The low variation of CTOD for $0°C$ shows that the material exhibits some brittle characteristics. As discussed in Section 2.6, the material will cleave when it is more energetically efficient than energy dissipation through plastic deformation. Hence, the RKR-criterion will be met before substantial ductile tearing has occurred at this temperature.

For room temperature ($21°C$), however, the resulting CTOD varies with critical distance, shorter distance gives higher CTOD-value. Shorter distance corresponds to higher critical stress, which implies that the SENB specimen must undergo a certain amount of crack growth to achieve constraint sufficient to push the stress field far enough upwards to meet the RKR-criterion. CTOD values increase with increasing crack growth, giving higher fracture toughness values for lower critical distance. Figure 5.9 show that the CTOD value converges as the critical distance is shortened. Table 5.2 shows that for x_c-values between 50μm and 30μm, the difference in σ_c is small. It is reasonable to believe that all these cleavage criteria

Figure 5.9: Parametric study of x_c for the RKR-criterion.

are met at the same increment in the simulations, making the obtained CTOD value equal for the three last criterion the same. The criterion with x_c at 30μm and corresponding σ_c at $2411MPa$ was chosen as the brittle fracture criterion competing with the damage induced ductile crack growth from the Gurson model.

5.5   Combined Model: Gurson + RKR

In summary, the model for simulating the transition from completely brittle to completely ductile behaviour using the Gurson model in combination with the RKR-criterion as described in Sections 4.4 and 4.5 has the following constitutive parameters:

- elastic parameters, E and ν

- yield curve (power law: σ_{ys}, n)

- initial void volume fraction, f_0

- mesh size, l_c

- critical distance, x_c

- critical stress, σ_c, found from the critical distance

The constitutive parameters can be identified as follows:

1. Tensile tests at temperature in the ductile-to-brittle transition range

    (a) Determine Young's modulus, E, Poisson's ratio, ν and σ_{ys}.

Table 5.3: Constitutive parameters for the combined Gurson-RKR model.

T	E	υ	σ_{ys}	n	f_0	l_c	x_c	σ_c
[°C]	[GPa]		[MPa]			[mm]	[µm]	[MPa]
21			667					
0	210	0.3	676	0.1	0.0014	0.1	30	2411
-60			697					

    (b) Determine the true stress-strain curve and establish the Ramberg-Osgood power law parameters (*n* and *K*) to find material input data for the simulation.

2. Fracture toughness tests at temperatures in the ductile-to-brittle transition range

    (a) Determine f_0 by trial and error of fitting simulated force-CMOD curves to experimental ones in the ductile regime.

    (b) Verify the chosen mesh size by fitting fracture resistance curves.

    (c) Determine the characteristic fracture resistance value in the brittle regime.

3. Brittle region

    (a) Find the increment in simulation that corresponds to the characteristic value and determine x_c and σ_c.

5.5.1 Ductile-to-Brittle Transition

The constitutive parameters for the model used in this thesis are shown in Table 5.3. The RKR-criterion has been fitted from $-60°C$ and the Gurson model from $21°C$. It was determined that a stress criterion alone could not show the ductile-to-brittle transition, but needed an underlying model that accounted for ductile softening of the material. Figure 5.10 shows how the combined Gurson-RKR model captures the change of material behaviour with temperature. Ductile tearing from the experimental results is plotted along with the results from the simulations, which clearly shows the difference in behaviour over the temperature range. At $-60°C$ there is nearly no ductile tearing. This increases with the temperature, at $0°C$ there is roughly $0.09mm$ ductile tearing and at $21°C$ there is $0.1mm$ tearing. This clearly shows that the material is more ductile at higher temperatures. The simulated curve account for this behaviour as the predicted fracture toughness increase with temperature. As mentioned in Section 5.4.1, the CTOD-value obtained from the combined model should ideally lie over all experimental unloading points at $21°C$ to account for the lack of cleavage at this temperature. The model predicts cleavage at a CTOD $0.376mm$, which is still underestimates the findings from the experimental results. The experimental data clearly show that there are no cleavage fractures at this temperature.

