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Micromechanics of Fatigue with Application to Stents

Caoimhe A. Sweeney B.E. (2010)

Supervisors: Prof. Sean Leen and Prof. Peter McHugh

A thesis submitted to the National University of Ireland as fulfilment of the requirements for the Degree of Doctor of Philosophy.

Mechanical Engineering, National University of Ireland, Galway.

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Abstract

This thesis describes the development of a computational framework, based on experimental characterisation and validation, for the microstructure-sensitive modelling of fatigue crack initiation, with a focus placed on its application in stent fatigue design. The framework developed utilises crystal plasticity constitutive formulations for describing slip in individual grains in the microstructure. Coupled with realistic finite element microstructure geometries and microstructure-sensitive parameters, crack initiation is predicted for different loading conditions and microstructures. Extensive experimental testing is carried out for the calibration and validation of the micromechanical framework for the L605 CoCr alloy, typically used in modern stents. Grain structure, crystallographic texture and precipitate content are characterised via microscopy, while low cycle fatigue testing allows calibration of crystal plasticity constants, via comparison of macroscopic hysteresis behaviour, and identification of critical parameter values for prediction of fatigue crack initiation.

The calibrated framework is applied to the assessment of the high cycle fatigue performance of a generic stent design for both 316L stainless steel and the L605 alloy. The importance of size-scale consistency between fatigue predictive techniques and application is demonstrated. The micromechanical framework is also used to redesign the generic stent geometry for the L605 alloy, for which the original geometry is shown to be over-conservative. The framework is later val-
idated for use in the high cycle fatigue regime via comparison of predictions against stress-life data for L605 foil micro-specimens, representative of the stent size-scale.

Studies on the microstructural mechanisms influencing fatigue are also investigated. A study on ferritic steel four-point bending fatigue tests, in which the specific grain topography and crystallographic texture in the notch region of individual specimens is explicitly modelled, highlights the influence of elastic anisotropy and accumulated plastic slip on the location of fatigue crack initiation sites. In another study, a strain-gradient plasticity formulation is adopted to predict, for the first time, the experimentally-observed effect of grain size on the low cycle fatigue behaviour of as-received and heat-treated L605 CoCr material, where higher geometrically necessary dislocation density in fine-grain specimens is shown to play a key role.
Acknowledgements

First, I would like to thank my supervisors Prof. Sean Leen and Prof. Peter McHugh for their constant support, enthusiasm and willingness to impart knowledge and expertise over the last four years. A special thanks also to Prof. Fionn Dunne for his invitation to carry out research at the University of Oxford, during which time he imparted to me valuable knowledge on strain-gradient crystal plasticity modelling, which would become a key part of my thesis. I would also like to thank Dr. Barry O’Brien for his insights into heat treatment, microscopy and polishing of the L605 CoCr alloy, Dr. Wim Vorster for his initial work on the four-point bending fatigue study and Dr. Pat McGarry for his advice on stent modelling early in the project.

Thanks to the Irish Research Council (IRC) and College of Engineering and Informatics at NUI Galway for providing funding for the undertaking of this research. Without the support of many people, the experimental component of this research would not have been the success it was. Firstly, I would like to thank the technicians here in the Engineering Building at NUI Galway, Mr. Bonaventure Kennedy, Mr. Pat Kelly and Mr. William Kelly, for specimen manufacture and preparation, test set-up and generally being there to give a helping hand. Thanks to Mr. James Cotter of the Chemistry Department for preparation of all etching and electro-polishing solutions used in this research and to Dr. Eadaoin Timmins from the National Centre for Biomedical Engineering Science (NCBES)
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List of Publications

The work presented in this thesis has resulted in the following publications:


The following paper has been submitted to the Journal of Mechanical Behavior of Biomedical Materials for consideration for publication:

Chapter 8: C. A. Sweeney, B. O’Brien, F. P. E. Dunne, P. E. McHugh, S. B. Leen, “Micro-scale testing and micromechanical modelling for high cycle fatigue of CoCr stent material”.

List of Publications
1. Introduction

1.1. Chapter Summary

Fatigue of devices is of great concern in many industries. The factors which affect fatigue performance can vary, dependent on the type of fatigue loading applied, the geometry of the device subjected to fatigue, the material, environmental effects etc. In the case of small devices, with dimensions comparable in size to microstructural features of the material, such as cardiovascular stents, fatigue is highly dependent on the microstructure and microstructural evolution during the fatigue process.

Traditional techniques for prediction of fatigue performance of devices are largely macro-scale approaches, typically tending towards empirical methods, based on large-scale testing and, thus, neglect the underlying microstructure-based mechanisms which cause fatigue. The purpose of this research is to investigate these mechanisms and develop predictive computational capabilities for microstructure-sensitive fatigue.

This chapter details the motivation and foundation for this research, starting with an introduction to fatigue in Section 1.2, including an overview of the driving physical mechanisms and existing computational approaches for fatigue.
1. Introduction

Section 1.3 introduces the cardiovascular stent, and the topic of stent fatigue and the resulting potential adverse effects, as well as the typical industry-standard techniques for assessing stent fatigue performance. Motivation gathered from previous sections is discussed in Section 1.4, from which the aims and objectives of the thesis are cultivated, and a summary of each chapter is provided in Section 1.5.

1.2. Fatigue: Importance, Mechanisms and Modelling

1.2.1. What is fatigue and why is it important?

Fatigue refers to gradual degradation in material behaviour over time, caused by repetitive or cyclic loading on a component for many repetitions or cycles. Fatigue can often result in the partial or complete failure of the material, manifesting in the fracture of the component or structure for the latter. In general, fatigue is not desirable and components are designed to withstand the anticipated in-service fatigue loading for as long as is economically feasible. Different approaches for fatigue design can be adopted [1], depending on the application. Components can be designed to have infinite fatigue life (i.e. such that stresses are well below the fatigue limit) or a finite safe-life, after which the component should be replaced. For example, cutting tools and ball bearings are rated for a minimum life under specified operational conditions, after which they are replaced. Other approaches design for the presence of cracks, where either features are included in component structure to prevent a fatigue crack propagating to failure prior to routine inspection (fail-safe design), or the design process includes fracture mechanics calculations which indicate that a potential crack cannot propagate
1. Introduction

to failure prior to inspection (damage-tolerant approach). The wing of a plane, for example, is designed to tolerate the presence of cracks, where cracks above a threshold size are checked for regularly. In the case of many components, premature failure can have catastrophic effects, e.g. failure of a bridge or building, fracture of a plane wing, stent fatigue fracture, etc.

For all cases mentioned above, knowledge of fatigue performance is desirable prior to placement of a component in service and, in the majority of cases, it is a requirement. A designer should know if a component is expected to fail in operation and, if so, after how long in operation (number of fatigue cycles) and in what manner (i.e. gradual ductile or sudden brittle fracture). Experimental testing can provide much information on expected fatigue performance, but it is often expensive, including both manufacture of specimens and execution of tests. Computational modelling offers a method of assessing feasibility of a component design well in advance of testing. Potential designs can be explored, both in terms of material choice, including heat-treatment etc. being considered for application to the material, and component dimensions, without the commitment required for prototyping.

1.2.2. Underlying Mechanisms

The fatigue of any metallic device or structure is dictated by the initiation and propagation of a critical crack, which causes eventual failure. Fatigue crack initiation (FCI) occurs as a result of continuous build-up of fatigue damage. Once a crack forms, the initial stage of propagation is heavily dependent on the surrounding microstructure. However, once a crack reaches a certain size relative to the microstructure, propagation becomes less dependent on microstructure and growth path is dictated by the loading direction, as illustrated in the schematic of Fig. 1.1(a). The influence of microstructure on crack growth rate can also be
1. Introduction

Figure 1.1: (a) Schematic of crack growth from the free surface of a specimen under uniaxial loading and (b) a plot of crack growth rate versus crack size, including influence of microstructure and modelling approaches for each stage.

seen in Fig. 1.1(b). Crack initiation and propagation can have varying degrees of relative importance depending on the proportion of fatigue life governed by each, determined by the specific device and loading sequence. In the case of small devices, for which dimensions are comparable in size to microstructural features, the number of cycles for a crack to propagate to failure is small and thus crack initiation is expected to dominate fatigue life.

A metallic microstructure consists of crystallographic grains, each composed of a structured crystal lattice of atoms. Irreversible slip or glide of dislocations (irregularities in the lattice, such as a missing half plane of atoms) across the crystal lattice takes place during fatigue in the microstructure. Over many cycles, these dislocations build up at grain boundaries, free surfaces and other barriers to form dislocation structures, such as the persistent slip bands shown in Fig. 1.2(a), which themselves become sites for crack initiation. Examples of slip bands observed in 316LN steel and nickel are provided in Figs. 1.2(b) and (c), respectively. Dislocation motion and, thus, crack initiation are heavily influenced by microstructural features, including grain boundaries, particles within the lattice, orientation mismatch between grains, multi-phase regions, etc. The early stages of crack propagation are similarly affected by microstructure until
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Figure 1.2: (a) Schematic of slip band formation along a grain boundary, (b) slip bands observed in a 316LN steel after 60000 cycles of fatigue loading [2] and (c) formation of cracks along slip bands in nickel after 140000 cycles of fatigue loading [3].

the crack size is larger than several grain sizes, when microstructural features have less influence on crack path.

1.2.3. Fatigue Prediction

Modelling techniques for fatigue vary from the empirical type to approaches describing the physical mechanisms involved. Prediction of large crack growth is well established via use of the power law Paris equation based on linear-elastic fracture mechanics (LEFM). The $J$ integral technique for prediction of physically small crack growth based on elastic-plastic fracture mechanics (EPFM) is also considered sufficiently established. The stages of crack growth at which LEFM
and EPFM are used is illustrated in Fig. 1.1(b). However, in the case of microstructurally small crack growth and crack initiation, the approaches available are less established. One approach for prediction of microstructurally small crack growth is to alter equations of LEFM and EPFM to include an effective crack length, which captures crack growth below the threshold stress intensity factor and increased growth rates at smaller crack sizes. Prediction of FCI tends towards the use of damage approaches, where damage is assessed via use of indicator damage parameters and crack initiation is predicted to occur at critical values of these parameters. Traditionally, these parameters were developed based on macro-level stresses or strains or a combination of the two. However, especially for the case of crack initiation dominated fatigue, microstructure has significant influence on the formation of cracks and, thus, micro-level parameters are required. Additionally, the macro-scale approaches mentioned cannot capture the scatter observed experimentally in fatigue performance. Despite being manufactured from the same material and with identical geometry, no two components will exhibit the same fatigue behaviour, owing to microstructural inhomogeneity. Therefore, representation of the variability introduced by microstructure is necessary to fully understand and reasonably predict the range of fatigue behaviour observed experimentally.

1.3. Fatigue of Stents

1.3.1. What is a Stent?

A stent is a tubular metallic or polymeric mesh, as shown in Fig. 1.3(a), with micro-scale dimensions, evident from the stent strut shown in Fig. 1.3(b). Stents are key components used in the modern treatment of ischemic heart disease.
IHD is a condition describing a reduction in cross-sectional area in a coronary artery available for blood flow, or lumen, due to the build-up of plaque, also known as atherosclerosis. Symptoms of IHD manifest in the form of heart pain, or angina, due to insufficient blood flow to the heart muscles, and can result in a heart attack, or myocardial infarction, due to complete blockage of blood flow to the heart muscles, leading to the development of scar tissue. Percutaneous coronary intervention (PCI), also known as angioplasty, is a non-surgical procedure, developed in the last two decades for the treatment of IHD. The procedure involves the use of catheters to navigate the vascular system to the site of the blockage, followed by inflation of a balloon to reopen the lumen and, often, installation of a stent to provide long-term support to the artery. A simple illustration of stent deployment is provided in Fig. 1.4. The development of the angioplasty procedure has revolutionised the treatment of IHD, providing an alternative to coronary artery bypass surgery, where the blocked artery is bypassed via grafts of arteries or veins from elsewhere in the body.
1. Introduction

Figure 1.4: Installation of a stent in a coronary artery (adapted from [6]) showing (a) stent crimped on deflated balloon and catheter at site of plaque blockage prior to deployment, (b) inflated balloon causing expansion of stent into artery, (c) expanded stent maintaining lumen after balloon is removed.

1.3.2. Evolution of Coronary Stents

Over the past two decades, several factors have influenced and driven the design of stents. Self-expanding nitinol stents and bare metal stents (BMSs) were the first to be used in coronary arteries [7]. However, issues surrounded these initial stents, primarily related to a thickening of the vessel wall or neointimal hyperplasia, causing a narrowing of the lumen or in-stent restenosis (ISR). Revascularisation was often needed. Metal ion release into surrounding tissue has been highlighted as an inducer of neointimal hyperplasia for BMSs [8]. These issues prompted the development of drug-eluting stents (DESs). First and second generation DESs were coated with a polymeric layer containing anti-proliferative drugs, released over controlled periods, resulting in a reduction of rates of ISR [7,9]. Complications related to late events, such as formation of a blood clot or thrombus on a stent, presented with first generation DESs. Second generation DESs
were designed to provide greater endothelial coverage of stent struts, thus preventing clot formation. In more recent times, research has been carried out on biodegradable polymeric and non-polymeric DESs to further improve endothelialization [9,10]. Much interest has also been generated in biodegradable stents, composed of magnesium or polymers, allowing the provision of scaffolding only for the period required, thus removing triggers for late cardiac events and reducing the need for long-term dual anti-platelet therapy, as required with permanent stents [10]. Interest has also been renewed in self-expanding nitinol stents, which lost popularity with the introduction of DESs. Self-expanding stents offer superior conformability to balloon-expanded stents and boast a lower incidence of edge dissections [10].

Stent materials have also evolved to improve mechanical performance, biocompatibility and visibility, and to reduce stent profile. With a focus on permanent, balloon-expandable stents, biomedical grade 316L stainless steel (SS) was the material of choice for initial BMSs and first generation DESs, offering good strength and corrosion resistance. However, imaging of these stents was difficult due to a low density and their ferromagnetic nature. Also, a high release rate of metal ions, primarily nickel, from 316L SS stents can trigger inflammatory reactions leading to neointimal hyperplasia [8,9,11]. While still employing SS, other materials were also used for second generation DESs. Cobalt chromium (CoCr) alloys L605 and MP35N are two such materials, which are commonly used in coronary stents today [7,9,11]. The high Young’s modulus of CoCr alloys limits recoil effects and high radial strength allows design of thinner struts than 316L SS stents, reducing stent profile and improving deliverability. CoCr alloys show superior biocompatibility to 316L SS and higher density, resulting in improved radio-opacity for X-ray imaging. Despite large percentages of nickel content in CoCr alloys, the rate of metal ion release is less than for 316L SS [9]. Tantalum (Ta) and titanium (Ti) have been investigated as potential stent materials due to
their excellent corrosion resistance, having highly stable oxide surface layers, and Ta also exhibits excellent properties for magnetic resonance imaging and X-ray fluoroscopy. However, owing to the yield and tensile strengths of Ta being close together and the low tensile strength of Ti, a high probability of fracture during deployment exists for these two materials. They are, therefore, more commonly used as coatings for 316L SS stents \[8, 11\]. Similarly, platinum (Pt) alloys have also shown excellent biocompatibility, with good properties for imaging and support of endothelialization; however, owing to their poor mechanical properties, Pt alloy stents exhibit a high recoil percentage, which can cause inflammatory responses \[8, 11\].

Innovation surrounding the treatment of stent surfaces has allowed much improvement in biocompatibility. While, for the most part, this involves surface coatings for dispensing anti-proliferative drugs, other approaches involve modification of the base metal surface. One approach makes use of a microtextured or roughened stent surface to which the drug can be attached \[9\]. Similarly, the use of microporous stent surfaces has been investigated; the drug is loaded into micro-pores, which later promote endothelialization once the drug has been eluted \[10\]. Macro-reservoirs laser-cut from the stent surface, which penetrate through the complete strut thickness, containing a biodegradable polymer and drug mix, have also been used \[9, 10\].

### 1.3.3. Stent Fatigue Fracture

It is clear from above that the primary drivers of stent design are (i) surface modifications for the prevention of ISR and stent thrombosis, and promotion of endothelialization, (ii) reduction of stent profile and (iii) mechanical performance during stent deployment and recoil. Fatigue does not appear to have been a major driver of design in the stent industry. Stents undergo multiple stages of
deformation in their lifetime, including crimping or crushing of the stent over a
deflated balloon on a delivery catheter, deployment into the destination blood
vessel via expansion of the balloon, recoil after removal of the balloon and a
pulsatile cyclic pressure due to pumping of the blood. Indeed, in the past, stent
fracture was associated with stent deployment, during which a stent sustains the
largest proportion of deformation, and fatigue was not considered as important.
However, awareness of the occurrence of stent fatigue fracture has come to the
fore in recent times with the development of DESs [12–14]. DESs are coated with
a layer of anti-proliferative drugs, which prevent restenosis or the re-growth of
tissue over exposed stent surfaces. As such, instances of stent facture have been
revealed, which previously went unnoticed, before DESs.

Various studies have reported on stent fracture from a few months to several
years after implantation in patients. Sianos et al. [15] reported on fracture of
316L Cypher sirolimus-eluting stents (SESs) in two separate cases after 6 months
and 5 months of implantation, with neointimal formation indicating ISR at the
fracture sites only, requiring further PCI. Yagi et al. [14] reported on observed
hinge movement of a BMS implanted in the right coronary artery (RCA) due to
pulsatile motion, and postulated that the mechanical stimulation of the vessel
wall by this movement contributed towards the development of a blood clot, or
thrombus, near the site of hinge movement, 9 years after implantation. Shaikh
et al. [16] investigated the occurrence of stent fracture for PCI cases in ISR,
within a 12 month period, in which DESs were implanted. The study reported
that stent fracture had occurred in 35 out of 188 cases of ISR and statistically
identified higher risk of stent fracture associated with (i) implantation in the
RCA, (ii) male patients, (iii) smaller diameter blood vessels, (iv) overlapping
stent sections and (v) stenting on bends greater than 70°. A study by Almasood
et al. [17] reports cases of stent fracture for two patients. In the case of the
first patient, stent fracture was observed 4 months after implantation of a CoCr
1. Introduction

Figure 1.5: SEM images of a 316L SS stent installed in the RCA [18], showing (a) strut fracture and plastic deformation, (b) HCF fracture surface (c) plastic deformation of another strut and (d) formation of slip-band extrusions and intrusions which are considered susceptible to fracture.

Xience DES. Multiple stent fractures occurred in the case of the second patient after 5 months implantation, including fracture of CoCr and PtCr stents. In both cases, patients presented with angina and ISR was revealed at the sites of stent fracture. Halwani et al. [18] carried out an investigation of 7 cases of stented calcified coronary arteries, in which 18 stents were retrieved by chemical removal of surrounding tissue and analysed. Stent fracture was observed in 9 out of 11 DESs and 3 out of 7 BMSs, including both 316L stainless steel (SS) and CoCr stents, from between 19 to 84 months after implantation. Slip bands were observed in several cases, an example of which is provided in Fig. 1.5, indicating fracture by high cycle fatigue (HCF). A review of further reported incidences of stent fracture has been carried out by Nair and Quadros [19].

Serious consequences can result from stent fracture. The risk of ISR is higher in cases of stent fracture [19], corroborated by evidence in the studies above.
Irritation of the vessel wall by a fractured strut may cause inflammation leading to neointimal hyperplasia, reducing the lumen. Exposure of fractured surfaces can also trigger platelet activation, causing stent thrombosis [19], which can lead to myocardial infarction and, in some cases, sudden cardiac death [20–23]. Stent fracture of BMSs may go unnoticed altogether as tissue re-growth covers and supports the stent [13,19]. While this restenosis acts to reduce the lumen, fractured BMS surfaces are protected from exposure, reducing the risk of thrombus formation and irritation of the vessel wall. In the case of DESs, however, re-growth of tissue over stent surfaces is prevented. Thus, fracture surfaces are exposed to the lumen, increasing the risk of stent thrombosis and neointimal hyperplasia. DES fractures are unsupported by tissue re-growth and can, therefore, result in a loss of radial strength and reduction in lumen. Fracture can cause a maldistribution of the drug [12] and focal ISR at the exposed fracture site. While reduction of lumen and stent thrombosis can be treated via revascularisation, the outcome of such procedures is not always successful and can begin a new cycle leading to a recurrence of symptoms.