    A competing criterion is needed to establish whether the material undergoes cleavage or not. From the simulations, CTOD from the increment corresponding to maximum force for

Figure 5.10: The change of material behaviour captured by the combined Gurson-RKR model. Experimental CTOD values and RKR+Gurson results refer to the principal axis, while the measured Δa-tearing values refer to the secondary axis.

the characteristic value from experiments can be found. This can be plotted along with the combined model's prediction of DBTT. If the CTOD at maximum force lies under the Gurson+RKR curve, then the material has not undergone cleavage. The results are presented in Figure 5.11. The Gurson model forces plasticity for all temperatures, and will therefor over-predict CTOD at maximum force for both $-60°C$ and $0°C$. At $21°C$, however, the maximum CTOD from the simulation is $0.193mm$, which corresponds well with the experimental value at $0.187mm$.

Figure 5.11: Competing criteria for DBT.

Following the RKR+Gurson curve from $-60°C$ until it crosses the CTOD at maximum force curve at roughly 5°C, and then following the latter curve gives the ductile-to-brittle transition as predicted by the combined model. The result is shown in Figure 5.12. The model fits well at both $-60°C$ and 21°C, which is expected as these temperatures have been used for calibration. The intermediate region is where the results are interesting. The experimental results at 0°C are scattered, and determining the characteristic value is not straightforward. The lowest cleavage fracture toughness value at this temperature is $0.101\,mm$. Another specimen has been unloaded at a CTOD value of $0.133\,mm$, which indicates that the lowest cleaved CTOD value is too conservative to be representative for the material. The second lowest cleavage fracture toughness is at $0.175\,mm$, which is significantly higher than the lowest cleavage fracture toughness value. The model should hit in between these two values, which it does at a cleavage fracture toughness of $0.117\,mm$. The conservative predicted value indicates that the combined Gurson+RKR model overestimates the brittleness of the material at intermediate temperatures as well as at the upper shelf, 21°C.

Figure 5.12: The thick, black line shows the ductile-to-brittle transition predicted by the combined Gurson-RKR model.

Incorporating temperature changes solely through the plastic flow curve might not be sufficient to show the correct ductile-to-brittle transition for the steel. At $-60°C$, the results are only affected by x_c and σ_c as the material is completely brittle. These values are fitted from this temperature, making it possible to choose the fracture toughness value predicted by the combined model. For 21°C, the brittle fracture criterion should never be met, and the fracture toughness is solely determined by f_0 and l_c, which are fitted from the same temperature. The intermediate region takes into account all material parameters. Figure 5.12 shows that the cleavage fracture criterion is met too early at 0°C. The model should predict more ductile crack growth and, consequently, higher fracture toughness at this temperature. The

possible temperature dependency of the Gurson model parameter, f_0 should therefore be investigated.

5.5.2   Criticalities of the Combined Model

Although the combined Gurson-RKR model is able to predict a conservative ductile-to-brittle transition for the selected steel, there are some issues with the simulation scheme and the validity of the results. There are a total of eight constitutive parameters needed for the scheme: E, v, σ_{ys}, n, f_0, l_c, x_c and σ_c. Half of these, namely E, v, σ_{ys} and n, can be found from material testing. The remaining four parameters have to be fitted from simulations.

The initial void volume fraction, f_0, can be uniquely determined from force-CMOD curves. This, however, assumes that all voids are nucleated simultaneously at the onset of plasticity and that no voids are nucleated after this. The material is seen as an assembly of cells of equal size that all contain a single void that grows under deformation. This might not be the right nucleation model for the material. The CGHAZ contains second-phase particles that serve as nucleation sites, which is not accounted for by the nucleation model. Additionally, other microstructural effects such as shape and distribution of voids can only be taken into account through calibration to experimental results, rather than through their physical impact on the material. This is a known problem in continuum mechanics models. The initial void volume fraction, f_0, should in theory be the same for all temperatures since the same material is simulated. However, growth and coalescence is not the same over the temperature range. The model does not account for this other than through limitation of plastic flow as temperature decreases, and an investigation of the possible temperature dependency of the parameter is required for further development.

The length scale, l_c is incorporated as a material parameter. The main problem with this is that the mesh size served two purposes: i) it geometrically represents the cracked parts and the direction of crack propagation and ii) it represents the materials characteristic length controlling crack extension. These functions, determining both crack growth and its resistance, are somewhat contradicting. The mesh size should in theory be related to the mean inclusion or void distance, but has rather been used to fit fracture resistance curves, which makes it possible to obtain any desired fracture resistance curve.