1.3.4. Fatigue Design - Industry Standards

The Food and Drug Administration (FDA) of the U.S. Department of Health and Human Services are the regulatory body for the design and testing of stents, including fatigue design. The FDA have published a set of recommendations for non-clinical tests to be carried out on intravascular stents for which approval is being sought [24]. Three steps pertaining to fatigue design are included among these recommendations:

- A finite element-based stress-strain analysis, including modelling of each loading step contributing to residual stress, and realistic physiological load-
1. Introduction

• Assessment of fatigue resistance via a Goodman analysis, or other appropriate fatigue analysis method, using mean and alternating stress inputs from stress-strain analysis results,

• Accelerated durability testing of the device for the equivalent of 10 years of operation, under pulsatile flow and other physiological conditions which replicate the implant environment \textit{in vivo}.

While the guidelines here cover both experimental and computational fatigue tests and recommend that both FE simulations and durability tests are carried out for worst case conditions, some shortcomings of the guidelines exist. Firstly, the concept of “test to fracture” is not enforced by these recommendations, instead a “test to success” approach is adopted [25]; it is not required to provide an expected life for the device, merely to demonstrate that it will last the specified 10 years operational life. Additionally, use of a Goodman analysis in determining fatigue resistance or fatigue factor of safety for the device is entirely dependent on the ultimate tensile strength and endurance fatigue limit used to form the Goodman line. However, endurance fatigue limits are often taken at $10^7$ cycles and, thus, factors of safety calculated based on these limits cannot be relied upon for a minimum \textit{in vivo} fatigue life of 10 years, corresponding to approximately $4 \times 10^8$ cycles (based on an average heart rate of 72 beats per minute). Secondly, consideration of microstructural effects is not explicitly included as a recommendation in relation to fatigue performance. While the guidelines recommend consideration and justification of constitutive models used, the examples provided refer to linear versus non-linear behaviour, isotropic versus anisotropic behaviour, temperature-dependency and raw versus processed material. As such, the guidelines do little to encourage a microstructure-sensitive investigation of fatigue performance; the need for such analyses has been raised in the literature [17, 26]. The drive towards smaller stent profiles and, thus, thinner stent struts has resulted in strut.
cross-sections with dimensions comparable in size to the microstructural features of the base metal, giving rise to inhomogeneous behaviour. An example of this is illustrated in Fig. 1.3(b), where as little as four grains can be seen in the cross-section of a 316L stent strut. The slip lines of Fig. 1.5(d) clearly testify to the micro-plasticity nature of stent fatigue, which is not accounted for by the macro-stress-based approach of a Goodman analysis.

1.4. Thesis Aims and Objectives

The aim of this work is to develop a micromechanical computational framework for investigation of the microstructural factors which influence fatigue and allow prediction of FCI life. The fatigue analysis of cardiovascular stents is used as a demonstrator application for this micromechanical framework.

Investigation of the effectiveness of different constitutive models for simulating microstructural phenomena affecting fatigue is a key objective. This primarily relates to a comparison of material hardening formulations and the mechanisms involved, but also includes treatment of elastic behaviour.

Another objective is the development of microstructure-sensitive methods for prediction of FCI life and the comparison of these methods with existing macro-scale methods. Particularly for HCF, traditional stress-based approaches, which assume elastic fatigue only, are challenged.

From the previous section, it can be seen that a need exists in stent design approaches for microstructure-sensitive methods for prediction of stent fatigue performance. Stent fatigue is, thus, a key theme in this thesis, both in response to this gap in stent design techniques, and as a demonstration of the applicability
1. Introduction

of the micromechanical framework.

Finally, calibration and validation via experimental work is another important objective in this thesis, to bring authenticity to predictions and conclusions made. The test program includes both microscopy for microstructural characterization, allowing development of FE polycrystalline geometries, and fatigue and tensile testing for calibration of cyclic hysteresis behaviour and parameters for predicting FCI, as well as validation.

1.5. Thesis Overview

The thesis begins with a review of the relevant literature in Chapter 2, including experimental observations of microstructural phenomena in fatigue, microstructure-sensitive modelling techniques and stent fatigue modelling. A description of finite element theory and constitutive models is given in Chapter 3.

Chapter 4 describes the development of a micromechanical model for 316L stainless steel and application of this framework to assess fatigue performance of a generic stent design. This work also explores the usefulness of kinematic hardening, particularly in modelling high initial deformation steps, followed by fatigue. The micromechanical approach is extended to assess the same generic design for a CoCr alloy, typically used in current generation stents, in Chapter 5. A comparison is made between the performance of the two materials, leading to redesign of the CoCr stent for optimised microstructure-sensitive fatigue.

Chapters 6 and 7 focus on exploring mechanisms contributing to FCI through the use of dislocation-based crystal plasticity constitutive models, which can capture strain-gradient effects. A four-point bending fatigue study is presented in
Chapter 6, in which computational predictions of FCI are compared directly with experimental observations for specific microstructures. Chapter 7 specifically studies the effect of grain size on low cycle fatigue for a CoCr alloy, via comparison of experimental and simulated data for fine-grain (as-received) material and coarse-grain (heat-treated) material.

Comparison of experimental results and computational predictions for a test representative of stent fatigue, both in terms of loading and specimen size, is presented in Chapter 8. The study facilitates validation of the micromechanical framework and a back-to-back comparative assessment of the power-law and strain-gradient crystal plasticity formulations.

Finally, a general discussion of the results is presented in Chapter 9, including key conclusions on the impact of findings for stent fatigue design.
2. Background

2.1. Chapter Summary

While Chapter 1 set out the objectives of the thesis and provided motivation for microstructure-sensitive fatigue modelling and improved fatigue design tools for cardiovascular stents, this chapter will build on this further. An overview of the different components of fatigue life and conventional methods for prediction of life and crack behaviour is first provided. This is followed by a review of experimental observations of fatigue crack initiation in the literature and the factors which influence crack initiation. Existing techniques for modelling fatigue, with emphasis on microstructure-sensitive approaches, are then appraised in the categories of constitutive models, predictive techniques and polycrystal geometry representation and generation. Finally, the standard practice for stent fatigue analysis is outlined, and new existing approaches for stent fatigue modelling and validation of those approaches are assessed.
2. Background

2.2. Fatigue Life and Stages of Crack Growth

Fatigue can be categorised into different regimes depending on the type of plasticity distribution incurred. At low stress amplitudes, strains appear to be macroscopically elastic, with only localised pockets of plasticity occurring at points in the microstructure favourable to slip (e.g. favourably oriented grains etc.). This is known as high cycle fatigue (HCF), as the accumulation of damage is slow due to the small amount of micro-plasticity, thus resulting in long fatigue lives. The empirical Basquin equation [27] was developed for the prediction of total life for a material in the HCF regime based on the applied stress-range:

$$N_f = \left( \frac{\Delta \sigma}{C_2} \right)^{-\gamma_2}$$  \hspace{1cm} (2.1)

where $C_2$ and $\gamma_2$ are material constants. High stress amplitudes trigger more widespread and uniform plasticity, resulting in a reduced number of cycles to failure and, thus, is referred to as low cycle fatigue (LCF). The Coffin-Manson relation can be used to predict number of cycles to failure in the LCF regime, based on the applied macroscopic plastic strain range:

$$N_f = \left( \frac{\Delta \epsilon_p}{C_1} \right)^{-\gamma_1}$$  \hspace{1cm} (2.2)

where $C_1$ and $\gamma_1$ are material constants. The traditional fatigue limit (i.e. maximum stress amplitude at which fatigue life is infinite) of a material is generally evaluated in the HCF regime at $10^7$ cycles. However, a third regime has been noted to exist, known as the ultra-high cycle fatigue (UHCF) regime [28], at $10^9 – 10^{10}$ cycles, during which failure can occur at the traditional fatigue limit evaluated at $10^7$ cycles. Further lowering of the stress amplitude reveals a second fatigue limit as illustrated in Fig. 2.1(a).
2. Background

Figure 2.1: (a) Schematic of traditional fatigue limit in HCF regime and second fatigue limit in the UHCF regime and (b) Kitagwa-Takahashi diagram for crack growth behaviour, where propagation is predicted to occur for all points above the curve and crack arrest is predicted for all points below the curve.

Across all aforementioned regimes, fatigue life can be defined in terms of the stages of the formation and growth of a crack. Total fatigue life, $N_f$, can be decomposed into components accordingly [29]:

$$N_f = N_i + N_{MSC} + N_{PSC} + N_{LC}$$  \hspace{1cm} (2.3)

where $N_i$, $N_{MSC}$, $N_{PSC}$ and $N_{LC}$ represent number of cycles during which crack initiation, microstructurally small crack growth, physically small crack growth and long crack growth occur, respectively. Crack initiation and propagation dominate different proportions of life for different regimes of loading. In HCF, $N_f$ is dominated by $N_i$, while for LCF crack propagation plays an increasing role.

Fracture mechanics is conventionally used to predict the growth behaviour of an existing crack. The plastic zone at the crack tip is small compared with crack size, $a$, in the long crack growth stage and can, thus, be predicted using linear elastic fracture mechanics (LEFM). According to LEFM, crack growth occurs when the stress intensity factor range, $\Delta K$ is greater than a threshold stress intensity factor range, $\Delta K_{th}$, where $\Delta K$ is calculated as a function of far field...
2. Background

stress range, $\Delta \sigma^\infty$, and specimen geometry factor $Y$:

$$\Delta K = Y \Delta \sigma^\infty \sqrt{\pi a}$$  \hspace{1cm} (2.4)

where $a$ is the crack size. As mentioned in Chapter 1, the Paris equation, relating $\Delta K$ to crack growth rate, $da/dN$, is widely accepted to capture long crack growth:

$$\frac{da}{dN} = C(\Delta K)^m$$  \hspace{1cm} (2.5)

where $m$ is a material constant identified from experimental data.

While use of the Paris equation for long cracks is appropriate, it has been observed experimentally that short cracks can propagate below $\Delta K_{th}$, while also exhibiting faster growth rates than long cracks at a given $\Delta K$. El Haddad [30] proposed that for small crack sizes $\Delta K$ can be evaluated as:

$$\Delta K = Y \Delta \sigma^\infty \sqrt{\pi (a + a_0)}$$  \hspace{1cm} (2.6)

where $a_0$ is found to correspond to the critical crack size for the fatigue endurance limit, $\sigma_e$:

$$a_0 = \frac{1}{\pi} \left( \frac{\Delta K_{th}}{\sigma_e} \right)^2$$  \hspace{1cm} (2.7)

The Kitagawa-Takahashi diagram, given in Fig. 2.1 (b) illustrates the significance of $a_0$ as it marks a transition between crack growth regimes.

For smaller cracks, the plastic zone at the tip of the crack is comparable in size to the crack length (i.e. physically small crack growth) and LEFM is no longer a reasonable assumption, as demonstrated by the requirement of the El-Haddad modification to the Paris equation above. The $J$ integral from elastic-plastic fracture mechanics (EPFM) can then be used for quantifying the strain field.
around a crack tip:

\[ J = \int_C \left( W \, dy - T \cdot \frac{\partial u}{\partial x} \, ds \right) \]  \hspace{1cm} (2.8)

where \( x \) and \( y \) are the directions parallel and perpendicular to the crack direction, \( ds \) is an increment on contour \( C \) around the crack tip, \( T \) is the stress vector acting on \( C \), \( u \) is the displacement vector and \( W \) is the strain energy density. The \( J \) integral range, \( \Delta J \), can be identified and used in a relation similar to Eq. 2.5 for prediction of physically small crack growth rate, where crack growth is not expected to occur below the threshold \( J \) integral range, \( \Delta J_{th} \).

While the techniques above can explain the driving factors for long crack growth and physically small crack growth, the prediction of crack behaviour via macro-based methods becomes difficult in the microstructurally small crack growth and crack initiation stages, as illustrated in the schematic of Fig. 1.1. Instead, mechanisms based in the heterogeneous microstructure dictate behaviour.

### 2.3. Fatigue Crack Initiation - Experimental Observations

Risbet and Feaugas [31] provide an overview of slip band formation and the relationship between irreversible strain and FCI. Sangid [32] provides a comprehensive overview of the physics of fatigue crack initiation (FCI), including a step-by-step description of the formation of persistent slip bands (PSBs) to give FCI. As introduced in Chapter 1, FCI in ductile metals can be attributed to dislocation mechanisms. When the resolved shear stress on a slip system reaches the critical resolved shear stress, \( \tau_c \), of the material, dislocations in the microstructure glide or slip along the close-packed planes or planes of least resistance in the metal until they reach an obstacle, such as a grain boundary or precipitate. Further
increase of stress can trigger the generation of more dislocations and can provide additional energy to impeded dislocations to overcome obstacles via cross-slip, climb, looping etc. Cyclic loading leads to the irreversible slip of dislocations along preferred low energy pathways and the eventual formation of dislocation structures which minimize energy. Slip bands form as a result of the increased dislocation density, manifesting in intrusions and extrusions at free surfaces and grain boundaries, as illustrated in Fig. 1.2. This results in stress concentrations and highly localized strain, leading to FCI.

Lukáš and Kunz review experimental studies on the formation on PSBs in fcc single crystals [33]. One of the highlighted studies reports an increase in volume fraction of PSBs with increasing plastic strain amplitude for copper single crystals, for symmetric strain or stress controlled loading. However, the response was found to depend strongly on the regime of cycling, as cell structures instead of PSBs were observed to form along the primary slip system (i.e. slip system with highest Schmid factor) for a non-zero mean stress under stress-controlled loading. For symmetric loading, the stress fatigue limit is found to be the same as the stress required to form PSBs. In the UHCF regime, where stresses are below the traditional stress fatigue limit, cyclic slip irreversibility is responsible for generating surface roughness, that may lead to FCI. For fcc single crystals, FCI is observed to occur at the free surface, where higher stresses and less constraints exist, or at pores lying near the surface, which behave as points of stress concentration and whose inner surfaces are akin to free surfaces. Three requirements for FCI are identified; a peak-valley topography at the surface, higher plastic strain at the intrusion root and a suitable dislocation configuration at the intrusion (i.e. a structure which prevents local stress relaxation by disallowing unobstructed glide).

Buque [34] carried out a study on PSB formation in nickel polycrystals, cyclically loaded at constant plastic strain amplitude ranging from $5 \times 10^{-5}$ to $5 \times 10^{-3}$. Three
range sets were identified; $<1\times10^{-4}$ (range I), $>1\times10^{-3}$ (range III) and range II between ranges I and III, where a quasi-plateau in saturated stress amplitude is observed. Slip markings were removed from each specimen surface after saturation of the stress amplitude and SEM was used to record the evolution of PSBs, recording both grain orientation via electron back-scattering patterns and dislocation structures via electron channelling contrast (ECC). While PSBs were not observed in range I, ladder-like structures were evident for range II after 10 cycles of loading. Due to the high density of dislocations in range III, PSB ladders were difficult to distinguish from the matrix. Location of PSBs were found to correlate with slip markings observed in the first stage of testing prior to re-polishing. The PSBs observed were found to increase with increasing plastic strain and to be inhomogeneously distributed. Slip traces predominantly occurred along primary and secondary slip planes, i.e. slip planes with the two highest Schmid factors. Spacing of dislocations was observed only to increase in range III testing, above plastic strain amplitudes of $1\times10^{-3}$, where the saturation stress amplitude begins to increase after the quasi-plateau of range II, suggesting a dependence of dislocation spacing on stress. Schwartz et al. [2] observed the formation and evolution of PSBs in 12 grains via scanning electron microscopy (SEM) of a notched 316LN specimen during interrupted LCF testing. After initial cyclic softening (20 cycles), PSBs were observed along the primary and secondary slip systems, as in [34]. PSBs formed at twin and grain boundaries, and at the grain interior for one case of PSBs along the primary slip system. Extrusions were already evident at this early stage. After cyclic softening (200 cycles), PSBs in the primary systems were observed to increase in width and height, while PSBs in secondary systems showed less activity. At half life (3000 cycles), cracks were observed to initiate at twin or grain boundaries where PSBs are present. Fujimura et al. [35] focused on the evolution of surface roughness during low cycle fatigue of an austenitic stainless steel (fcc structure) across three strain ranges; 8%, 4% and 1%. The surface roughness was observed to change with formation of extrusions.
and intrusions caused by irreversible dislocation cyclic motion. For all strain ranges a linear increase in surface roughness was observed up to $N/N_f = 0.4$, while the surface roughness appeared to saturate at $N/N_f = 0.6$ for the higher two strain ranges.

While surface PSBs are preferred locations for FCI, the site of FCI can vary further, depending on microstructure, surface roughness, temperature, mode of loading etc. In a study on modelling of FCI, Chan [36] included a summary of experimentally observed FCI for a range of materials in the literature, including, but not limited to, pure copper and aluminium, low carbon steels, carbon steels and titanium, nickel, cobalt and molybdenum alloys. Under various loading conditions and for a range of grain sizes, locations of FCI sites reported include slipbands, grain boundaries, alpha phase, pores, inclusions and carbides, thus conveying the extent of microstructural influence on FCI.

As mentioned in [33] above, non-symmetrical loading can influence the type of dislocation structures formed and thus FCI. Different preferred locations for FCI are also apparent in different regimes of loading [28]. While FCI in the HCF regime tends to occur at the surface, in the UHCF regime, at stresses below the traditional fatigue limit, FCI tends towards sub-surface mechanisms, at pores and inclusions in interior grains.

Surface roughness is evidently a direct effect of the formation of extrusions and inclusions in PSBs, as demonstrated in [35] above. Surface FCI is, therefore, more likely in specimens with high surface roughness. Twin boundaries are also shown to create an environment which promotes FCI. Man et al. [37] reported observations of preferential formation of persistent slip markings parallel to twin boundaries, in polycrystalline nickel under cyclic loading at constant plastic strain amplitude.
Dislocation glide and, thus the formation of PSBs, is heavily dependent on crystallographic orientation. Grains can be labelled 'soft' or 'hard' depending on whether they are favourably or unfavourably oriented for slip. Crystallographic orientation combinations can also have a significant influence, where the degree of orientation mismatch between adjacent grains can result in low angle grain boundaries (LAGBs), which can be overcome by dislocations, or high angle grain boundaries (HAGBs), which impede further slip of dislocations and thus can cause a build-up. The possibility of a 'rogue' grain combination can give rise to significantly higher stresses at the grain boundaries [29]. Crystallographic texture, i.e. a polycrystal composed of grains with preferential crystallographic orientation, can also have an effect on FCI. Mineur et al. [38] demonstrated this for 316L stainless steel specimens, where textured specimens with preferentially soft grains exhibit a higher crack density at failure than specimens with preferentially hard grains, and thus a higher tendency for FCI. Interestingly, while soft grain specimens were also shown to have lower stress amplitudes at a given plastic strain range, a difference in total fatigue life was not observed, suggesting a difference also in the crack propagation stage. Mineur et al. also reported on the detrimental environmental effect on fatigue performance, where fatigue lives were three times higher for specimens tested in a vacuum than in air for the same crystallographic texture and plastic strain range.

2.3.1. Size Effects

Various size effects on mechanical performance of metallic materials have been observed. Murphy et al. [39] demonstrated the size dependence of tensile behaviour of 316L micro-specimens with strut widths ranging from 60 to 500 µm, as illustrated in Fig. 2.2 (a), where thicker struts exhibited higher ductility with higher elongation at tensile fracture. Simons et al. [40] reported a similar ef-
2. Background

Figure 2.2: (a) Effect of specimen width on strain at necking for monotonic loading of 316L stainless steel wire specimens [39]. (b) Effect of foil thickness and annealing on the tensile behaviour of copper foils. [40].

fect for tensile testing of copper foils for thicknesses ranging from 10 to 100 µm, as seen in Fig. 2.2 (b); a more ductile response was observed for thicker foil specimens, while thinner specimens exhibited higher ultimate tensile strength. This study also looked at the effect of annealing on tensile behaviour, where the equiaxed, coarser-grained microstructure of the annealed material exhibited increased ductility, compared with the highly-textured, finer-grained, as-received material. Connelley et al. carried out a review on mechanical behaviour of micro-scale components across a broad range of applications [41], reporting similar size effects to those mentioned above for monotonic behaviour, while studies on fatigue performance were also reviewed. One example looked at the effect of film thickness (0.2 to 1.5 µm) on fatigue of silver films and demonstrated improved fatigue resistance for thinner film thickness. Results of in situ fatigue tests on 20 µm diameter titanium alloy specimens were reported by Szczepanski et al. [42], in which the superior fatigue performance of the micro-specimens in comparison with conventional bulk specimen data was demonstrated. Morrison and Moosbrugger [3] carried out an important study on the effect of grain size on the fatigue performance of polycrystalline nickel, across both the LCF and HCF regimes. In Fig. 2.3 (a), a harder cyclic response for fine grain nickel \(d = 24 \text{ µm}\) is shown, compared with the coarse grain material \(d = 290 \text{ µm}\), corresponding to higher stress amplitudes at applied plastic strain amplitudes. The fine grain nickel was also observed to provide superior fatigue performance, as shown in Fig. 2.3 (b).
2. Background

Figure 2.3: Effect of grain size on (a) stress amplitude and (b) fatigue life for nickel specimens under an applied cyclic plastic strain amplitude \[3\].

The life data of Fig.2.3 (b) also indicates an increase in effect of grain size at lower amplitudes of plastic strain, i.e. towards the HCF regime. Monotonic tensile and force-controlled fatigue tests were carried out by Järvenpää et al. \[43\] on coarse grain \(d = 14 \mu m\) and ultra fine grain \(d = 1.3\) and \(1.6 \mu m\) austenite for a 301LN stainless steel, revealing a higher yield strength for the ultra-fine grain austenite, with little compromise on ductility, and a higher fatigue limit for the ultra-fine grain material, compared with the coarse grain austenite. A difference in crack initiation sites was also noted for the two materials; FCI was noted to occur at slipbands for the coarse-grain austenite and at grain boundaries for the ultra-fine-grain austenite. This observed effect of grain refinement was applied by Roland et al. \[44\] to improve the fatigue performance of 316L stainless steel specimens. A mechanical attrition treatment was applied to specimens, leaving them with a nanostructured surface. High compressive residual stresses were observed as well as a significant reduction in grain size from between 10 and 50 \(\mu m\) to 20 nm. The treated specimens exhibited significantly improved behaviour under fully-reversed stress-controlled fatigue tests, while annealing was shown to further improve performance.

Geers et al. \[45\] categorised size effects into (i) strain-gradient effects, (ii) intrin-
2. Background

Figure 2.4: (a) Schmid factor map and (b) GND map for a Ti-6Al-4V polycrystal after 3000 cycles of loading [46].

Strain-gradient effects result from the storage of geometrically necessary dislocations (GNDs) to allow lattice curvature. Littlewood and Wilkinson imaged the formation of GNDs for Ti-6Al-4V under cyclic loading, as shown in Fig. 2.4, via cross-correlation-based electron backscattering diffraction analysis [46]. Intrinsic effects refers to the influence of intrinsic length scales in the microstructure, such as Burger’s vector magnitude, obstacle size and spacing, grain size and grain boundary width [47, 48]. For example, strengthening due to the Orowan mechanism, describing the bowing of dislocations between obstacles to overcome them, is dependent on obstacle spacing and, thus, can be classified as an intrinsic size effect. Strengthening at yield as a function of grain size due to the pile-up of dislocations at grain boundaries is another such effect (empirically captured using the Hall-Petch relation $\sigma_y = \sigma_0 + 1/\sqrt{d}$). An example of this can be seen clearly in Fig. 2.2 (b) for the 100 µm specimens, where the as-received specimen (fine-grained) exhibits a higher yield strength than the annealed specimen (coarser-grained) [40]. Statistical size effects arise when device or specimen dimensions are
comparable to grain size. The mechanical performance of such devices is often dictated by the behaviour of relatively few grains. Hence, features such as crystallographic orientation can significantly affect mechanical performance. Finally, surface constraints become increasingly important in the presence of a high ratio of surface area to volume. The behaviour of material at an interface or along a free surface can significantly affect the behaviour of a thin specimen. In the examples of experimental observations provided previously, both grain size and specimen dimensions are shown to have an effect on fatigue performance and, by extension, FCI. It can be postulated that all categories of size effects above play a role in these observations.

2.4. Fatigue Crack Initiation - Modelling

Approaches to modelling of FCI are varied, with studies focusing on different contributing mechanisms and loading regimes. The most common approach, typically using finite element (FE) analysis, can be broken into three components: constitutive formulation, predictive method (e.g. indicator parameters) and model geometry. Each of these components contributes to the ability of a model to predict FCI, both in terms of number of cycles to FCI and FCI location. Other approaches tend towards a smaller scale again, including molecular dynamics simulations.

2.4.1. Constitutive Models

Use of an appropriate constitutive model is key to the prediction of FCI. Experimental evidence in Section 2.3 clearly demonstrates the importance of capturing plasticity in a model. PSBs, commonly cited as a location for FCI, are formed
as a result of dislocation glide and, thus, are directly related to plastic strain. Accurate representation of the stress field is equally important, as the driving force for dislocation glide. Therefore, it follows that constitutive formulations used should include phenomena observed in the stress-strain relationship. For example the Armstrong-Frederick relation for hardening is often used to simulate the Bauschinger back-stress observed upon reversal of loading, corresponding to shifting of the yield surface in principal stress space [49].

Many fatigue studies choose to use macroscopic material formulations for defining stress-strain behaviour, such as $J_2$ plasticity models, for which the yield surface is defined by the von Mises yield criterion, where von Mises stress, $\sigma_{\text{mises}}$, is related to the second invariant of deviatoric stress $\sigma_{\text{mises}} = \sqrt{3 J_2}$. Fatigue indicator parameters (FIPs) can be combined with macro-scale constitutive models to predict FCI; however, such an approach is based on the assumption of a homogeneous material. As demonstrated in Section 2.3, FCI is a highly microstructure-sensitive event and, therefore, such an assumption is not valid.

Micromechanical constitutive models are, therefore, more scale-consistent for prediction of FCI. Crystal plasticity (CP) constitutive formulations, modelling of dislocation glide in a slip system as a function of the applied shear stress in individual crystallographic grains, are commonly used for this purpose [29,50]. Various CP formulations have been developed; some are phenomenologically-based formulations, e.g. [51, 52], while others include evolution laws for dislocation density, e.g. [53–56], and are, thus, more mechanistically or physically-based. CP modelling offers the opportunity to use microstructure-based variables in predictions and has the ability to capture scatter in fatigue behaviour due to microstructural features, such as crystallographic orientation, grain boundaries, precipitates etc. Przybyla and McDowell [57, 58], have predicted the influence of different microstructural attributes on FCI via CP modelling and correlation functions for proximity of attributes to extreme values of FIPs, considered to be driving forces.
for FCI. Dislocation-based CP formulations have the added benefit of the inclusion of geometrically necessary dislocation (GND) density, which form as a result of plastic strain gradients in the microstructure. Strain-gradient CP modelling has been used by Dunne and co-workers to investigate the stress-strain state as a result of strain-gradients at grain boundaries in a titanium alloy under cyclic loading [56] and to capture the GND density field surrounding a precipitate in a titanium alloy matrix [59]. Strain-gradient CP was used in another study to model the monotonic behaviour of copper and aluminium polycrystals for different grain sizes, capturing the Hall-Petch effect for yielding via inclusion of unique initial statistically-stored dislocation density for different grain sizes [60]. Dislocation-based CP formulations have also been adapted to include a physically-based back-stress as a function of gradient in GND density, to capture the experimentally observed back-stress as a result of internal stresses [61].

While much emphasis is placed on the capture of plasticity for prediction of FCI, the choice of isotropic versus anisotropic elasticity can also have a significant influence on FCI predictions. This is particularly the case for HCF, during which plastic strains are small compared with LCF, as highlighted by [62]. A study by Sauzay and Jourdan demonstrates the influence of anisotropic elasticity on the stresses developed in fcc and bcc polycrystals via investigation of the normal and shear stresses in a grain as a result of different orientations of the neighbouring grains. Another study by Guerchais et al. [63] on modelling of HCF for copper plain notched and holed specimens found that the use of cubic elastic constants versus isotropic elasticity had a significant influence on the stress distributions predicted.
2.4.2. Fatigue Prediction

Indicator parameters are a useful tool for predicting fatigue performance, whereby the accumulation of an FIP at a given material point indicates a likely location for FCI and the rate of accumulation of the FIP can be used to assess the number of cycles to FCI. FIPs are typically linked to damage mechanics; an increase in FIP value correlates to an increase in damage, where damage, $D$, is the fraction of compromised cross-sectional area in the affected region, resulting in an effective stress:

$$\tilde{\sigma} = \frac{\sigma}{1 - D} \quad (2.9)$$

Various relations have been developed for the relationship between $N/N_f$ and $D$, as outlined in a review by Fatemi and Yang [64]. One example is the well-known Palmgren-Miner rule for cumulative damage:

$$D = \sum \frac{N_{\alpha}}{N_{f,\alpha}} \quad (2.10)$$

where $N_{\alpha}$ and $N_{f,\alpha}$ are the number of cycles and total fatigue life for loading condition $\alpha$. Puchi-Cabrera et al. [65] demonstrate usage of the Palmgren-Miner rule for multi-phase loading of 316L SS specimens. In Fig. 2.5 (a) is shown one of the loading sequences tested and a comparison of predictions using the Palmgren-Miner relation against experimental data is shown in Fig. 2.5 (b).

FIPs for modelling damage accumulation were initially based on either strain or stress parameters, reflected by the Coffin-Manson relation for LCF and the Basquin relation for HCF. The Sines equation [66] is a stress-based fatigue criterion, developed specifically for multiaxial fatigue:

$$\frac{\sqrt{2}}{3} \sigma_{\text{mises,a}} \leq A - 3\alpha \sigma_{H,m} \quad (2.11)$$
2. Background

Figure 2.5: (a) Low-high loading sequence applied in [65] to 316L specimens and (b) comparison of predictions using the Palmgren-Miner cumulative damage rule with experiments.

Based on von Mises alternating stress, $\sigma_{\text{mises,a}}$, related to the octahedral shear stress, and mean hydrostatic stress, $\sigma_{\text{H,m}}$. Smith, Watson and Topper (SWT) [67] first developed a combined stress-strain criterion, based on the product of maximum tensile stress and strain amplitude, which was successfully validated for LCF and HCF behaviour of various materials. Use of a stress-strain approach accounts for both the formation of PSBs via slip (strain component) and material hardening (stress component). However, while the criterion was shown to be effective for mean stress cases as well as fully reversed loading, the stress and strain quantities used do not account for multiaxial fatigue. Brown and Miller [68] later developed a criterion for multiaxial fatigue failure, based on both shear and tensile components. Their criterion proposed that fatigue failure is related to the maximum shear strain and the normal strain on the plane of maximum shear strain, i.e.:

$$\frac{\varepsilon_1 - \varepsilon_3}{2} = f \left[ \frac{\varepsilon_1 + \varepsilon_3}{2} \right]$$  \hspace{1cm} (2.12)

where $\varepsilon_1$, $\varepsilon_2$ and $\varepsilon_3$ are the principal strains. Brown and Miller use the criterion to predict different behaviour for cracks which grow along a plane (i) oriented away from the surface or (ii) oriented along the surface, where the latter is shown to be better for fatigue. Fatemi and Socie (FS) [69] later modified the approach of Brown and Miller to replace normal strain with normal stress on the plane of
2. Background

maximum shear strain:

$$\frac{\Delta\gamma_{\text{max}}}{2} \left( 1 + n \frac{\sigma_{n}^{\text{max}}}{\sigma_y} \right) = \text{constant} \quad (2.13)$$

where $\Delta\gamma_{\text{max}}$ is the range of maximum shear strain and $n$ is a constant. Inclusion of stress in the criterion accounts for cyclic hardening which can occur in multiaxial fatigue, particularly in out-of-phase loading. Dang Van also developed a multiaxial fatigue criterion based on crack initiation in critically oriented grains. The criterion is based on the shear stress on a plane of potential crack initiation, $\tau$, and hydrostatic stress, $p_H$, accounting for crack opening:

$$\tau = \pm (\beta - \alpha p_H) \quad (2.14)$$

where $\tau$ is calculated from a microscopic stress tensor, which itself is evaluated as a function of the macroscopic stress tensor, via an elastic localisation tensor, and a residual stress field.

All of the above criteria for fatigue are still in use today for the prediction of damage in fatigue. In macro-scale modelling for example, Leen and co-workers [70, 71] have successfully applied the SWT parameter to fretting fatigue for Ti-6Al-4V. The Dang Van criterion has recently been applied by Aurrichio et al. [72] to HCF for 316L micro-scale components. Due to lack of directionality in macro-scale (e.g. $J_2$) modelling (e.g. via slip systems in CP modelling) a critical plane approach has been developed for FIPs, to determine direction of a crack initiated, as demonstrated by McCarthy and co-workers [73, 74] for the SWT parameter with application to fretting fatigue. The plane with maximum FIP value, is considered to be the critical plane along which an initiated crack may propagate. Techniques have been developed to deal with the influence of stress-gradient on fatigue behaviour, as opposed to FIPs at a single point. Araújo and Nowell [75] applied averaging to SWT and FS FIPs over both a critical depth
2. Background

Figure 2.6: (a) Application of TCD to fracture prediction for a nuclear graphite corner component for different corner radii, $r$, where the stress-distance curves shown represent the state at fracture for each component [77]. The critical stress, which corresponds to the plain specimen strength, for each component coincides at the critical distance from the notch root.

and critical volume for prediction of fretting fatigue life for Ti-6Al-4V. Critical values identified to give good correlation to experimental life data for the two averaging methods were related by authors to the grain size of the material. Fouvry et al. [76] employ a similar technique for a different FIP. Taylor developed the theory of critical distances (TCD) to capture the stress-gradient effect [77], based on a similar concept to the previous two studies. Multiple methods are developed for different stress concentration types, for which a critical distance is identified and used to make predictions. For example, the stress used for predictions can be taken at the critical distance from a stress concentration for the point method, or can be averaged along the critical distance for the line method. The predictive ability of the point method is demonstrated in Fig. 2.6. Use of the TCD has been successfully demonstrated for fretting fatigue, for which it was proven more effective than fatigue assessment based on FIPs directly at the stress concentration [78].

Many of the FIPs and techniques developed above for fatigue prediction have been extended to the micromechanical framework, allowing the influence of microstructural inhomogeneity to be captured in predictions, as reviewed by McDowell and
Dunne [29]. Neu and co-workers have carried out a series of studies on CP modelling in fretting fatigue in which FCI is predicted using the FS parameter and additional parameters modified to capture ratchetting [79–81]. Castelluccio and McDowell [82] used the FS FIP to investigate the effect of twin boundaries on FCI formation by comparing FIP distributions for single crystal and polycrystal models with and without twin boundaries. The study revealed an increase in FIP values due to the presence of twin boundaries, with a larger influence of twin boundaries evident for single crystals.

Additional microstructure-sensitive FIPs have been developed for micromechanical modelling of FCI. Dunne et al. [62] developed a crystallographic effective plastic strain parameter, $p$, which sums plastic slip over individual slip systems. The parameter has been successfully used by Dunne and co-workers to predict the location of experimentally observed FCI for an LCF tested nickel alloy polycrystal [62], as illustrated in Fig. 2.7 (a). FCI is predicted to occur for the parameter when a critical value, $p_{\text{crit}}$, is reached. Manonukul et al. [83] successfully demonstrated use of the FIP to predict number of cycles to FCI across both LCF and HCF regimes for a nickel-base alloy in which FCI is known to dominate fatigue life, as illustrated in Fig. 2.7 (b) and (c), respectively. McCarthy and co-workers have demonstrated use of $p$ in predictions of FCI for fretting fatigue [73, 74, 84, 85], which allowed CP models to distinguish between cracking and wear at the fretting surface [85] among other microstructural effects. Another microstructure-sensitive parameter developed is the crystallographic work parameter of Korsunsky et al. [86], $W$, which, similar to $p$, sums strain energy dissipation over each slip system. Use of this FIP has been demonstrated by Li et al. [87] along with the FS parameter, where FIP distributions generated via CP modelling corresponded with surface observations of deformation for fatigue of 304L austenitic steel.
2. Background

Figure 2.7: Application of the $p$ FIP to prediction of FCI for nickel-base alloys. (a) Prediction of experimentally observed FCI site [62] and comparisons of predicted number of cycles to FCI against experimental data for both (b) LCF and (c) HCF testing [83].

Dislocation-based Techniques

Other techniques developed for FCI prediction focus on dislocation mechanisms and the formation of structures such as PSBs which are preferred sites for FCI. Mura developed an FCI criterion based on the stability of the dislocation dipole structure in a PSB [88], known as the Tanaka-Mura criterion. Brückner-Foit and Huang [89] successfully applied the Tanaka-Mura criterion to the prediction of FCI for a martensitic steel, where excellent correlation was observed between simulated and experimental risk of FCI. Anahid et al. [90] developed a CP based FIP for prediction of the initiation of a wedge shape crack at the grain boundary of a 'hard' grain as a result of dislocation build up at the grain boundary in a neighbouring 'soft' grain. Polák and Man [91, 92] use physically-based models for dislocation generation, annihilation and migration to model the formation of surface extrusions and intrusions within PSBs as a result of relaxation of
2. Background

compressive stresses in the PSB and tensile stresses in the matrix at the PSB-matrix interface.

While computationally expensive, dislocation dynamics simulations can be used to model the formation of slip bands and offer insight into factors of influence. For example, Brinckmann and Van der Giessen [93] modelled the evolution of dislocation structures in a surface grain with grain boundaries and were able to capture the build-up of dislocations at the grain boundary and a corresponding accumulation in stress. Another study by Déprés et al. [94] reports on the capture of intrusions and extrusions at the free surface under applied cyclic loading in dislocation dynamics simulations. Sangid [95–97] and co-workers have developed a criterion for FCI formation in a PSB based on the stability of an energy balance. The criterion sums energy terms relating to all contributing factors, including the applied stress field, work hardening, formation of dislocation dipole structures, dislocation nucleation at grain boundaries, penetration of grain boundaries by dislocations to form extrusions and shearing of the matrix and precipitates by dislocations. Atomistic simulations were used to calculate variables relating to dislocation-grain boundary interactions in the model for different grain boundary characters. This energy balance criterion for FCI has been used in polycrystal simulations to successfully predict $N_i$ and scatter in $N_i$ for a nickel superalloy [95]. The contribution of each energy term can be used to identify the mechanisms which are dominant at different loading regimes and for different microstructure attributes [97]. The model has also been used to investigate the influence of parameters such as grain boundary character (degree of misorientation), Schmid factor and grain size on $N_i$ [96].
2. Background

2.4.3. Simulation of Polycrystal Geometries

While the choice of constitutive formulation and predictive technique is fundamental to the success of fatigue prediction, another important aspect is the use of an appropriate model geometry. Particularly for microstructure-based constitutive models, such as CP, but also for $J_2$ models, the capture of microstructural effects relies heavily on the detail of the geometry chosen and the degree to which it reflects the real microstructure. Owing to the nature of CP formulations (i.e. modelling crystallographic slip on individual slip systems, dependent on the orientation of the crystal lattice) the inclusion of grain morphology in the FE geometry is a necessity in order to allow for different crystallographic orientations. In $J_2$ formulations with anisotropic material descriptions, the inclusion of a grain morphology can offer a means of capturing some degree of microstructural inhomogeneity. For example, Soppa et al. [98] modelled the development of anisotropic strain fields in a silver/nickel composite loaded in tension, via $J_2$ flow theory applied to a polycrystal model for the composite material. Anisotropy was introduced by multiplying the yield curve defining $J_2$ behaviour of each grain by an orientation factor, based on measured Schmid factors for the composite microstructure. Other microstructural features such as precipitates or other defects can also be included to reflect the measured microstructure and allow investigation of their effect on fatigue performance.

In some microstructure-sensitive fatigue studies, explicit microstructure morphologies are modelled enabling direct comparison of predictions with experimental fatigue. For example You et al. [99] model the explicit polycrystal morphology for a 316LVM SS strut to investigate the effectiveness of CP modelling at capturing macro-stress-strain behaviour, micro-strain fields and reorientation of grains during tensile loading, via direct comparison with experiments. In the area of fatigue, Dunne et al. [62] successfully predicted the FCI site for an exper-
imental three-point bending fatigue test on a directionally-solidified nickel-base superalloy by modelling the explicit microstructure observed in the region of highest bending moment, measured via electron backscatter diffraction (EBSD) techniques. Another study reports the modelling of the dislocation density and strain fields which develop around a precipitate embedded in a nickel alloy for an experimental case [59], again by using the geometry measured in EBSD. However, a large amount of work is required to fully characterise the microstructure for a specimen, proceeded by a fatigue test on the same specimen. This process is time consuming, even for a single specimen, and difficult to complete without incurring damage to the specimen between characterisation and fatigue testing. Therefore, microstructure morphologies are often generated which are statistically similar to the measured microstructure. In this way a statistical comparison of predictions can be made, i.e. results from several simulated microstructures can be compared against data for a similar number of fatigue specimens.

Different approaches exist for the generation of polycrystal morphologies for FE analyses. Some studies make use of hexagonal grains in 2D morphologies, e.g. [5, 73, 100], allowing for inclusion of triple points at grain boundary intersections. Similarly, rhombic dodecahedron-shaped grains have been used in 3D morphologies, e.g. [101]. However, in both cases, polycrystal morphologies are subject to the limitation of uniform grain size and shape throughout. Voronoi Tessellation algorithms are used in many different fields for the generation of 2D polygon or 3D polyhedron geometries, based on the isotropic growth of cells from a set of nuclei points, as illustrated in Fig. 2.8(a) for a 2D microstructure. Thus, this algorithm can be used to generate random crystallographic FE morphologies, e.g. [102–104].