A third challenge with the model is the determination of the critical distance, x_c, and the critical stress, σ_c, for the RKR-criterion. Cleavage initiation is described by dechoesion or breaking of a second-phase particle, the propagation of the formed mircrocrack in the grain and through the next grain boundary. Grain size is the relevant length scale for the RKR-criterion. The critical distance has in this thesis been viewed as a material fitting parameter independent of microstructure. This enables the possibility of adjusting the RKR-criterion to fit as desired, without considering the material in question. The issue that arises is that the predicted fracture toughness is not uniquely determined, and can be adjusted as required.

The combination of these issues implies that the model itself is unstable and inaccurate. It is not difficult to simulate the ductile-to-brittle transition when both the Gurson model

and the RKR-criterion can be adjusted to give desired output. It is questionable whether the model can predict DBTT for other materials without the need of similar adjustments, and consequently extensive material testing. To be able to predict the ductile-to-brittle transition for a material to avoid cost inefficient lab-based research, the model needs to be further developed.

6 | Conclusion

An attempt to determine a simulation scheme covering the whole range of the ductile-to-brittle transition of steel from completely brittle to completely ductile, has been made. The upper shelf region that constitutes ductile behaviour has been modelled by the complete Gurson model, which accounts for void growth and coalescence induced softening and rupture. The lower shelf with brittle characteristics has been simulated by the RKR-criterion, a cleavage stress criterion. The ductile model has been fitted from experimental results at $21°C$, where the steel in question is completely ductile, while the RKR-criterion has been fitted to experimental results from $-60°C$, where the steel is completely brittle. Experimental data from $0°C$, which is in the intermediate region where the steel exhibits both ductile and brittle characteristics, have been used as verification of the modelling scheme.

The investigation of whether changing constraint and temperature would be sufficient to show the ductile-to-brittle transition through solely a stress based fracture criterion revealed that implementing a model that accounts for material softening was necessary to simulate the full transition regime. The change in constraint linked to crack growth will elevate the stress field at the crack tip. In the upper shelf the stresses need to be dissipated into plastic flow for ductile tearing, and for this reason, not accounting for material softening leads to severe underestimation of the fracture resistance.

The combined Gurson-RKR model was found to predict cleavage for all temperatures in the ductile-to-brittle transition curve, even at the upper shelf. A competing criterion was needed to establish whether the material underwent cleavage at the predicted fracture resistance value or if the fracture resistance corresponded to that from the highest applied force in the experiments. The results showed that the change from cleavage to maximum force occurred at approximately $5°C$. The combined model is able to capture the change of fracture mechanism over the temperature range with the temperature dependent plastic flow curves as the only temperature adjustment in the model. The results, however, show that the combined model still over accounts for brittleness in the material. An investigation of the temperature dependency of the Gurson parameter f_0 is a necessary step to further develop the model.

The determination of the constitutive parameters for the combined model proved to be problematic. There are two length scales involved in the model that ideally should be linked to microstructure and inclusion density. These have rather been used as material fitting parameters, which indicates that the simulated ductile-to-brittle transition curve is not uniquely determined. The transition curve can be adjusted as required, and does not give a representative presentation of the DBT as it is. The model needs to be further developed in order to accurately predict the full transition from ductile to brittle behaviour in other material than the one treated in this thesis.

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A | Derivation of Equations

A.1 Equations 2.8 and 2.9

Engineering strain from tensile testing is defined as:

$$e = \frac{\Delta L}{L_0} \tag{A.1}$$

True stress can be found through the following equation.

$$\epsilon = \int \frac{dL}{L_0} = ln\left(\frac{L}{L_0}\right) \tag{A.2}$$

Inserting $L = L_0 + \Delta L$ gives the following:

$$\epsilon = ln\left(\frac{L_0 + \Delta L}{L_0}\right) = ln\left(\frac{L_0}{L_0} + \frac{\Delta L}{L_0}\right) \tag{A.3}$$

Inserting A.1 gives:

$$\epsilon = ln\left(\frac{L_0}{L_0} + e\right) = ln(1 + e) \tag{A.4}$$

True stress from tensile testing is defined as:

$$\sigma = \frac{F}{A} \tag{A.5}$$

This can be rewritten as:

$$\sigma = \frac{F}{A} \times \frac{A_0}{A_0} = \frac{F}{A_0} \times \frac{A_0}{A} \tag{A.6}$$

where $\frac{F}{A_0}$ is the engineering stress, s. The material volume is constant, which gives

$$A_0 L_0 = AL \tag{A.7}$$

Inserting this into Equation A.6 gives

$$\sigma = s \times \frac{L}{L_0} = s \times \frac{L_0 + \Delta L}{L_0} \tag{A.8}$$

Inserting Equation A.1 gives

$$\sigma = s(1 + e) \tag{A.9}$$

A.2 Equation 2.21

Cottrell[20] and Petch[54] derived an energy balance for crack nucleation in the presence of slip. This can be expressed as:

$$\sigma_F n\mathbf{b} = \beta\gamma_s \tag{A.10}$$

The displacement, $n\mathbf{b}$ may be expressed through:

$$n\mathbf{b} \cong \frac{(\tau - \tau_i)}{G}d \tag{A.11}$$

where G is the shear modulus. The friction stress, τ_i, in polycrystals deforming by slip only can be determined by the following relation between flow stress and grain size:

$$\tau_y = \tau_i + k_s d^{-1/2} \tag{A.12}$$

where k_s is a constant describing the grain boundary contribution to strength. Substituting Equation A.12 into Equation A.11 gives:

$$n\mathbf{b} = \frac{k_s d^{1/2}}{G} \tag{A.13}$$

Further substituting Equation A.13 into Equation A.10 gives the following condition for crack nucleation at yield stress, i.e $\sigma_F = \sigma_y$:

$$\sigma_y k_s d^{1/2} \geq \beta G\gamma_s \tag{A.14}$$

Substituting Equation 2.4 into Equation A.14 gives the following equation for energy balance:

$$(\sigma_i d^{1/2} + k_y)k_s \geq \beta G\gamma_s \tag{A.15}$$

The constants from Equations 2.4 and A.12 have the following relationship, $k_y = mk_s$, where m is a factor relating the average normal-to-shear stress ratio in the slip plane. This must not be mistaken for β which relates to the overall stress state[25][45].

B | Experimental Force-CMOD Curves

Figure B.1: Experimental force-CMOD curves for room temperature.

Figure B.2: Experimental force-CMOD curves for 0°C.

Figure B.3: Experimental force-CMOD curves for −60°C.

C | Risk Assessment

NTNU		Kartlegging av risikofylt aktivitet	Utarbeidet av	Nummer	Dato	
☐			HMS-avd.	HMSRV2601	22.03.2011	
HMS			Godkjent av		Erstatter	
			Rektor		01.12.2006	

Enhet: Institutt for produktutvikling og materialer   **Dato:** 1/2 – 17

Linjeleder: Torgeir Welo

Deltakere ved kartleggingen (m/ funksjon): Odd M. Akselsen (veileder), Ingrid Holte (student)

(Ansv. veileder, student, evt. medveiledere, evt. andre m. kompetanse)

Kort beskrivelse av hovedaktivitet/hovedprosess: Masteroppgave student xx. Tittel på oppgaven. Modelling the Ductile-to-Brittle Transition in Steel

Er oppgaven rent teoretisk? (JA/NEI): JA   «JA» betyr at veileder innestår for at oppgaven ikke inneholder noen aktiviteter som krever

risikovurdering. Dersom «JA»: Beskriv kort aktiviteten i kartleggingskjemaet under. Risikovurdering trenger ikke å fylles ut.

Signaturer: Ansvarlig veileder: Odd M Akselsen -   Student: Ingrid Holte

ID nr.	Aktivitet/prosess	Ansvarlig	Eksisterende dokumentasjon	Eksisterende sikringstiltak	Lov, forskrift o.l.	Kommentar

Figure C.1: Risk assessment for the master's thesis.

D | A3 Posters

Figure D.1: The A3-poster presented at the start of the semester.

Figure D.2: The A3-poster presented at the end of the semester.