Various studies have been published on the modification of the VT algorithm to facilitate more control over the grain size distribution of the polycrystal geometries generated, including minimisation of an objective function via an inverse
2. Background

Figure 2.8: (a) Generation of a Voronoi Tessellation from a set of nuclei points, whereby grains are assumed to grow isotropically from their respective nuclei, i.e. a point is considered part of a grain if it is closer to that grain’s nucleus than to any other nucleus. (b) Periodic RVE in a fatigue specimen.

Monte Carlo method [105,106], a maximum entropy approach [107,108] and use of a regularity control parameter based on the one-parameter gamma distribution representing the measured grain size distribution [109,110]. Other studies look at alternative methods to Voronoi Tessellation for improved polycrystal morphology generation. For example, the association of an ellipse, rather than just a nuclei point, to each grain allows control over grain area and shape as well as seed location, and has been successfully shown to generate morphologies with distributions which more closely resemble the real microstructure [111,112].

Representative Volume Elements

Unless a specimen’s dimensions are on the scale of the grain size, it is not generally feasible to use CP modelling for the entire specimen or even a full cross-section, due to the computational expense associated with CP simulations. Thus, a representative volume element (RVE) is instead modelled, which statistically represents the specimen microstructure and has a sufficient number of grains such that the macroscopic response of the RVE is unaffected by a variation of the polycrystal morphology or crystallographic orientations [113,114]. The size of an RVE differs for different materials, depending on average grain size and
the degree of microstructural heterogeneity. The microstructure itself can be generated via Voronoi Tessellation to be periodic to facilitate the application of periodic boundary conditions, in order to simulate the behaviour of a repeatable volume in the microstructure [103,115], as illustrated in Fig. 2.8(b).

2.5. Stent Fatigue Modelling

As demonstrated in Chapter 1, the design of stents for improved performance in vivo is an ever-expanding area in the medical devices industry. Modelling has become a key aspect of stent design, providing a relatively cheap method for virtual testing and improving design, assessing causes for failure, investigating potential materials etc. Much focus has been placed in the past on the modelling of the initial stages of stent deformation, in the deployment process, and identifying aspects of modelling required to simulate the process in vivo. For example, Migliavacca and co-workers identified the need to model the balloon in the deployment process to realistically simulate the transmission of applied pressure and stresses applied by the expanded stent to the arterial wall [116,117]. Grogan et al. utilised FE modelling to simulate bench testing of different stent designs for different materials [118], including assessment in the areas of deployment, radial strength, longitudinal resistance and flexibility.

As highlighted in Chapter 1, stent dimensions are comparable in size to the grain size of the material and, thus, are highly sensitive to the microstructure. McHugh and co-workers have carried out a series of studies on CP modelling of the monotonic deformation of stent struts under uniaxial loading and bending [5,39,99,101,119–122]. Results from these studies demonstrated the ability of CP modelling to capture strut necking [5,101,119–121] and the dependence of monotonic behaviour on strut thickness [5,39,121] and experimentally observed
2. Background

maps of surface strains and stresses [99]. One study also demonstrated the use of design curves for different strut thicknesses, generated from CP modelling of individual struts, in $J_2$ design modelling of full stents [122]. Following on from this, Grogan et al. [123] investigated the statistical size effects, as outlined in Section 2.3.1 observed in stent strut behaviour using CP modelling. The effect of changing strut width and thickness for a given grain size, and inclusion of precipitates on the strain at ultimate tensile strength was assessed and a set of design rules for the monotonic loading of stents were generated. This microstructure-sensitive approach to stent modelling is particularly desirable for stent fatigue performance, particularly due to the importance of FCI in stent fatigue; the micro-dimensions involved cannot support long and physically small crack growth as highlighted in [124]. Fatigue life, instead, consists of FCI and microstructurally small crack growth. However, as outlined below, few of the existing approaches for stent fatigue modelling include representation of the microstructure.

2.5.1. Traditional Approach

As outlined in Chapter 1, application of the Goodman relation to the results of an FE model, in which one cycle of pulsatile loading is simulated, is sufficient to meet the recommendations set out by the FDA for the computational aspect of stent fatigue design. The Goodman relation defines a line in the alternating stress ($\sigma_a$) - mean stress ($\sigma_m$) plane, as shown in Fig. 2.9 (a), below which a design is considered 'safe' and above which a design is predicted to fail:

$$\sigma_a = \sigma_e \left( 1 - \frac{\sigma_m}{\sigma_{TS}} \right)$$

(2.15)

where $\sigma_e$ is the traditional endurance fatigue limit and $\sigma_{TS}$ is the ultimate tensile strength. Typically, calculated ($\sigma_a$, $\sigma_m$) data points or loading paths are plotted on the Goodman diagram corresponding to all material points, to assess the
durability of a fatigue design. This is the common approach of many published studies which consider fatigue as part of stent modelling, e.g. [125–130] (example of Goodman diagram provided in Fig. 2.9 (b)), while one study assessed the durability of a stent design simply by comparing the predicted maximum stress amplitude to the fatigue limit for the material [131]. One key study acknowledges the need for a micromechanics approach to stent fatigue modelling, in order to account for inhomogeneity effects caused by microstructure [129].

2.5.2. New Approaches

A number of studies have addressed the need for improved computational methods in stent fatigue design. Marrey et al. applied a fracture mechanics approach to assess the effect of a crack on the performance of a L605 CoCr alloy stent [26]. A global stent model was used to identify the most critical location in the stent design, as illustrated in Fig. 2.10 (a), via a Goodman analysis. The authors then introduced centre and corner cracks, as shown in Fig. 2.10 (b), of different sizes into the stent geometry in a submodel of the critical region and applied a fracture mechanics approach to determine if the crack would propagate under the applied stress intensity factor range. Attention was drawn to the need to use
2. Background

Figure 2.10: Modelling methodology used by Marrey et al. [26] to assess the fatigue performance of a CoCr alloy stent, including (a) identification of critical region for submodel geometry, (b) crack types applied to submodel and (c) curves of life versus initial crack size for different final crack sizes.

the El-Haddad modification to the traditional LEFM approach, as described in Section 2.2, due to the small size of the cracks involved. The approach allowed the generation of design curves defining the size of safe (i.e. non-propagating) and unsafe cracks, shown in Fig. 2.10 (c). While this study represented a step forward, one of the key conclusions cited the need for CP approaches in future work on stent fatigue, to capture the effect of microstructure.

Wiersma et al. [132,133] applied the theory of critical distances, which accounts for stress-gradient effects, as described in Section 2.4.2, to the prediction of the fatigue limit for 316L SS micro-specimens with different notch geometries. While the critical distance used is identified from micro-specimen data and is argued to be related to the grain size, the modelling approach does not include inhomogeneous microstructural effects. Barrera and co-workers [134] applied the Dang Van relation along with a critical plane approach, described in Section 2.4.2, to assess the fatigue performance of a 316L SS stent, as illustrated in Fig. 2.11. However, while the shear and hydrostatic stresses used in calculations were evaluated at a mesoscopic level, the FE model used to generate the data used a macroscopic material description, omitting the influence of microstructural features. A dam-
2. Background

Figure 2.11: Application of the Dang Van criterion to assess the durability of a 316L SS stent [134].

age mechanics approach has been applied in another study to predict number of cycles to FCI for two 316L SS stents [135]. This approach employed cycle jumping based on a plastic strain FIP to reach a critical damage in the model, and simulated FCI lives which were comparable to experimental tests on the same stent designs. However, the material description used in the framework was, again, a macroscopic formulation and does not have the ability to capture microstructural inhomogeneity.

Finally, a micromechanics approach has been applied to assess a generic stent design for 316L SS [100]. The geometry consisted of a polycrystalline morphology applied to a single repeatable unit in the stent design, modelled using both a CP constitutive model and a $J_2$ plasticity model for comparison. While the study revealed the ability of CP modelling to capture surface roughness and a non-smooth stress distribution, as expected from inhomogeneous microstructure, the CP material description was based on a monotonic calibration and a basic Goodman analysis was the only tool applied to assess fatigue performance.
2. Background

![Figure 2.12: Flat notched and slotted tube micro-specimens tested by Wiersma et al. to validate their methodology for micro-fatigue predictions [132].](image)

2.5.3. Micro-Specimen Testing

Validation is an important aspect of the development of computational tools for the design of any component and is highlighted in a review by Morlacchi and Migliavacca [136] on modelling of coronary arteries as a key requirement to improve acceptance of such tools in stent design. One form of validation is the comparison of predicted fatigue lives against data from \textit{in vitro} studies, e.g. [135], while another approach compares deformed stent geometries simulated by a model against the real stent geometry, reconstructed from fluoroscopy images for a patient-specific case [126]. These approaches serve as validation for macroscopic behaviour at the global level. However, use of material properties and formulations based on macroscopic validation only neglects the microstructure-sensitivity of stent fatigue. Micromechanical methods are required for stent fatigue assessment, which are validated against micro-scale experiments.

The concept of a representative test, in which a sub-component of the stent design is tested, can provide a means of investigating the ability of a model to capture microstructural effects. Selection of a micro-specimen, smaller than the
global stent, to simulate and compare against the representative test allows more detailed modelling. Wiersma et al. carried out a series of micro-specimen HCF tests on plain and notched flat specimens and slotted tube specimens, shown in Fig. 2.12, at different cyclic loading ratios for 316L stent material [132, 133]. The tests allowed the identification of a micro-based critical distance for the stress-gradient approach applied in the study and validation of predictions of fatigue limit for the range of micro-specimen geometries tested. Pelton et al. [137] developed a subcomponent specimen for a nitinol stent, shown in Fig. 2.13 (a) and (b), respectively. Displacement-controlled fatigue tests were carried out on the subcomponents and full stents were also tested under equivalent conditions of loading. Results showed that fatigue behaviour of the subcomponent micro-specimen reflected that of full stent specimens for different combinations of strain amplitude and mean strain, as illustrated in Fig. 2.13 (c), thus endorsing the representative specimen concept. The representative test concept can be used for simulating the complex behaviour of full-scale components across a range of applications, for which testing of the full-scale component is not feasible due to expense or other inhibiting factors. For example, Leen et al. [138] and Houghton et al. [139] describe the development and validation of a representative test for fretting fatigue in spline coupling joints.
In summary, there is a lack in the published literature of a computational design tool for stent fatigue, which has representation of the microstructure to account for microstructural inhomogeneity effects, and has been validated against micro-experiments. As devices which undergo high cycle fatigue loading and whose cross-section dimensions prevent crack growth going beyond the microstructurally small crack growth regime before fracture, the prediction of crack initiation in stent fatigue is of primary interest. The experimental observations of Section 2.3 illustrate the dependence of slip band formation and, thus, crack initiation on dislocation mechanisms, and, also, the influence of different microstructural and specimen attributes on these mechanisms. The various computational approaches presented in Section 2.4, which are based on these observations, are adopted and developed in this thesis to build a micromechanical framework for the microstructure-sensitive assessment of stent fatigue.
3. Theory

3.1. Chapter Summary

The development of a computational framework is central to the work presented in this thesis. This chapter outlines the methods of numerical modelling adopted. A brief background to continuum mechanics is provided, followed by a description of the constitutive formulations used, including a $J_2$ flow model for macroscopic behaviour and both phenomenological and physically-based crystal plasticity models. The finite element method is introduced, including the fundamental equilibrium balance used in finding the solution for an increment. Finally, the use of element shape functions to calculate key spatial gradients of variables required in strain-gradient CP formulations is outlined.

3.2. Continuum Mechanics

A brief overview of the mechanics upon which the numerical simulations of this thesis are based is provided here. A more complete development of the framework can be found in Dunne and Pertrinic [140] and Crisfield [141], for example.

The deformation of a body is shown schematically in Fig. 3.1, including both the
reference or undeformed configuration and the current or deformed configuration.
The position of a point on the undeformed body, $P$, can be described by the vector $X$. Similarly, the position of the corresponding point $P'$ on the deformed body can be described by the vector $x$, while the displacement, $u$, relates $X$ and $x$:

$$x = X + u$$  \hspace{1cm} (3.1)

The deformation gradient $F$ defines the transformation of the vector $dX$ in the reference configuration to the corresponding vector $dx$ in the current configuration:

$$F = \frac{\partial x}{\partial X} = \frac{\partial u}{\partial X} + I$$  \hspace{1cm} (3.2)

The Green-Lagrange strain tensor, $E$, a strain measure defined relative to the undeformed (reference) configuration, is given as:

$$E = \frac{1}{2} (F^T F - I) = \frac{1}{2} \left( \left[ \frac{\partial u}{\partial X} + I \right]^T \left[ \frac{\partial u}{\partial X} + I \right] - I \right)$$

$$= \frac{1}{2} \left( \frac{\partial u}{\partial X} + \left( \frac{\partial u}{\partial X} \right)^T \right) + \left( \frac{\partial u}{\partial X} \right)^T \frac{\partial u}{\partial X}$$  \hspace{1cm} (3.3)
where Eq. 3.2 is substituted to give the final form. For small strains the product of partial derivatives in Eq. 3.3 is negligible, giving rise to the infinitesimal strain:

\[ \varepsilon = \frac{1}{2} \left( \frac{\partial u}{\partial X} + \left( \frac{\partial u}{\partial X} \right)^T \right) \]  

(3.4)

For rate-dependent constitutive models it is useful to define the framework above in terms of rate quantities, where the velocity of a point in the current configuration is given by:

\[ v = \frac{\partial x}{\partial t} \]  

(3.5)

and the velocity gradient can be used to define the spatial rate of change of an increment in velocity \( dv \):

\[ L = \frac{\partial v}{\partial x} = \frac{\partial v}{\partial X} \cdot \frac{\partial X}{\partial x} = \frac{\partial F}{\partial t} \cdot F^{-1} = \dot{F} F^{-1} \]  

(3.6)

where a relationship with the deformation gradient is also defined above. The symmetric and asymmetric components of \( L \) define the rate of deformation \( D \) and the continuum spin \( W \), respectively:

\[ D = \frac{1}{2} \left( L + L^T \right) \]  

(3.7)

\[ W = \frac{1}{2} \left( L - L^T \right) \]  

(3.8)

Different measures of stress can be defined within the framework above. The Cauchy stress tensor, \( \sigma \) can be related to a stress vector, \( t \), acting on a surface with normal \( n \):

\[ t = \sigma n \]  

(3.9)

The Cauchy stress can be considered to represent the true stress tensor, as it is evaluated in the current configuration, thus taking into account a changing
cross-sectional area. It can be coupled with the rate of deformation, $D$ of Eq. 3.7, to form a work conjugate pair. Another common stress measure, defined relative to the undeformed (reference) configuration, is the second Piola-Kirchoff stress, $S$:

$$
S = \det(F)F^{-1}\sigma F^{-T}
$$

(3.10)

which forms a work conjugate pair with the Green-Lagrange strain tensor of Eq. 3.3. For rate-dependent formulations, the Jaumann rate of Cauchy stress is a useful quantity:

$$
\nabla \sigma = \dot{\sigma} - W\sigma + \sigma W
$$

(3.11)

where $\dot{\sigma}$ is the rate of Cauchy stress with respect to the material undeformed (reference) frame.

### 3.3. $J_2$ Plasticity Theory

The Cauchy stress, $\sigma$, can be decomposed into both hydrostatic and deviatoric components:

$$
\sigma = \frac{1}{3}\text{Tr}(\sigma)I + \sigma' = PI + \sigma'
$$

(3.12)

where $P$ is the hydrostatic pressure and $\sigma'$ is the deviatoric stress. In multiaxial plasticity, yield criteria are commonly defined as a function of the von Mises stress, defined as:

$$
\sigma_e = \left(\frac{3}{2}\sigma' : \sigma'\right)^{1/2}
$$

(3.13)

The second invariant of the deviatoric stress tensor, $J_2$, is defined as:

$$
J_2 = \frac{1}{2}(\sigma' : \sigma')
$$

(3.14)
Figure 3.2: Schematics of (a) the displacement of the yield surface as a result of kinematic hardening and (b) the expansion of the yield surface as a result of isotropic hardening in 2D principal stress space, (c) the von Mises yield surface in 3D principal stress space and (d) the effect of isotropic hardening, $r$, and kinematic back-stress, $x$, on a cyclic hysteresis curve.

Thus, the von Mises stress can be written as $\sqrt{3}J_2$. Plasticity flow theories with yield functions based on the von Mises stress are, therefore, referred to as $J_2$ flow theory constitutive models. The simplest yield surface in $J_2$ flow theory is defined by the equation:

$$f = \left(\frac{3}{2} \sigma' : \sigma'\right)^{1/2} - \sigma_y$$  \hspace{1cm} (3.15)$$

where $\sigma_y$ is the material yield stress. This yield function corresponds to an ellipse in 2D principal stress space, as seen in Figs. 3.2 (a) and (b) and a cylinder in 3D principal stress space, as illustrated in 3.2 (c).

A $J_2$ flow theory constitutive model is used in two studies in the thesis, for
calibration purposes and to facilitate comparison of CP model results with a macro-scale approach. The $J_2$ formulation used incorporates the key phenomena of cyclic hardening and Bauschinger effect, via non-linear isotropic and kinematic hardening models, respectively, where the yield surface is defined by the function:

$$f = \left( \frac{3}{2} (\sigma' - x') : (\sigma' - x') \right)^{1/2} - \sigma_y - r(p) \quad (3.16)$$

where $\sigma'$ and $x'$ are the deviatoric stress and back-stress tensors, respectively, and $r(p)$ is the isotropic hardening function. The kinematic back-stress is used to capture the Bauschinger effect, whereby the yield surface is shifted or displaced in principal stress space in the direction of applied loading, as illustrated in Fig. 3.2 (a). One or multiple back-stresses can be used in the model, which are summed to give an overall back-stress:

$$x = \sum_i x_i \quad (3.17)$$

where use of multiple back-stresses can aid in capturing the complex kinematic hardening response of a material. The non-linear evolution of each back-stress tensor, $x_i$, is defined by the Armstrong-Frederick rule:

$$dx_i = \frac{2}{3} c_i d\varepsilon_p - \gamma_i x_i dp \quad (3.18)$$

where $c_i$ is the initial hardening modulus, $\gamma_i$ is the rate of decay and $dp$ is the increment in an effective plastic strain defined as:

$$dp = \left( \frac{2}{3} d\varepsilon^p : d\varepsilon^p \right)^{1/2} \quad (3.19)$$

Isotropic hardening allows capture of the isotropic expansion of the yield surface in response to cyclic hardening as illustrated in Fig. 3.2 (b), by an amount equal to the isotropic hardening parameter $r$, defined as a function of the effective plastic strain, $p$:

$$dr(p) = b(Q - r) dp \quad (3.20)$$
where $Q$ is the saturation value of the isotropic hardening parameter and $b$ controls the rate of decay leading to saturation; both $Q$ and $b$ are constitutive constants. The respective effects of kinematic back-stress $\mathbf{x}$ and isotropic parameter $r$ on the cyclic hysteresis stress-strain curve is illustrated in Fig. 3.2 (d).

The elastic relation for the $J_2$ constitutive model is defined simply as:

$$d\sigma = C d\varepsilon^e = C (d\varepsilon - d\varepsilon^p) \quad (3.21)$$

where $d\varepsilon^e$ is the elastic strain increment and $C$ is the fourth order tensor of elastic modulii. This can easily be represented for Voigt (matrix/vector) notation as:

$$C_{iso} = \frac{E}{(1 + \nu)(1 - 2\nu)} \begin{bmatrix} 1 - \nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1 - \nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1 - \nu & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(1 + \nu) & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(1 + \nu) & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(1 + \nu) \end{bmatrix} \quad (3.22)$$

for isotropic elasticity, where $E$ is Young’s modulus and $\nu$ is Poisson’s ratio. For cubic crystals, elastic behaviour along the $x$, $y$ and $z$-axes is identical due to symmetry in the crystal, while a separate modulus is needed to define shear behaviour. When the local cubic axes coincide with the coordinate directions, the
3. Theory

The stiffness matrix for cubic elasticity can be defined, for Voigt notation, as \[ C_{\text{cubic}} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} \] (3.23)

where $C_{11} = \frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)}$; $C_{12} = \frac{E\nu}{(1 + \nu)(1 - 2\nu)}$; $C_{44} = \mu$

3.4. Crystal Plasticity Theory

Deformation of a crystal lattice occurs via glide or slip of line defects called dislocations in the lattice. Examples of edge and screw dislocations are depicted in Figs. 3.3 (a) and (b), respectively, where the Burger’s vector $b$ associated with a dislocation indicates the lattice distortion caused by the dislocation, and also a unit of slip. Crystal plasticity (CP) \[143-147\] describes deformation in the crystal lattice via dislocation motion along slip systems in the crystal lattice.
3. Theory

Figure 3.4: Schematic of glide of an edge dislocation through the crystal lattice.

![Figure 3.4: Schematic of glide of an edge dislocation through the crystal lattice.](image)

Figure 3.5: Examples of a single slip system from each slip system family for (a) a fcc crystal and (b) a bcc crystal.

![Figure 3.5: Examples of a single slip system from each slip system family for (a) a fcc crystal and (b) a bcc crystal.](image)

in response to shear stresses applied to those slip systems, as illustrated for an edge dislocation in Fig. 3.4. Slip systems, along which slip or dislocation glide occurs, correspond to the close-packed planes in a crystal structure. Face-centred cubic (fcc) and body-centred cubic (bcc) crystals are considered in this thesis. An example of a slip system in each slip system family for fcc and bcc crystal structures are illustrated in Figs. 3.5 (a) and (b), respectively, via Miller indices and unit crystal depictions. Each slip system is defined by a slip direction, $\mathbf{s}$ and a normal to the slip plane $\mathbf{m}$, and each slip system family includes all slip systems which are symmetrically identical to the slip system shown. For the fcc crystal the slip system shown belongs to the family $\{111\} \langle 110 \rangle$ and the bcc slip systems of Fig. 3.5 (b) belong to the slip system families $\{101\} \langle 11\bar{1} \rangle$, $\{112\} \langle 11\bar{1} \rangle$ and $\{123\} \langle 11\bar{1} \rangle$, respectively.

Slip occurs in response to the resolved shear stress on a slip system. Given a tensile stress $\sigma$ applied to a body with cross-sectional area $A$, as illustrated in Fig. 3.6, the force applied along unit vector $\mathbf{t}$ is given by $\sigma A$. For a slip system
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Figure 3.6: Schematic of the resolved shear stress, $\tau$, on a slip plane with normal, $m$, and along slip direction $s$ in response to an applied stress, $\sigma$.

with slip direction $s$, this force can be resolved to a force $\sigma A \cos \lambda$ parallel to the slip direction. For slip plane normal $m$, the relevant cross-sectional area is given by $A / \cos \phi$. Therefore, the resolved shear stress on the slip system shown in Fig. 3.6 is defined by Schmid’s law:

$$
\tau = \sigma \cos \lambda \cos \phi = \sigma (t \cdot m) (t \cdot s) \quad (3.24)
$$

Slip occurs on a slip system when the resolved shear stress, $\tau$, reaches a critical resolved shear stress, $\tau_c$, for the material.

CP formulations describe deformation of the crystal lattice through the use of the deformation gradient $F$ which can be decomposed into components:

$$
F = F^* \cdot F^p \quad (3.25)
$$

where $F^*$ includes both stretching of the lattice (or elastic deformation) and rotation of the lattice [148] and $F^p$ represents plastic deformation of the crystal lattice, as illustrated in Fig. 3.7. The rate of deformation and spin, from Eqs.
3.7 and 3.8, respectively, can be similarly decomposed:

\[
D = D^* + D^p
\]  
(3.26)

\[
W = W^* + W^p
\]  
(3.27)

Crystal plasticity models are often based on rate-dependent formulations and, thus, use the plastic velocity gradient \( L^p \), which is related to the plastic deformation gradient, \( F^p \), in a similar fashion to the relationship between \( L \) and \( F \) in Eq. 3.6. The plastic slip rate \( \dot{\gamma}^\alpha \) on a slip system \( \alpha \) can be related to \( L^p \) by Schmid’s law:

\[
L^p = \dot{F}^p \cdot F^{p^{-1}} = \sum_{\alpha} \dot{\gamma}^\alpha s^\alpha \otimes m^\alpha
\]  
(3.28)

where \( s^\alpha \) and \( m^\alpha \) define the slip direction and slip plane normal, respectively, for slip system \( \alpha \).

CP modelling is an important component of the micromechanical computational methodologies presented in this thesis. Two types of CP formulations are used: a phenomenological formulation, which uses a power law relationship between slip rate and resolved shear stress, and physically-based, strain-gradient formulations, which use equations based on dislocation mechanics.
3. Theory

3.4.1. Power-Law Formulation

The phenomenological CP constitutive model was previously implemented into a user-defined material subroutine (UMAT) in Abaqus/Standard by Huang [148], and is used in Chapters 4, 5 and 8 of this thesis. The visco-plastic power law flow rule defining the relationship between slip rate on a slip system $\alpha$, $\dot{\gamma}_\alpha$, and the slip system resolved shear stress $\tau_\alpha$ is given by:

$$
\dot{\gamma}_\alpha = \dot{a} \text{sgn}(\tau_\alpha) \left\{ \frac{\tau_\alpha}{g_\alpha} \right\}^n 
$$

(3.29)

where $\dot{a}$ is a reference strain rate, $n$ is a rate sensitivity exponent and $g_\alpha$ is the slip system strain hardness. The resolved shear stress on a slip system is defined as:

$$
\tau_\alpha = (m^{\alpha*} \otimes s^{\alpha*}) : \sigma
$$

(3.30)

where $\sigma$ is the Cauchy stress tensor, and $m^{\alpha*} = m^{\alpha} F^{*-1}$ and $s^{\alpha*} = F^* s^{\alpha}$ are the slip plane normal and slip direction, respectively, in the deformed configuration, as illustrated in Fig. 3.7. The slip system hardening function in Eq. 3.29 is based on that of Asaro and co-workers [147,149,150], given by:

$$
g(\gamma_\alpha) = g_0 + (g_\infty - g_0) \tanh \left| \frac{h_0 \gamma_\alpha}{g_\infty - g_0} \right|
$$

(3.31)

where $h_0$ is the initial hardening modulus, $g_0$ is equal to the critical resolved shear stress, $g_\infty$ is the saturation stress and $\gamma_\alpha$ is the accumulated plastic slip. Evolution of the slip system hardness can be defined as:

$$
\dot{g}_\alpha = \sum_\beta h^{\alpha\beta} \dot{\gamma}_\beta
$$

(3.32)
where $h^{\alpha \beta}$ represents self ($\beta = \alpha$) and latent ($\beta \neq \alpha$) hardening moduli, derived from Eq. 3.31 as:

$$h^{\alpha \alpha} = h^{\alpha \beta} = h(\gamma^\alpha) = h_0 \text{sech}^2 \left( \frac{h_0 \gamma^\alpha}{g_\infty - g_0} \right)$$

(3.33)

Accumulated plastic slip, used in Eqs. 3.31 and 3.33, is given by:

$$\gamma_a = \sum_\alpha \int_0^t |\dot{\gamma}^\alpha| \, dt$$

(3.34)

Kinematic hardening has been introduced into the CP constitutive formulation for improved capture of cyclic and tensile behaviour, as will be discussed and demonstrated in Chapters 4 and 5. Various formulations for kinematic hardening have been proposed for implementation into different CP flow rules. Most commonly employed is the Armstrong-Frederick rule for non-linear kinematic hardening [80, 81, 102, 151], which will be used in this work. Other formulations include a superposition of linear and non-linear kinematic hardening rules [52] and a combination of the Armstrong-Frederick rule with the Ohno-Wang model for improved modelling of ratchetting behaviour [152]. The Armstrong-Frederick rule for describing non-linear kinematic hardening is implemented here on a slip system basis and, as for the $J_2$ constitutive model, a single or multiple back-stresses can be used:

$$x^\alpha = \sum_i x_i^\alpha$$

(3.35)

$$\dot{x}_i^\alpha = C_{kini} \dot{\gamma}^\alpha - D_{kini} x_i^\alpha |\dot{\gamma}^\alpha|$$

(3.36)

where $x_i^\alpha$ is the $i^{th}$ kinematic back-stress on a slip system, $\alpha$, $C_{kini}$ is the associated initial hardening modulus and $D_{kini}$ is the rate of decay. Adaptation of the flow rule in Eq. 3.29 to incorporate kinematic hardening leads to the following equation:

$$\dot{\gamma}^\alpha = \dot{\gamma}_{\alpha} \text{sgn}(\tau^\alpha - x^\alpha) \left\{ \left| \frac{\tau^\alpha - x^\alpha}{g^\alpha} \right| \right\}^n$$

(3.37)
Implementation of the kinematic back-stress into the CP UMAT is discussed in Appendix A.1.

The elastic relation for the formulation, as described by Huang [148], is defined as:

\[
\nabla \sigma^* + \sigma(I : D^*) = C : D^* \quad (3.38)
\]

where \( C \) is the fourth order tensor of elastic modulii, introduced in Eq. 3.21 and illustrated in Eqs. 3.22 and 3.23 for isotropic and cubic elasticity, respectively, and \( \nabla \sigma^* \) is the Jaumann rate of Cauchy stress on axes that rotate with the crystal lattice, related to the Jaumann rate of Cauchy stress on axes that rotate with the material in Eq. 3.11 by:

\[
\nabla \sigma^* = \nabla \sigma + (W - W^*) \sigma - \sigma (W - W^*) \quad (3.39)
\]

The vectors:

\[
\mu^\alpha = \frac{1}{2} [s^{\alpha*} \otimes m^{\alpha*} + m^{\alpha*} \otimes s^{\alpha*}] \\
\omega^\alpha = \frac{1}{2} [s^{\alpha*} \otimes m^{\alpha*} - m^{\alpha*} \otimes s^{\alpha*}] \quad (3.40)
\]

can be used to defined the plastic components of the rate of stretch and spin as:

\[
D^p = \sum_\alpha \mu^\alpha \dot{\gamma}^\alpha \quad (3.41)
\]
\[
W^p = \sum_\alpha \omega^\alpha \dot{\gamma}^\alpha \quad (3.42)
\]

Substituting Eqs. 3.26, 3.27 and 3.38 into Eq. 3.39 gives the Jaumann stress rate in the deformed configuration:

\[
\nabla \sigma = C : D - C : D^p - \sigma (I : D) + \sigma (I : D^p) - W^p \sigma + \sigma W^p \quad (3.43)
\]

where Eqs. 3.41 and 3.42 can also be substituted into the expression above to
3. Theory

Figure 3.8: Schematic of immobile dislocations behaving as obstacles to the glide of a mobile dislocation.

give:

\[
\mathbf{\nabla} \sigma = C : \mathbf{D} - \sigma (I : D) - \sum_{\alpha} \dot{\gamma}^\alpha [C : \mu + \omega \sigma - \sigma \omega]
\] (3.44)

The stress increment for the formulation is calculated using the form of the Jaumann rate of Cauchy stress defined in Eq. 3.44 above.

The above formulation is implemented via an implicit integration scheme, whereby the slip increment on a slip system \(\alpha\), \(\Delta \gamma^\alpha\), is solved for iteratively via the Newton-Raphson method, as discussed further in Appendix A.1 for the implementation of kinematic hardening.

3.4.2. Strain-Gradient Formulations

Two physically-based strain-gradient CP models are used in this thesis: a small strain kinematics formulation is used in Chapter 6 and a large deformations formulation is used in Chapters 7 and 8. Both constitutive models describe the glide of mobile statistically stored dislocations (SSDs) as a function of applied stress, where dislocation glide is impeded by immobile dislocations, including both geometrically necessary dislocations (GNDs) and immobile SSDs, as illustrated in the schematic of Fig. 3.8. GNDs introduce the strain-gradient component into the constitutive models, as they are present due to spatial gradients in plastic deformation, corresponding to lattice curvature, as illustrated in Fig. 3.9 for a bending beam example. The user-material subroutine facility in Abaqus
Figure 3.9: Formation of GNDs to accommodate a gradient in plastic strain in a bending beam.

does not provide information on the spatial gradients of the deformation gradients at element Gauss integration points, which are required for calculating the evolution of GND. Thus, the strain-gradient CP formulations are implemented in user-element subroutines (UELs), allowing access to Gauss integration point information, as will be discussed further later in the Chapter.

The basis for the physically-based formulations is a creep rate equation, first developed by Gibbs [153], based on a statistical-thermodynamic analysis of dislocation glide impeded by obstacles in the lattice, as described by [154]. The slip rate is a function of dislocation glide velocity of mobile dislocations [155]:

\[
\dot{\gamma} = b v_g \rho_{SSD,m}
\]  

(3.45)

where \( b \) is Burger’s vector magnitude, \( v_g \) is the average dislocation glide velocity and \( \rho_{SSD,m} \) is the density of mobile SSDs. The average dislocation glide is a product of the rate of escape of pinned dislocations, \( \Gamma \), and the length of the thermal activation event, \( d_{act} \). The rate of escape includes an exponential probability function for the event of an energy fluctuation at a given temperature that could allow a dislocation to overcome a peak Gibbs free energy barrier, \( \Delta G \) [156], expressed by:

\[
\Gamma = \frac{\nu b}{2l} \exp \left( -\frac{\Delta G}{kT} \right)
\]  

(3.46)

where \( l \) is the pinning distance, \( b/2l \) is the number of degrees of freedom in the pinned dislocation segment, \( \nu \) is the frequency of attempts of dislocations to jump
3. Theory

energy barriers, $k$ is the Boltzmann constant and $T$ is temperature. The average dislocation glide velocity is, therefore, defined as:

$$v_g = \frac{\nu b d_{act}}{2l} \exp \left( -\frac{\Delta G}{kT} \right)$$ (3.47)

By making the approximation that $d_{act} \approx l$, the slip rate on a slip system $\alpha$ is then given by:

$$\dot{\gamma}_\alpha = \frac{\rho_{SSD,m} b^2 \nu}{2} \exp \left( -\frac{\Delta G}{kT} \right)$$ (3.48)

Gibbs free energy can be further broken down into:

$$\Delta G = \Delta H - \tau \Delta V \gamma_0$$ (3.49)

where $\Delta V$ is the activation volume, $\gamma_0$ is the shear strain that is work conjugate to the resolved shear stress [59], $\tau \Delta V \gamma_0$ is the work carried out by the stress field and the Helmholtz free energy, $\Delta H$, is associated with the activation of pinned dislocation jumps, successful or otherwise, utilised by Gibbs, in order to establish average dislocation glide speed. The shear stress, $\tau$, includes both slip system resolved shear stress, $\tau^\alpha$, and critical resolved shear stress, $\tau_c$:

$$\tau = |\tau^\alpha| - \tau_c$$ (3.50)

Combining Eqs. 3.49 and 3.50 with Eq. 3.48 gives:

$$\dot{\gamma}_\alpha = \frac{\rho_{SSD,m} b^2 \nu}{2} \exp \left( -\frac{\Delta H - (|\tau^\alpha| - \tau_c) \Delta V \gamma_0}{kT} \right) \text{sgn}(\tau^\alpha)$$ (3.51)

where the $\text{sgn}(\tau^\alpha)$ term is introduced to ensure that slip is symmetric with regard to positive and negative values of $\tau^\alpha$. By considering both forward and backward activation events in a symmetrical arrangement, achieved by a hyperbolic sine
type term $e^x - e^{-x}$, the flow rule then becomes:

$$\dot{\gamma} = \rho_{SSD,m} b^2 \nu \exp \left( -\frac{\Delta H}{kT} \right) \sinh \left( \frac{(|\tau^\alpha| - \tau_c) \Delta V \gamma_0}{kT} \right) \text{sgn}(\tau^\alpha) \quad (3.52)$$

The activation volume can be expressed as:

$$\Delta V = lb^2 \quad (3.53)$$

where the pinning distance $l$ can be expressed as a function of the density of immobile dislocations:

$$l = \frac{1}{\sqrt{\rho_{SSD,i} + \rho_{GND}}} \quad (3.54)$$

where $\rho_{SSD,i}$ and $\rho_{GND}$ are the immobile SSD and GND densities, respectively.

By combining Eqs. 3.54, 3.53 and 3.52, the flow rule becomes:

$$\dot{\gamma} = \rho_{SSD,m} b^2 \nu \exp \left( -\frac{\Delta H}{kT} \right) \sinh \left( \frac{(|\tau^\alpha| - \tau_c) \gamma_0 b^2}{kT \sqrt{\rho_{SSD,i} + \rho_{GND}}} \right) \text{sgn}(\tau^\alpha) \quad (3.55)$$

### Small Strain Kinematics Formulation

The small strain kinematics formulation, used in the work of Chapter 6 of this thesis, was implemented by Dunne et al. [56] in a user-element subroutine (UEL) in the Abaqus/Standard framework. A yield condition is used to define the occurrence of slip on a slip system:

$$|\tau^\alpha| > \tau_c + r \quad (3.56)$$

where $r$ is an isotropic hardening parameter. The flow rule of Eq. 3.55 has been modified to include the isotropic hardening parameter and to reflect an
assumption that the mobile and immobile SSD densities are equal, to give:

$$
\dot{\gamma}^\alpha = \rho_{SSD} b^2 \nu \exp \left( -\frac{\Delta H}{kT} \right) \sinh \left( \frac{(|\tau^\alpha| - \tau_c - r)\gamma_0 b^2}{kT\sqrt{\rho_{SSD} + \rho_{GND}}} \right) \text{sgn}(\tau^\alpha) 
$$

(3.57)

where the resolved shear stress on a slip system $\alpha$ is defined as:

$$
\tau^\alpha = (m^\alpha \otimes s^\alpha) : \sigma 
$$

(3.58)

and the elastic relation is defined as:

$$
\sigma = C \varepsilon^e 
$$

(3.59)

where $C$ is the global elastic stiffness tensor and $\varepsilon^e$ is the global elastic strain tensor. The isotropic hardening variable is the same for all slip systems, defined by the equation:

$$
\dot{r} = h(q - r)\dot{p} 
$$

(3.60)

where $q$ and $h$ are hardening constants and $p$ is an accumulated effective plastic strain, defined using the plastic velocity gradient $L^p$:

$$
\dot{p} = \left( \frac{2}{3} L^p : L^p \right)^{1/2} 
$$

(3.61)

$$
p = \int_0^t \dot{p} dt 
$$

(3.62)

The density of GNDs, $\rho_{GND}$, used in the flow rule of Eq. 3.57, corresponds to the magnitude of the GND density vector obtained by summing over all slip systems:

$$
\dot{\rho}_{GND} = \sum_\alpha \dot{\rho}_{GND}^\alpha = \sum_\alpha \frac{\dot{\gamma}^\alpha}{b} \text{curl} [m^\alpha F^p] 
$$

(3.63)

where the slip system GND density vector accounts for screw dislocations in the slip direction, $s^\alpha$, and edge dislocations in the direction of the slip plane normal.
$m^\alpha$ and in the direction $s^\alpha \times m^\alpha$ [157]:

$$\dot{\rho}_{GND}^\alpha = \dot{\rho}_{GND,em}^\alpha m^\alpha + \dot{\rho}_{GND,es,xm}^\alpha (s^\alpha \times m^\alpha) + \dot{\rho}_{GND,s}^\alpha s^\alpha$$

(3.64)

The same GND density is used for calculation of the slip rate across all slip systems, allowing latent hardening effects to be taken into account.

A Newton-Raphson iterative scheme is again employed for implementation of this formulation, this time to identify the increment in stress, $\delta\sigma$, as discussed in [56]. However, due to calculation of the GNDs at an element level (discussed later in the chapter), GND density is calculated at the start of the increment only and is not included in the implicit integration scheme.

**Large Deformation Formulation**

A large deformation formulation for strain-gradient CP, implemented for a 3D 20-noded, reduced-integration, brick element by Dunne et al. [59], is used in the studies of Chapters 7 and 8. A complete description of the implementation is provided in the thesis of Kiwanuka [158]. As for the small strain kinematics formulation, a yield condition is used to define the occurrence of slip on a slip system:

$$|\tau^\alpha| > \tau_c$$

(3.65)

The specific flow rule used in Chapters 7 and 8 is given by:

$$\dot{\gamma}^\alpha = \rho_{SSD,m} b^2 \nu \exp \left(-\frac{\Delta H}{kT}\right) \sinh \frac{(|\tau^\alpha| - \tau_c)\gamma_0 b^2}{kT \sqrt{\sum_\alpha (\rho_{SSD,i}^\alpha + \rho_{GND}^\alpha)}} \text{sgn}(\tau^\alpha)$$

(3.66)
3. Theory

where the shear stress on a slip system $\alpha$ is defined as a function of the second Piola-Kirchhoff stress, $S$, defined in Eq. 3.10:

$$\tau^\alpha = (s^\alpha \otimes m^\alpha) : S$$

where superscript ‘*’ denotes the intermediate frame of Fig. 3.7, in which the stress-update takes place, as described in [158]. The elastic relation for the large deformation implementation is defined as:

$$S^{*\text{tr}} = C_R E^*$$

where $C_R$ is the fourth order elasticity tensor referred to the reference frame, $E$ is the Green-Lagrange strain tensor and $S^{*\text{tr}}$ refers to the trial stress tensor. The slip system GND density of Eq. 3.66 is defined here as a function of $F^*$:

$$\sum_\alpha (b^\alpha \otimes \rho_{GND}^\alpha) = \text{curl}(F^{*-1})^T$$

where $b^\alpha$ is Burger’s vector and $\rho_{GND}^\alpha$ is comprised of both edge and screw dislocation density components. Eq. 3.69 is solved via a least squares minimisation scheme, described fully in [59] and [158], whereby the sum of the squares of dislocation densities is minimised. The implementation has been modified to include an evolution equation for the immobile SSD density, similar to that presented by Evers et al. [159], to account for both accumulation and annihilation (illustrated in Fig. 3.10) of dislocations:

$$\dot{\rho}_{SSD,i}^\alpha = \frac{|\dot{\gamma}|^\alpha}{b} \left[ \sum_\alpha (H^{\alpha\beta} \rho_{SSD,i}^{\beta} + H^{\alpha\beta} \rho_{GND}^{\beta}) - 2c y_c \rho_{SSD,i}^{\alpha} \right]$$

where $H^{\alpha\beta}$ are interaction coefficients describing the mutual immobilisation between dislocations of different slip systems, $c$ is a constant and $y_c$ is the critical annihilation distance. The rationale of Ohashi et al. [160] is adopted for assign-
3. Theory

Figure 3.10: Schematic of annihilation of two edge dislocations of opposite sign.

ing $H^{\alpha \beta}$; dislocations on the same slip system and on coplanar slip systems are assumed not to contribute to the mean free path and, thus a coefficient of 0 is assigned, while a coefficient of 1 is assigned for all other combinations.

Similar to the small strain kinematics implementation, a Newton-Raphson implicit integration scheme is used to calculate the second Piola Kirchhoff stress in the intermediate frame, $S^*$ at the end of the time increment. Again evolution of GND dislocation, and the additional evolution of SSD density, are included in the implementation explicitly.

3.5. The Finite Element Method

Numerical simulations in this thesis are carried out via the finite element method (FEM) using the commercial Abaqus FE solver (DS SIMULIA USA). While the basic principles of FEM for solid structures is discussed here, more thorough descriptions of the FEM can be found in Dunne and Petrinic [140], Crisfield [141,161] and the Abaqus Theory Manual [162], amongst others.

The FEM allows calculation of deformation or change in other variables throughout a body in response to external stimuli. Rather than considering a body as a whole, the solid structure is discretized into elements which are defined and connected by nodes to form an FE mesh, as illustrated in Fig. 3.11. Discrete
values of variables at the nodes, such as displacement, \( \mathbf{u} \), can be interpolated to find a distribution of the variable throughout the body via:

\[
\mathbf{u} = \mathbf{N}^{(e)} \mathbf{u}^{(e)}
\]  

(3.71)

where \( \mathbf{N}^{(e)} \) is a matrix containing shape functions for an element ‘e’ and \( \mathbf{u}^{(e)} \) contains the element nodal displacements. Other variables can be similarly calculated from discrete values at the nodes. The rate of deformation can be calculated at any point as a function of the nodal velocities by:

\[
\mathbf{D} = \mathbf{B}^{(e)} \mathbf{v}^{(e)}
\]  

(3.72)

where \( \mathbf{B}^{(e)} \) is a matrix containing derivatives of shape functions for an element with respect to the parent coordinate system for the element.

Hamilton’s principle for conserving energy provides a means of finding a solution for the equations of motion for an increment of an FE simulation. The variation of the kinetic energy, potential energy and work done by non-conservative forces in the system within any time increment must be zero, giving rise to the principle of virtual work, as described in Dunne and Petrinic [140]. For the quasi-static analyses of primary interest in this thesis, the kinetic energy term can be removed.
and the principle of virtual work can be defined as:

\[ \delta W = \int_{\Omega} \sigma : \delta D dV - \int_{\partial \Omega} t \delta v dA = 0 \] (3.73)

where \( \Omega \) and \( d\Omega \) are domains of volume, \( V \), and area, \( A \), and the work conjugate pair of Cauchy stress, \( \sigma \), and rate of deformation, \( D \), are used. Eq. 3.73 can be written using another work conjugate pair. For example, the principle of virtual work could be formed based on the reference configuration, using the second Piola Kirchoff stress and the rate of Green-Lagrange strain. Eq. 3.73 can be re-written using Voigt notation as:

\[ \delta W = \int_{\Omega} \delta D^T \sigma dV - \int_{\partial \Omega} \delta v^T t dA = 0 \] (3.74)

A similar substitution to that for \( u \) in Eq. 3.71 can be made for the virtual velocity, \( \delta v \) and, likewise, a similar substitution to that for \( D \) in Eq. 3.72 can be made for the virtual rate of deformation \( \delta D \). Eq. 3.74 then becomes:

\[ \delta W = \int_{\Omega^{(e)}} \delta \mathbf{v}^{(e)^T} \mathbf{B}^{(e)^T} \sigma^{(e)} dV^{(e)} - \int_{\partial \Omega^{(e)}} \delta \mathbf{v}^{(e)^T} \mathbf{N}^{(e)^T} t dA^{(e)} = 0 \] (3.75)

By removing the arbitrary \( \delta \mathbf{v}^{(e)^T} \), the above equation becomes a force balance for an element:

\[ \int_{\Omega^{(e)}} \mathbf{B}^{(e)^T} \sigma^{(e)} dV^{(e)} - \int_{\partial \Omega^{(e)}} \mathbf{N}^{(e)^T} t dA^{(e)} = 0 \] (3.76)

A summation can be performed over all elements in the model to give the global force balance:

\[ \mathbf{G}(u) = \int_{\Omega} \mathbf{B}^T \sigma dV - \int_{\partial \Omega} \mathbf{N}^T t dA = 0 \] (3.77)

where \( \mathbf{G}(u) \) is solved as a function of the global nodal displacement vector, \( u \). The FE analyses of primary interest in this thesis use the Abaqus implicit solver,
which solves for $u_{t+\Delta t}$ via the iterative Newton-Raphson integration scheme:

$$u_{t+\Delta t}^{(i+1)} = u_{t+\Delta t}^{(i)} - \left[ \frac{\partial G(u_{t+\Delta t}^{(i)})}{\partial u} \right]^{-1} G(u_{t+\Delta t}^{(i)})$$

(3.78)

where superscript “($i$)” and “($i+1$)” indicate consecutive estimates of $u_{t+\Delta t}$ and iterations are repeated until a converged solution for $u_{t+\Delta t}$ is found.

While the Abaqus solver carries out the calculation of elemental contributions to the global force balance and the Jacobian, $\frac{\partial G(u_{t+\Delta t}^{(i)})}{\partial u}$, of Eq. 3.78 above, for the $J_2$ plasticity and power-law CP (implemented in a UMAT) models, these contributions must be calculated within the UELs, used for implementation of the strain-gradient CP models. Further details of the specific equations used for calculation of the elemental contributions can be found in [56] and [158] for the small and large strain kinematics implementations, respectively.

### 3.5.1. Spatial Gradients Calculations

Calculation of the terms $\text{curl} [m^s F^p]$ in Eq. 3.63 and $\text{curl} (F^s)\!^{-1}$ in Eq. 3.69 in the strain-gradient CP formulations of Section 3.4.2 require knowledge of the spatial gradients of the components of $F^p$ and $F^s\!^{-1}$ for the small and large strain kinematics implementations, respectively. Element shape functions allow the calculation of these spatial gradients. The small kinematics formulation is implemented in a UEL for a 2D, reduced integration, 8-noded element, while the large strain kinematics formulation is implemented for a 3D, reduced integration, 20-noded brick element. For each implementation, a second internal element is introduced, with nodal coordinates equal to the coordinates of the Gauss integration points of the external element, as illustrated for a 2D element in Fig. 3.12. For an arbitrary scalar $\rho$, the discrete values of $\rho$ are known at the Gauss points of the external element and, thus at the nodes for the internal element. For a
Figure 3.12: Internal element with nodes at the Gauss integration points of an external element for a 2D example, used for the calculation of spatial gradients.

Gauss point in the internal element the spatial gradients of \( \rho \) can be calculated by:

\[
\frac{\partial N}{\partial \alpha} \begin{bmatrix} x^{(n)} \frac{\partial N}{\partial \alpha} \end{bmatrix}^{-1} \rho^{(n)} = \frac{\partial x}{\partial \alpha} \begin{bmatrix} \rho^{(n)} \end{bmatrix}^{-1} \rho^{(n)}
\]

\[
\frac{\partial N}{\partial \alpha} \frac{\partial x}{\partial \alpha} \left( \rho^{(n)} \right) \rho^{(n)} = \frac{\partial x}{\partial \alpha} \rho^{(n)}
\]

(3.79)

where \( \frac{\partial}{\partial x} \) and \( \frac{\partial}{\partial \alpha} \) denote partial derivatives with respect to the current global coordinate system and the parent shape coordinate system, respectively, \( \rho^{(n)} \) contains the discrete values of \( \rho \) at the internal element nodes, \( x^{(n)} \) contains the current nodal coordinates for the internal element and \( |_{i} \) denotes evaluation at a Gauss point \( i \) of the internal element. The spatial gradients can be back-calculated at the nodes of the internal element (i.e. at the Gauss points of the external element) using the spatial gradients calculated at the internal element Gauss points and an inverse of the shape functions for the internal element.

In the following chapters, the theory described here is applied to predict the fatigue behaviour of different materials for varying loading histories and model geometries. The crystal plasticity formulations of Section 3.4 are incorporated into a micromechanical framework for the microstructure-sensitive prediction of fatigue crack initiation, while the \( J_2 \) plasticity theory of Section 3.3 is used for the calibration of the micromechanical framework in Chapter 4 and provides
an industry standard approach for stent fatigue modelling to compare against in Chapters 4 and 5. The importance of different features of the constitutive models presented here for the capture of cyclic plasticity behaviour and prediction of fatigue crack initiation, in particular the kinematic hardening terms in the power-law CP formulation and evolution of geometrically necessary dislocation density in the strain-gradient CP formulations, is demonstrated and discussed.
4. Assessment of Fatigue 
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Design

4.1. Chapter Summary

A finite element based micromechanical methodology for cyclic plasticity and fatigue crack initiation (FCI) in cardiovascular stents is presented in this chapter. The methodology is based on the combined use of a (global) three-dimensional continuum stent-artery model and a local micromechanical stent model, to which micro-structure sensitive crack initiation parameters are applied. The methodology is applied to 316L stainless steel stents with random polycrystalline microstructures, based on scanning electron microscopy images of the grain morphology, under realistic elastic-plastic loading histories, including crimp, deployment and in-vivo systolic-diastolic cyclic pressurisation. Identification of the micromechanical cyclic plasticity and failure constants is achieved via application of an objective function and a unit cell representative volume element for 316L stainless steel. Cyclic stent deformations are compared with the $J_2$-predicted response and conventional fatigue life prediction techniques. It is shown that micromechanical fatigue analysis of stents is necessary due to the significant predicted effects.
of material inhomogeneity on micro-plasticity and micro-crack initiation. Implementation of damage, based on the accumulation of a microstructure-sensitive parameter, facilitates the prediction of the critical fatigue crack location, given multiple locations of potential crack initiation sites.

4.2. Introduction

The use of balloon expandable stents as part of the angioplasty procedure has revolutionised the treatment of heart disease. Although stent design is a relatively mature topic, numerous instances of stent fatigue fracture have been reported. This is particularly the case recently with the advent of drug eluting stents where tissue in-growth over stent struts is impeded, allowing deformed geometries and fractures to be more clearly revealed than before. Shaikh and co-workers [16] and Sianos and co-workers [15] provide intravascular ultrasound images depicting cases of stent fracture in the right coronary artery allowing the artery to collapse. Such severe fracture indicates a clear need to gain a deeper understanding of stent fracture and fatigue behaviour and to develop failure prediction methods to aid stent design refinements.

As a minimum requirement stent components are designed to have an operational life in excess of 10 years as recommended by the US Food and Drug Administration (FDA) [24]. This corresponds to a fatigue life in excess of approximately $4 \times 10^8$ systolic-diastolic pulsatile cycles (assuming a heart beat rate of 72 beats per minute). Such a fatigue life is considered to be in the high cycle fatigue (HCF) regime, corresponding to stress amplitudes below the macroscopic yield. However, as typical stent strut dimensions are comparable with microstructural geometry, such as grain size [5,26,99,121], it can be anticipated that inhomogeneity effects introduced by microstructure will cause localised (grain level) plastic de-
formation even at macroscopically elastic strains. Therefore crack initiation and microstructurally small crack propagation can occur during stent operational life. As a stent strut typically has only a few grains across its thickness [99, 100, 121] a crack is likely to cause fracture in the microstructurally small crack growth regime without ever entering the regime of physically small crack growth, indicating a need for microstructure-sensitive approaches to stent fatigue modelling. Crystal plasticity (CP) theory [163], which provides a means of explicitly modelling microstructural grains in a polycrystalline material, can be used for this purpose.

As a subject of growing interest, different approaches have already been proposed for stent fatigue analysis, outlined in Section 2.5 of the Background, briefly recounted here. Azaouzi et al. [129], Li et al. [127] and Schievano et al. [126] applied the traditional Goodman approach to 3D FE 316L stainless steel (SS), L605 and platinum stent models, respectively. Basic tensile properties were used to characterize constitutive behaviour and microstructural effects were neglected in all three cases, with the first study concluding that a micromechanical approach is essential in stent fatigue assessment. Wiersma et al. [133] applied the theory of critical distances [77], a continuum approach, which takes into account stress- gradients, to assess the fatigue performance of a biomedical grade 316L, however again, microstructural effects are not considered using this approach. A continuum fracture mechanics approach has been used by Marrey et al. [26] to assess the effect of a crack introduced on a L605 stent strut during fatigue. A key conclusion of this work was the need for CP modelling for stent fatigue assessment. Argente dos Santos et al. [135] employ a multi-scale damage-mechanics approach for prediction of micro-crack initiation during fatigue for two 316L stent designs. While micro-scale damage is a key contribution of this study, microstructural inhomogeneities introduced by grain boundaries and different crystallographic orientations are ignored, evident by the lack of scatter in predictions. The Dang
Van approach has been applied in another study to assess the fatigue of a 316L stent [134], again claiming the ability to capture grain-level phenomena; however, evaluation of mesoscopic stresses as a function of macro-scale models again ignores the inhomogeneous nature of the microstructure. The common drawback of these methodologies is the use of macroscopic continuum material models which are incapable of explicitly capturing microstructural effects. CP theory has been applied to the monotonic loading of 316L stainless steel stent material [5, 39, 99, 101, 121–123], giving good correlation to experimental work and capable of capturing statistical size effects in the macroscopic response. Finally, a quasi-3D CP model has been used to assess stent fatigue life via the Goodman diagram [100], but this work (i) did not use a cyclic plasticity model, (ii) assumed a regular crystal lattice, (iii) did not predict life and (iv) only employed continuum fatigue methods.

Methodologies for the modelling of crack initiation are less firmly established than those for crack growth. Section 2.4.2 of the Background provides an overview of fatigue indicator parameters (FIPs), used for predictions of fatigue crack initiation. Various parameters using macroscopic stress and strain values have been developed, such as the Fatemi-Socie parameter [69] and the Smith-Watson-Topper parameter [70, 73], often used in conjunction with a critical plane approach. Volume averaging techniques have also been applied to macroscopic FIPs to avoid over-conservative predictions for crack initiation based on FIPs at discrete points, e.g. [75]. However, while these techniques can give reasonable results they are based on continuum mechanics and are incapable of capturing microstructural inhomogeneity effects. Attempts to meet the need for microstructural representation in crack initiation predictions have been made, such as the Dang Van approach for predicting damage in multiaxial fatigue based on local microscopic stresses, evaluated as a function of macroscopic stress [164] and the Tanaka and Mura criterion for crack initiation in a slip band, based on the accumulation
of dislocation dipoles [88]. However, inhomogeneity effects observed in explicit modelling of random crystalline microstructures cannot be captured by these methodologies. Finally, a number of microstructure-sensitive FIPs, such as crystallographic effective plastic strain [62,83], used in conjunction with CP theory in micromechanical models have proved successful in the prediction of FCI observed experimentally. A similar approach is adopted in this study as the basis for stent fatigue analysis.

In this study, a finite element (FE)-based stent fatigue methodology is presented, based on CP theory for prediction of crack initiation using microstructural FIPs. A Voronoi Tessellation methodology is developed for the automated generation of realistic polycrystalline microstructures for real 316L stainless steel (SS) stent material. A combined kinematic-isotropic hardening CP constitutive material model for microscopic cyclic plasticity analysis is developed and calibrated via simulation of macroscopic 316L SS cyclic behaviour. A 3D stent-artery model is developed to identify boundary conditions for a unit cell (micromechanical) stent sub-model. Two candidate microstructure-sensitive FIPs are implemented in the CP formulation for prediction of FCI, where critical FIP values are calibrated and validated for LCF 316L data, and then applied to the prediction of crack initiation for different stent microstructure realizations. Damage is later implemented, based on accumulation of one of the FIPs, to facilitate cycle jumping analyses for two realizations of the stent sub-model, allowing identification of the critical crack location, where initial FIP distributions indicate the possibility of multiple crack initiation sites.
4. Assessment of Fatigue Performance for a 316L Stent Design

Figure 4.1: Flowchart illustrating the interaction between the different levels of material and geometry idealisations of the present study.

4.3. Methodology

The development and calibration of a micromechanical methodology is outlined in this section, along with application of the methodology to assess the fatigue behaviour of 316L SS for a generic stent design. A flowchart illustrating the methodology is provided in Fig. 4.1. Referring to Fig. 4.1, a crystal (cyclic) plasticity constitutive model is coupled with an FE model of a realistic polycrystalline geometry for calibration (via a least squares objective function). This is achieved via comparison of the strain-controlled response of this periodic microstructure model against a target (cyclic) $J_2$ continuum (macroscopic) response for 316L SS. Once calibrated, the CP material model and the $J_2$ continuum (macroscopic) model are both implemented within a 2D unit cell sub-model of the stent, where fatigue boundary conditions for the sub-model are extracted from a global 3D continuum stent-artery model. Finally, the fatigue life predictions of the microstructure-sensitive approach and the traditional continuum approach are compared for the stent sub-model.
4.3.1. Constitutive Models

Both a $J_2$ plasticity model and a CP model are employed in this study. The $J_2$ flow theory formulation is used to (i) generate a target response for the calibration of the CP model, (ii) define the behaviour of a global stent model and (iii) allow comparison of the CP micromechanical approach for stent fatigue analysis against a macroscopic constitutive model approach. The $J_2$ formulation used is described by Eqs. 3.16 – 3.21 of Chapter 3, where one kinematic back-stress is employed.

The power-law CP formulation of Section 3.4.1 is also used in this study. Use of a CP constitutive model allows microstructure-sensitive analysis of stent fatigue to be carried out. Stent fatigue behaviour is affected by (i) the initial deformation due to the crimp and deployment processes and (ii) systolic-diastolic cyclic loading. Therefore a material model must be adopted which simulates both monotonic and cyclic loading behaviour of a real material. Cyclic behaviour of a material can be defined by (i) evolution of the stress-strain curve prior to a stabilised response and (ii) the stabilised cyclic stress-strain curve (CSSC). Isotropic hardening (allowing yield surface expansion) defines the evolution of stress magnitudes reached in a cyclic stress-strain response and controls the rate at which saturation, and thus a stabilised response, is achieved. A CP constitutive model with isotropic hardening only has been used in previous work for modelling the monotonic loading of 316L SS stent material [5, 99]. Calibration of the isotropic CP model against stabilised cyclic behaviour of a $J_2$ continuum 316L SS material model has also been carried out [73]. However the isotropic CP model, once calibrated for stabilised cyclic behaviour, is unable to capture the initial monotonic behaviour of the $J_2$ continuum model, which represents the target response, or cyclic evolution before stabilisation. Furthermore, significant discrepancies exist between the stabilised hysteresis loop shapes of the two models. It has been shown that crack initiation and propagation can be correlated
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against cyclic strain energy dissipation \([86,165]\), calculated by the area bounded by a hysteresis loop. Therefore, the discrepancies between hysteresis loop shapes need to be rectified. Kinematic hardening introduces a back-stress into the cyclic stress-strain response. This facilitates capture of the Bauschinger effect, i.e. a decrease in yield stress upon reversal of loading, and, thus, influences the shape of the stabilised hysteresis curve. Hence, to facilitate computational studies of cyclic and monotonic behaviour of 316L SS it is necessary that both isotropic and kinematic hardening are included in the material model employed.

Kassner et al. \([166]\) proposed that the experimentally observed Bauschinger effect can be attributed, in physical terms, to a combination of (i) the Orowan-Sleeswyk mechanism, where dislocations surmounted in “forward” direction straining are more easily overcome upon reversal of straining direction, resulting in a lower flow stress, and (ii) long range internal stresses due to heterogeneous dislocation structures, formed as a result of strain incompatibility between differently oriented grains. Pham and Holdsworth \([61]\) further differentiated between inter- and intra-granular back-stresses as a result of internal stresses, based on experimental observations for 316L SS. Inter-granular back-stress was attributed to the difference in geometrically-necessary dislocation density at the grain boundaries, formed due to incompatibility between grains, and dislocation density at the interior of the grain, which increases at a slower rate. However, with cycling, the difference in boundary and interior dislocation density diminishes, reducing the effect of inter-granular back-stress. As dislocation density at the grain interior increases, dislocations rearrange to form stable configurations and, thus, an intra-granular back-stress is formed as a result of strain incompatibilities between high and low density regions caused by these dislocation structures. While it may be argued that inclusion of crystallographic orientation in polycrystal models can capture strain incompatibility at grain boundaries and, thus, an inter-granular back-stress, the same cannot be said for the intra-granular back-stress. Hence,
the Armstrong-Frederick formulation for kinematic hardening has been implemented into the power-law CP formulation for the phenomenological capture of the Bauschinger effect.

As described in Chapter 3, the power-law CP model was first implemented by Huang [148] in a UMAT. The kinematic hardening component is developed and implemented in this study, for which details of the implementation are provided in Appendix A.1. As for the $J_2$ model, one CP kinematic back-stress is used.

Two microstructure-sensitive FIPs are implemented to predict crack initiation in the CP stent fatigue model based on (i) effective plastic strain, which sums plastic strain due to slip over all slip systems, and (ii) crystallographic work, which sums strain energy dissipation over all slip systems. The effective plastic strain FIP, $p$, has been shown to be successful in predicting number of cycles to crack initiation in both the low and high cycle fatigue regimes for different mean stress levels for a C263 nickel alloy based on identification of a critical value of effective plastic strain from low cycle fatigue data [83]. It is defined as a function of the plastic velocity gradient (Eq. 3.28) integrated over time:

$$\dot{p} = \left( \frac{2}{3} L^p : L^p \right)^{1/2} ; \quad p = \int_0^t \dot{p} dt \quad (4.1)$$

An accumulative crystallographic work parameter is the second FIP implemented [86], defined by the equation:

$$W = \sum_{\alpha} \int_0^t \tau^\alpha \dot{\gamma}^\alpha dt \quad (4.2)$$

4.3.2. Realistic Microstructure Generation

A Voronoi Tessellation (VT) and Delaunay Triangulation methodology is developed here for the generation of random crystalline microstructures based on real
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Figure 4.2: SEM of a 316L SS stent strut, showing scale of strut dimensions and morphology of material microstructure.

316L SS stent material. Fig. 4.2 shows a scanning electron microscopy (SEM) image of a typical stent strut which illustrates the material microstructure. The methodology is implemented in a Python script coupled with the commercial finite element package Abaqus for automatic generation of microstructure FE models. Given a random array of nuclei points the VT algorithm generates a grain boundary geometry based on the assumption that all grains grow at a uniform rate from their respective nuclei, as illustrated in Fig. 2.8 of Chapter 2. Delaunay Triangulation allows the identification of sets of nuclei belonging to grains which share grain boundaries and form a triple point; a set of three nuclei points form a triangulation if no other nuclei point lies within the circle circumscribed by these three nuclei points. Microstructural samples are generated such that periodic boundary conditions can be applied to them [103]. The algorithm generates a set of random nuclei points in a cell with the desired sample dimensions. This set of nuclei points is then copied into a 3×3 cell matrix, as shown in Fig. 4.3(a). A microstructure sample is then generated in the central cell only. The unit cell model of Fig. 4.3(b) is an example of a generated periodic microstructure. Due to the VT process the grain boundaries on opposite faces of the generated microstructure are aligned, allowing for application of periodic boundary conditions.

The average grain area of a generated microstructure can be controlled by specifying an appropriate nuclei point density. A Matlab program is developed for
Figure 4.3: (a) Process of generation of a periodic microstructure and (b) FE model of a generated periodic microstructure, subsequently employed for calibration of the crystal (cyclic) plasticity material model.

the extraction of average grain area and grain area distribution from a given microstructural geometry. The number of grain measurements needed to acquire a statistical distribution of grain sizes for a material is dependent on the variability of the microstructure, e.g. variability of grain size and shape. An ASTM standard for determining average grain size and distribution of grain sizes [167] recommends that at least 500 grains are measured from at least five different fields. Due to the limited SEM data available, the Matlab program is applied here to measure approximately 300 grains in images of three 316L SS stent struts [5] (e.g. Fig. 4.2), with average grain areas for each image of 73, 91 and 108 $\mu m^2$ and lowest correlation between area distributions for two images of 86 %. The extracted overall average grain area is used to generate realistic 316L SS microstructures. The 316L stent material and the generated periodic microstructure of Fig. 4.3(b) both have an average grain area of 89 $\mu m^2$ and a correlation to within 7% between their grain area distributions.

Due to unavailability of data on the crystallographic orientations of grains in the 316L stent struts, it is assumed for this study that there is no crystallographic texture and, thus, random grain orientations will be assigned in the micromechanical model in the next section. However, while tubes used for the manufacture of
4. Assessment of Fatigue Performance for a 316L Stent Design

Table 4.1: Material constants for the 316L SS $J_2$ continuum material model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_y$</td>
<td>265 MPa</td>
</tr>
<tr>
<td>$E$</td>
<td>200 GPa</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.3</td>
</tr>
<tr>
<td>$Q$</td>
<td>35 MPa</td>
</tr>
<tr>
<td>$b$</td>
<td>3.85</td>
</tr>
<tr>
<td>$c$</td>
<td>30 GPa</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>60</td>
</tr>
</tbody>
</table>

Stents undergo an annealing process, the presence of a crystallographic texture from the fabrication of the tubes is still a possibility. This could have an effect on the fatigue performance of the stent and would, thus, need to be accounted for in the stent fatigue design process.

4.3.3. Crystal Plasticity Model Calibration

Calibration of the combined kinematic-isotropic CP material model is carried out by iteratively comparing the uniaxial macroscopic response for strain-controlled cyclic loading ($R_\varepsilon = \frac{\varepsilon_{\min}}{\varepsilon_{\max}} = -1$) across a range of five material parameters ($g_0$, $g_\infty$, $h_0$, $C_{\text{kin}}$, $D_{\text{kin}}$) against the target $J_2$ macroscopic response for 316L SS, for which the constants are given in Table 4.1 [168]. Convergence of the constants with respect to the calibration process was tested via the objective function:

$$F(x_k) = \sum_{j=1}^n \sum_{i=1}^m [(\sigma_{i\text{CP}}^j) - (\sigma_{i\text{\text{J2}}}^j)]^2$$  \hspace{1cm} (4.3)

where $x_k$ represents the material parameters to be calibrated, $n$ is the number of strain ranges considered, $m$ is the number of data points per strain range and $\sigma_{i\text{CP}}^j$ and $\sigma_{i\text{\text{J2}}}^j$ are the CP and $J_2$ continuum macroscopic stress values at the data points respectively. This methodology facilitates calibration of the five constants with...
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respect to: (i) the monotonic response, (ii) the evolution of stress-strain response prior to stabilisation and (iii) the hysteresis loop shapes for the stabilised stress-strain curves. Twelve potentially active slip systems are considered in the CP material model corresponding to the fcc crystalline structure of 316L SS, including four slip planes and three possible slip directions on each plane, described by the Miller indices \{111\}\langle110\rangle. Isotropic elasticity (Eq. 3.22) is assumed in the CP material model for the purposes of calibration against the $J_2$ continuum model, using a Young’s modulus of 200 GPa and a Poisson’s ratio of 0.3. The reference strain rate is taken to be 0.002 s$^{-1}$ and the rate sensitivity exponent, $n$, is set at a high value of 50, corresponding to low rate dependency as observed for experimental 316L SS behaviour [119].

A representative volume element (RVE), as introduced in Section 2.4.3, of 316L SS microstructure is developed to achieve uniform macroscopic behaviour independent of grain orientation and morphology. The FE model of the generated microstructure in Fig. 4.3(b), although having smaller dimensions than RVEs reported for 316L SS [168], has a reasonably uniform macroscopic response for different grain orientation sets while remaining practical computationally. The RVE contains 126 grains with random crystallographic orientation. While automatic meshing is applied to the bulk of the model, manual meshing is required to facilitate application of periodic boundary conditions to the model’s free edges; as for the grain boundaries, nodes on opposite faces of the model must be aligned. Therefore, an equal number of nodes, with equal spacing, is required along the edges of corresponding grains on opposite faces of the geometry, in order to apply the following periodic equations [169]:

\[
\begin{align*}
    u_E(x) &= u_{SE}(x) + u_W(x) \\
    u_N(y) &= u_{NW}(y) + u_S(y) \\
    \mathbf{u}_{NE} &= \mathbf{u}_{NW} + \mathbf{u}_{SE}
\end{align*}
\]
Figure 4.4: Application of periodic boundary conditions for periodic microstructure model.

where N, S, E and W refer to nodes along the edge faces and NW, NE, SW and SE refer to the corner nodes shown Fig. 4.4 and \( u(x) \) and \( u(y) \) are the \( x- \) and \( y- \) components of the nodal displacement vector, \( \mathbf{u} \). The final mesh for the RVE contained 12454 plane strain reduced-integration 4-noded quadrilateral elements.

4.3.4. Global Stent Model

A global 3D continuum model of stent deployment and fatigue in an artery is developed for the identification of fatigue boundary conditions for the unit cell sub-model. The Abaqus/Explicit FE solver is used for this analysis. A generic stent geometry based on the commercial Medinol NIR\textsuperscript{TM} stent is chosen for the analysis. The 3D macroscopic model consists of one complete ring of stent unit cells, as shown in Fig. 4.5(a), and employs the \( J_2 \) continuum constitutive model. The artery is modelled as a three-layered cylinder (shown in Fig. 4.5(a)) with an internal diameter of 2.65 mm, including the intima, media and adventitia layers. Layer thicknesses are based on measured coronary artery geometries [170]. A hyperelastic isotropic constitutive model, built into the Abaqus/Explicit FE solver, is employed to describe the material behaviour of the arterial layers. The
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Figure 4.5: (a) 3D stent ring model inside 3-layered artery and (b) von Mises stress distribution after deployment of stent into artery.

constitutive law uses a reduced polynomial strain energy density function of sixth order, for which further details and constants for each arterial layer are provided in the literature [117]. The stages modelled include crimping, post crimp recoil, deployment, post deployment recoil and fatigue. Pressure is applied to the external (crimp) and internal (deploy) stent surfaces corresponding to a change in stent diameter from 0.851 mm to 0.676 mm for crimp and expansion to a diameter of 3 mm during deployment. In Fig. 4.5(b) can be seen the deformed stent in the artery after deployment. Fatigue is simulated by applying an alternating internal pressure of maximum magnitude 7.98 kPa (60 mmHg), for a cyclic load ratio \( R_p = \frac{p_{\text{min}}}{p_{\text{max}}} = 0 \), to both the stent and artery [100]. A change in diameter of 0.00491 mm is recorded between the systolic and diastolic stages of fatigue in the 3D global macroscopic model.

4.3.5. Unit Cell Stent Sub-Model

A sub-model is developed of a unit cell, shown highlighted in a stent section both in 3D form and rolled out in 2D in Fig. 4.6(a) and Fig. 4.6(b) respectively, [100]
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Figure 4.6: (a) Stent section with unit cell highlighted, (b) rolled out stent section and (c) unit cell nodes and edges at which boundary conditions are applied.

for both the $J_2$ continuum and the calibrated CP material models. Crimp and deployment processes are modelled in addition to fatigue in order to capture the effect of initial deformation. The applied boundary conditions ensure periodicity of the unit cell within the stent geometry. Edge 1, as seen in Fig. 4.6(b), is fixed in the $x$-direction and node A is fixed in the $y$-direction. Edges 2 and 3 are coupled with nodes A and B respectively to ensure these edges remain plane. Nodes A and B are constrained such that their rotations are equal in magnitude and opposite in sign. Crimp and deployment are simulated via displacement of node B in the $y$-direction, calculated by:

$$|AB| = \frac{\pi D_{stent}}{n}$$  \hspace{1cm} (4.5)

where $D_{stent}$ is the stent diameter and $n$ is the number of unit cells required to form a ring. Removing these displacements simulates recoil after the crimp and deployment processes. Fatigue is simulated via an alternating displacement at node B of magnitude 1.29 $\mu$m, calculated using the change in stent diameter during fatigue, measured from the 3D global model. A schematic of the relative displacement between nodes A and B is provided in Fig. 4.7, corresponding to boundary conditions applied.
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Figure 4.7: History of relative displacement between nodes A and B, $d_{AB}$, for stent unit cell crimp, deployment and fatigue.

Due to the stochastic nature of inhomogeneous microstructures it is necessary here to model multiple possible stent microstructures in order to generate statistically significant results. Shown in Fig. 4.8 are two CP unit cell stent sub-models with different generated microstructural geometries, labelled RND1 and RND2. These microstructural geometries are designed to have optimum correlation with, i.e. be representative of, the measured microstructure of Fig. 4.2. A comparison of their grain area distributions with that of the measured microstructure can be seen in Fig. 4.8; all three microstructures have the same average grain area of 89 $\mu$m$^2$. Five different random distributions of crystallographic orientation are generated for each of the RND1 and RND2 CP unit cell sub-models to assess the effect of grain orientation. Therefore a total of ten stent microstructures are modelled. The RND1 and RND2 unit cells are meshed with 49007 and 47831 generalised plane strain, reduced integration, 4-noded elements while the $J_2$ continuum model contained 47610 elements of the same type. Adaptive meshing is implemented in the critical regions of the CP unit cell models during deployment due to excessive mesh distortion of individual elements within critically-loaded grains, caused by high deformation. Anisotropic cubic elasticity (Eq. 3.23) is used in the CP material model for the stent fatigue analysis using constants $C_{11} = 205$ GPa, $C_{12} = 138$ GPa and $C_{44} = 126$ GPa [5]. The unit cell sub-model developed can be considered a quasi-3D model [5] as (i) the CP material descrip-
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Figure 4.8: Stent unit cell microstructure geometries and their grain area distributions.

4.3.6. Life Prediction Approaches

Two approaches are adopted for the assessment of stent fatigue performance in this study. The first is a microstructure-sensitive approach, used to predict fatigue crack initiation, or failure of the material at a discrete point. The second is an industry-standard stress-based approach, used to predict fatigue failure, or stent fracture. Prediction of the number of cycles to FCI, $N_i$, in the CP model is carried out using the FIPs described in Section 4.3.1, $p$ and $W$:

$$N_i = \frac{p_{\text{crit}} - p_{\text{recoil}}}{p_{\text{cyc}}}; \quad N_i = \frac{W_{\text{crit}} - W_{\text{recoil}}}{W_{\text{cyc}}} \quad (4.6)$$
where $p_{\text{crit}}$ is an identified critical value of the effective plastic strain at which FCI is assumed to occur, $p_{\text{recoil}}$ is the initial effective plastic strain accumulated during the deployment process, $p_{\text{cyc}}$ is the effective plastic strain accumulated during one cycle of fatigue loading and $W_{\text{crit}}$, $W_{\text{recoil}}$ and $W_{\text{cyc}}$ are the corresponding values for crystallographic work. Calibration of $p_{\text{crit}}$ and $W_{\text{crit}}$ for generalised plane strain conditions is carried out via comparison with the Coffin-Manson equation for predicting number of cycles to failure in low cycle fatigue (LCF):

$$N_f = \left[ \frac{\Delta \epsilon_p C_1}{\gamma_1} \right]^{-\gamma_1} \quad (4.7)$$

where $\Delta \epsilon_p$ is the macroscopic plastic strain range, and $C_1$ and $\gamma_1$ are material constants. LCF simulations are carried out using the geometry of Fig. 4.3 (b) for generalised plane strain conditions to identify $p_{\text{cyc}}$ and $W_{\text{cyc}}$: there is no recoil contribution for fully-reversed cyclic loading. A mesh sensitivity study for the RVE, described in Appendix A.2, demonstrates an acceptably converged solution for the mesh density used, both in terms of macroscopic stress-strain response and FIP prediction. Assuming that crack initiation dominates fatigue life in LCF loading, values of $p_{\text{crit}}$ and $W_{\text{crit}}$ are identified as 43.3 and 12636 MJm$^{-3}$, respectively, using $N_f$ calculated for one plastic strain range. Life predictions using the FIPs are compared with the Coffin-Manson relationship for 316L in Fig. 4.9, in which good correlation is seen, validating the calibrated values of $p_{\text{crit}}$ and $W_{\text{crit}}$.

The stent design industry has a standard of carrying out a Goodman analysis using maximum principal stress to assess stent fatigue performance [24, 100]. Although a Goodman analysis can provide factors of safety for highly loaded points in a stent, these apply for a single fatigue life only. The modified Goodman equation is defined by:

$$\sigma_a = \sigma_e \left( 1 - \frac{\sigma_m}{\sigma_{TS}} \right) \quad (4.8)$$

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where $\sigma_a$ and $\sigma_m$ are the stress amplitude and mean stress of loading respectively, $\sigma_{TS}$ is the ultimate tensile strength, taken at 800 MPa, the saturated stress of the $J_2$ continuum constitutive model, and $\sigma_e$ is the fatigue limit for a given $N_f$. The Basquin equation for HCF loading provides a relationship between stress range at zero mean stress, $\Delta \sigma|_{\sigma_m=0}$, with number of cycles to failure, $N_f$:

$$\Delta \sigma|_{\sigma_m=0} = C_2 N_f^{-\frac{1}{\gamma_2}}$$ (4.9)

where $C_2$ and $\gamma_2$ are material constants. The fatigue limit, $\sigma_e$, for a given total life, $N_f$, can be calculated as half of $\Delta \sigma|_{\sigma_m=0}$. Hence, by combining the Goodman curve with Basquin’s equation, an equation relating $N_f$ to stress range and mean stress is formed:

$$N_f = \left[ \frac{\Delta \sigma}{C_2 \left( 1 - \frac{\sigma_m}{\sigma_{TS}} \right)} \right]^{-\gamma_2}$$ (4.10)

where $\Delta \sigma$ is the stress range due to loading. Another method used in stent fatigue analysis [171], which will also be used in this work, employs the Sines
4. Assessment of Fatigue Performance for a 316L Stent Design

Table 4.2: LCF and HCF constants for the 316L SS.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>0.34</td>
</tr>
<tr>
<td>$\gamma_1$</td>
<td>2.07</td>
</tr>
<tr>
<td>$C_2$</td>
<td>3280 MPa</td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>5.7</td>
</tr>
</tbody>
</table>

criterion for multiaxial fatigue [66]. The failure criterion can be expressed as:

$$\sigma_{\text{mises,a}} \leq \sigma_e \left(1 - \frac{3\sigma_{H,m}}{\sigma_{TS}}\right)$$  \hspace{1cm} (4.11)

where $\sigma_{\text{mises,a}}$ is the von Mises stress amplitude due to loading and $\sigma_{H,m}$ is the mean hydrostatic stress. The Sines criterion is typically used for assessing if a cyclically loaded component will fail before a fixed total life, defined by the fatigue limit, and not for life prediction. However, Basquin’s equation can once again be used to relate fatigue limit to total life, $N_f$, to give a combined Sines and Basquin equation:

$$N_f = \left[\frac{\Delta\sigma_{\text{mises}}}{C_2 \left(1 - \frac{3\sigma_{H,m}}{\sigma_{TS}}\right)}\right]^{-\gamma_2}$$  \hspace{1cm} (4.12)

where $\Delta\sigma_{\text{mises}}$ is the von Mises stress range due to loading. Hence, two methods will be used for prediction of total life in both the $J_2$ continuum and CP stent unit cell models: (i) the combined Goodman and Basquin formulation (Eq.4.9) using maximum principal stress values for stress range and mean stress, and (ii) the combined Sines and Basquin formulation (Eq.4.12) for multiaxial fatigue. LCF and HCF constants for 316L SS used in equations 4.7, 4.9 and 4.12 are provided in Table 4.2 [168].
4. Assessment of Fatigue Performance for a 316L Stent Design

Table 4.3: Identified CP constants for 316L SS.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_0$</td>
<td>90 MPa</td>
</tr>
<tr>
<td>$g_\infty$</td>
<td>104 MPa</td>
</tr>
<tr>
<td>$h_0$</td>
<td>30 MPa</td>
</tr>
<tr>
<td>$C_{kin}$</td>
<td>15836 MPa</td>
</tr>
<tr>
<td>$D_{kin}$</td>
<td>74</td>
</tr>
</tbody>
</table>

Figure 4.10: Comparison of tensile curves for $J_2$ continuum and kinematic-isotropic CP material models.

4.4. Results

4.4.1. CP Model Calibration

Table 4.3 contains the calibrated constants for the kinematic-isotropic hardening CP constitutive model which give monotonic and cyclic behaviour of excellent correlation to the $J_2$ continuum model, based on the objective function approach of Eq. 4.3. Comparisons of the tensile response and the macroscopic stabilised cyclic stress-strain curves of the $J_2$ continuum and CP material models are shown in Fig. 4.10 and Fig. 4.11 respectively. For the micromechanical CP material, this is the bulk stress-strain response of the unit cell model of Fig. 4.3(b).
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Figure 4.11: Comparison of cyclic stress-strain curves for the $J_2$ continuum and kinematic-isotropic CP material models.

Table 4.4: 316L identified constants for CP model with isotropic hardening.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_0$</td>
<td>70 MPa</td>
</tr>
<tr>
<td>$g_\infty$</td>
<td>250 MPa</td>
</tr>
<tr>
<td>$h_0$</td>
<td>60 MPa</td>
</tr>
</tbody>
</table>

Constants for the CP constitutive model with isotropic cyclic hardening only, corresponding to the flow rule of Eq. 3.29, have been previously identified for 316L SS stabilised cyclic behaviour [73], provided in Table 4.4. Fig. 4.12 shows a comparison of the predicted response for the first cycle of loading for the calibrated isotropic CP model and the kinematic-isotropic CP model with that of the $J_2$ continuum model. Isotropic hardening alone implemented in the CP model is unable to capture the initial stress-strain curve. However, introduction of kinematic hardening facilitates excellent correlation with the $J_2$ continuum model. This ability of the CP model to simulate the initial stress-strain behaviour of the $J_2$ continuum model is important in stent fatigue analysis for accurate representation of residual stresses and deformation due to deployment.

Fig. 4.13 shows a comparison of the stabilised cyclic hysteresis curve for the three material models. The kinematic-isotropic CP model still correlates excellently with the $J_2$ continuum model, taken here as the target macroscopic response.
4. Assessment of Fatigue Performance for a 316L Stent Design

Figure 4.12: Comparison of stress-strain curves for first cycle of loading for $J_2$ continuum, kinematic-isotropic CP and isotropic CP material models.

A loop shape parameter [3] is used to quantify this difference in hysteresis loop shape and the improvement to loop shape through the introduction of kinematic hardening, given by:

$$V_H = \frac{A_{hysteresis}}{A_{parallelogram}}$$  \hspace{1cm} (4.13)

where $A_{hysteresis}$ is the area within a hysteresis curve and $A_{parallelogram}$ is the area bounded by a parallelogram which circumscribes that curve. Values of the loop shape parameter for the three material models are given for the strain range of Fig. 4.13 in Table 4.5. It is clear that the introduction of kinematic hardening into the CP constitutive model significantly improves correlation with the $J_2$ continuum model. As mentioned in the previous section, cyclic crystallographic work, controlled by hysteresis loop area, has been proposed as a microscopic fatigue indicator parameter in crack initiation mechanisms. Thus, the excellent correlation of $V_H$ between the kinematic-isotropic CP model and the $J_2$ continuum model ensures similar strain energy dissipation contributing towards crack initiation in both material models.
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Figure 4.13: Comparison of stabilised macroscopic hysteresis curves for $J_2$ continuum, kinematic-isotropic CP and isotropic CP material models.

Table 4.5: Hysteresis loop shape parameters for $J_2$ continuum, isotropic CP and combined kinematic-isotropic CP models.

<table>
<thead>
<tr>
<th>Hysteresis Loop</th>
<th>$V_H$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J_2$ Continuum</td>
<td>0.627</td>
</tr>
<tr>
<td>Isotropic CP</td>
<td>0.946</td>
</tr>
<tr>
<td>Isotropic &amp; Kinematic CP</td>
<td>0.614</td>
</tr>
</tbody>
</table>

4.4.2. Stent Fatigue Model

Comparisons of the quasi-3D stent unit cell predictions for the $J_2$ continuum and CP material models (RND1 and RND2) show similar von Mises stress distributions for the bulk of the material, as depicted in Fig. 4.14 and Fig. 4.15 following post-crimp recoil and post-deployment recoil respectively. Overall, the predicted microscopic peak stresses are significantly higher than the macroscopic values.

The total life approach of the Goodman-Basquin and Sines-Basquin methods is predicated on macroscopic $J_2$ assumptions so that it is not consistent, in length scale, with micromechanical (CP) modelling. The constants used in Eq. 4.7 are conventionally identified using macroscopic fatigue data. This clearly contrasts
with the length scales and constitutive assumptions associated with plasticity due to inhomogeneous microstructure. Hence, peak von Mises stresses can be predicted at Gauss points in the CP model which exceed the macroscopic ultimate tensile strength. Therefore, a volume averaging technique, shown to be effective in dealing with steep stress-gradients \cite{75,76}, is implemented for homogenization of multiaxial mean stress and stress range values for \( N_f \) predictions for the CP model, where a grain is the averaging volume (grain-averaging). The volume-averaged value for a stress variable \( \sigma \) in a grain is defined as:

\[
\bar{\sigma} = \frac{\sum_i \sigma_i A_i}{\sum_i A_i}
\tag{4.14}
\]

where \( i \) is the number of elements in a grain and \( \sigma_i \) and \( A_i \) are the element integration point stress value and element area respectively. For comparative purposes a volume averaging approach is also adopted in the \( J_2 \) continuum model, where the averaging volume is based on the average grain area in the CP unit cell model of 89 \( \mu \)m \(^2\). \( N_f \) is predicted for a given element integration point based on volume-averaged stress values using all elements within a given radius, corresponding to average grain area, of that integration point.

Life predictions made for the \( J_2 \) continuum and CP unit cell models are given in Table 4.6. The Goodman-Basquin equation using maximum principal stress values predicts an average total life of \( 7.27 \times 10^8 \) cycles with standard deviation (SD) of \( 1.18 \times 10^9 \) cycles for the CP unit cell model across both grain morphologies with different grain orientation sets. The predicted \( N_f \) for the \( J_2 \) continuum model using the Goodman-Basquin equation lies within the lower end of the \( N_f \) range for the CP models. Predictions of number of cycles to FCI \( (N_i) \) for the CP models using the effective plastic strain FIP \( (p_{\text{crit}}) \) yield an average of \( 4.22 \times 10^6 \) with an SD of \( 5.69 \times 10^5 \). Using the crystallographic work FIP \( (W_{\text{crit}}) \), FCI is predicted to occur in the CP unit cell models at an average of \( 3.69 \times 10^6 \) cycles with an SD of \( 9.61 \times 10^5 \) cycles.
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Both the $J_2$ continuum and CP unit cell models give high mean hydrostatic stress values, despite the use of volume averaging methods, such that $3\sigma_{H,m}$ is higher than the ultimate stress, preventing the calculation of $N_f$ in the Sines-Basquin Eq. 4.12. It should be noted that these points of high hydrostatic stress are in the interior of the unit cell model, where stress amplitudes due to fatigue loading are low. A prediction using the Sines-Basquin equation is possible for the $J_2$ continuum unit cell model when the averaging volume is increased to 2.42 times the grain size, where the grain size is taken as the diameter of a circle which gives the average grain area.

Locations of the predictions for crack initiation in all RND1 and RND2 orientation sets are shown in Fig. 4.16, from which can be identified three critical regions, one of which corresponds to the location of lowest predicted $N_f$ in the $J_2$ continuum model. A plot of $N_i$ predictions, as shown in Fig. 4.17 for one CP unit cell model, illustrates the localisation of damage in these critical regions, while FCI is predicted to be unlikely to occur in the bulk of the material. In Fig.

Figure 4.14: Comparison of von Mises stress distributions after post-crimp recoil for the $J_2$ continuum model and one orientation set for both the RND1 and RND2 CP unit cell models.
4. Assessment of Fatigue Performance for a 316L Stent Design

Figure 4.15: Comparison of von Mises stress distributions after post-deployment recoil for the $J_2$ continuum model and one orientation set for both the RND1 and RND2 CP unit cell models.

4.18 can be seen a plot of $p_{\text{recoil}}$ for one CP unit cell model, with the region of highest deformation magnified. Unlike the $J_2$ continuum model whose surfaces remain smooth throughout loading, instances of surface roughening are observed in the CP model at locations of high effective plastic strain.

4.5. Discussion

Residual stresses introduced in the initial crimping and deformation processes can be seen clearly in the von Mises stress distributions of Fig. 4.14 and Fig.
## 4. Assessment of Fatigue Performance for a 316L Stent Design

Table 4.6: Unit cell model life predictions for $J_2$ continuum and CP material models.

<table>
<thead>
<tr>
<th>Model</th>
<th>$N_f$</th>
<th>$N_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$p_{crit}$</td>
<td>$W_{crit}$</td>
</tr>
<tr>
<td>$J_2$ continuum</td>
<td>7.63×10⁸</td>
<td></td>
</tr>
<tr>
<td>CP RND 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>orientation set 1</td>
<td>1.48×10⁹</td>
<td>5.27×10⁶</td>
</tr>
<tr>
<td>orientation set 2</td>
<td>9.78×10⁸</td>
<td>3.96×10⁶</td>
</tr>
<tr>
<td>orientation set 3</td>
<td>4.38×10⁸</td>
<td>3.94×10⁶</td>
</tr>
<tr>
<td>orientation set 4</td>
<td>1.23×10⁷</td>
<td>5.12×10⁶</td>
</tr>
<tr>
<td>orientation set 5</td>
<td>3.79×10⁹</td>
<td>4.36×10⁶</td>
</tr>
<tr>
<td>CP RND 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>orientation set 1</td>
<td>7.91×10⁷</td>
<td>3.49×10⁶</td>
</tr>
<tr>
<td>orientation set 2</td>
<td>1.58×10⁷</td>
<td>4.00×10⁶</td>
</tr>
<tr>
<td>orientation set 3</td>
<td>9.56×10⁶</td>
<td>4.34×10⁶</td>
</tr>
<tr>
<td>orientation set 4</td>
<td>1.87×10⁸</td>
<td>3.88×10⁶</td>
</tr>
<tr>
<td>orientation set 5</td>
<td>2.77×10⁸</td>
<td>3.86×10⁶</td>
</tr>
<tr>
<td>All Realizations</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Average</td>
<td>7.27×10⁸</td>
<td>4.22×10⁶</td>
</tr>
<tr>
<td>SD</td>
<td>1.18×10⁹</td>
<td>5.69×10⁵</td>
</tr>
</tbody>
</table>

4.15, with good qualitative agreement between the $J_2$ continuum and CP models. The struts of the stent unit cell sub-model can be considered to behave as thick curved beams undergoing bending. High stresses are generated through the width of the struts during crimp and deployment. Upon removal of the crimp and deployment loads (post-crimp and post-deployment recoil respectively), while the free surfaces are free to elastically recoil, residual deformation remains at the inner regions of the curved stent strut sections. The residual stress distribution after post-deployment recoil, shown in Fig. 4.15, represents the mean stress distribution present during fatigue loading of the stent unit cell model. Good quantitative agreement exists between the residual von Mises stress distribution for the bulk of material in the $J_2$ continuum and CP unit cell models. This can be attributed to appropriate choice of the kinematic-isotropic hardening CP material model and its calibration against the target $J_2$ continuum response. Use
4. Assessment of Fatigue Performance for a 316L Stent Design

Figure 4.16: Location of failure prediction in $J_2$ continuum model (left) and locations of predictions for crack initiation (indicated by green dots) for all orientation sets for the RND1 and RND2 CP unit cell models.

of a CP material model incorporating isotropic hardening only, calibrated against the $J_2$ continuum material model for cyclic behaviour, would result in a post-deployment residual stress distribution with peak and bulk values significantly lower than that of the $J_2$ continuum unit cell model. A good correlation between the post-deployment residual stress distributions of the CP and $J_2$ continuum unit cell models is critical as fatigue behaviour of the stent is affected by both stress range, due to systolic-diastolic pressure, and mean stress, due to the crimp and deployment processes. Results for one previous study [172] indicate that implementation of a strain gradient plasticity formulation would have negligible effect on the stress distribution predicted. However, it is intended that future work investigate this.

Experimental data available in the literature on bench testing of 316L SS stent fatigue is limited. One published study examines the evolution of stent microstructure due to fatigue [173]. Another study examines the HCF behaviour of 316L SS stent material in notched specimens [133]. However, in both cases, the tests were terminated in the $10^7$ cycles regime and did not report on micro-crack
initiation. To the authors’ knowledge, experimental data has not been published on micro-crack initiation during stent fatigue. It is probable that bench tests have been carried out commercially, to characterize fully the fatigue behaviour of 316L SS stents, and the data has not been published, for confidentiality reasons. However, it seems reasonable to assume that the present 316L NIR stent design conforms to recommendations by the FDA and therefore (i) has a minimum implantation life of 10 years ($4 \times 10^8$ cycles) and (ii) was based on a successful (i.e. safe) Goodman fatigue analysis. The $J_2$-continuum predicted $N_f$ of $7.63 \times 10^8$ cycles in the present study, based on a Goodman approach, corroborates this and therefore acts as a “representative bench-test” reference total life.

Inhomogeneity effects are observed in the CP models, shown clearly in Fig. 4.14 and Fig. 4.15, due to random crystal microstructure and crystallographic orientations. The magnified regions of the CP unit cell stress distributions clearly show microscopic peak stresses which exceed macroscopic peak stresses in the $J_2$ continuum unit cell sub-model. At certain locations, the peak microscopic
4. Assessment of Fatigue Performance for a 316L Stent Design

Figure 4.18: Plot of $p_{\text{recoil}}$ for one case of the CP unit cell model with region of highest crystallographic slip magnified.

stresses are larger than the macroscopic ultimate tensile strength of 800 MPa, used for total life predictions. This reinforces the necessity of grain averaging for homogenization of stress values in the CP unit cell models, to be used in conventional total life prediction methods, i.e. Goodman and Sines with Basquin. Total life predictions using the Goodman-Basquin approach for HCF, provided in Table 4.6, exhibit a large scatter ranging from $9.56 \times 10^6$ to $3.79 \times 10^9$ cycles, despite the reduction of inhomogeneity effects through use of grain averaging. Such broad scatter is unreliable for design purposes. Predictions are not possible using the Sines-Basquin approach for either the $J_2$ continuum or the CP unit cell models, due to residual (mean) stresses giving $3\sigma_{H,m} > \sigma_{TS}$. Although the Sines equation has been proven effective in multiaxial fatigue predictions, this suggests that it is ill-equipped to deal with very high mean stresses, as is the case for stent fatigue loading. Use of the grain size as a volume averaging diameter in the $J_2$ continuum unit cell model is inadequate in overcoming the steep mean stress gradient effects due to post-deployment residual stress distribution. Increase of the averaging diameter to 2.42 times the average grain size provides enough homogenization of stress in the $J_2$ continuum model such that a life prediction using the Sines-Basquin equation is possible. This suggests that an averaging parameter
of 2.42 times the average grain size can be used in \( J_2 \) continuum models for high mean stress fatigue applications.

In contrast to predictions using conventional methods, predictions of number of cycles to FCI using the microstructure-sensitive FIPs show more realistic (typical) scatter. For both the effective plastic strain and crystallographic work parameters the standard deviation of number of cycles to FCI is only a fraction of the average. This much narrower scatter is more reliable in design, as opposed to the broad scatter of predictions yielded by conventional stress-based approaches for HCF. The predictions for crack initiation are limited to three critical regions, identified clearly in Fig. 4.16 and in Fig. 4.17, one of which corresponds to the location of total failure predicted using the Goodman-Basquin method in the \( J_2 \) continuum unit cell model. Crack initiation is predicted to occur early in fatigue life, suggesting that microstructurally small crack growth will dominate fatigue life. From the distribution of predicted \( N_i \) for one CP unit cell sub-model, shown in Fig. 4.17, it can be seen that the initiation of more than one crack during stent operational life is quite possible. Modelling of damage can allow capture of softening due to material degradation, which in turn facilitates the capture of stress, strain and FIP redistribution in the locality of the damaged material. A simple damage coupling is, thus, implemented here in the CP constitutive model to investigate the effect of evolving FIP distributions on FCI prediction, in additional analyses for one grain orientation for each of the RND1 and RND2 CP sub-model grain morphologies. Evolution of damage, \( D \), is defined to be proportional to the FIP \( p \), using the calibrated \( p_{crit} \):

\[
D = \frac{p}{p_{crit}} \quad (4.15)
\]

and the effective stress \([168], \tilde{\sigma} \), due to damage is given by:

\[
\tilde{\sigma} = \frac{\sigma}{1 - D} \quad (4.16)
\]
Simulation of cycles is carried out until the maximum $p_{cyc}$ in the model stabilises according to a given tolerance:

$$\left| \left\{ p_{cyc,\text{max}} \right\}_n - \left\{ p_{cyc,\text{max}} \right\}_{n-1} \right|_{p_{cyc,\text{max}}^n} < \text{tolerance} \quad (4.17)$$

where subscript "n" and "n − 1" represent the current and previous time increment, respectively. Once convergence of $p_{cyc,\text{max}}$ is reached a cycle jumping approach is implemented for subsequent fatigue damage calculations. Simulation of large numbers of cycles is not feasible for CP modelling, due to the significant associated computational expense. Cycle jumping, however, offers a method for CP fatigue simulations, which is more computationally efficient, as every cycle is not explicitly modelled. The jump in cycles applied upon convergence of $p_{cyc,\text{max}}$ is defined by:

$$\Delta N = \frac{\Delta p_{\text{max}}}{p_{cyc,\text{max}}} = \frac{\Delta D_{\text{max}}}{p_{cyc,\text{max}}} \frac{p_{\text{crit}}}{p_{cyc,\text{max}}} \quad (4.18)$$

where $\Delta D_{\text{max}}$ is a constant increment in damage applied for each cycle jump at the material point with maximum $p_{cyc}$. The damage increment at all other material points is simply calculated by $\Delta D = \frac{p_{\text{crit}}}{\Delta N p_{cyc}}$. Cumulative parameters are updated to reflect the increase in cycles. The tolerance in Eq. 4.17 above and the maximum damage increment, $\Delta D_{\text{max}}$, are set at 0.05 and 0.001, respectively.

Plots of $p$ at different stages in the cycle jumping analysis for the two realizations are shown in Figs. 4.19 (a) and (b). In each case, the location of the critical crack is ambiguous from initial $p$ distributions; however one site in particular becomes dominant for each realization, shown in magnified views. The damage accumulation for the material point with maximum damage in each realization is illustrated in Figs. 4.19 (c) and (d). Maximum damage values of 46.8% and 48.7% are reached in the RND1 and RND2 realizations investigated, respectively, prior to analysis termination, at which the number of cycles is $1.9 \times 10^6$ and $1.5 \times 10^6$, respectively. FCI is predicted to occur when $p = p_{\text{crit}}$ or at a damage of 100%; from Figs. 4.19 (c) and (d), this occurs in the $10^6$ cycles regime for
Figure 4.19: Plots of $p$ at different numbers of cycles during the cycle jumping analysis for one grain orientation set for each of (a) RND1 and (b) RND2, and damage evolution at the point of highest $p$ for each of the two realizations in (c) and (d).

both realizations. Extension of the analysis presented here would facilitate the event of crack initiation to be explicitly modelled, followed by the prediction of microstructurally small crack growth thereafter. In the event of multiple cracks initiating, crack interaction could also be predicted. Such a methodology has been previously implemented for prediction of crack initiation and growth in a nickel-base superalloy [62].

Surface roughening observed in the CP unit cell model, as shown in Fig. 4.18, is directly associated with regions of high effective plastic strain and can be used as an indicator parameter for the formation of persistent slip bands on the surface of the stent, corroborated experimentally in Chapter 8 for representative L605 foil tests. Persistent slip bands are key visual indicators of FCI sites [28]. This reinforces the significance of the predictions for FCI using the microstructural
FIPs and reinforces the need for damage to be implemented for the prediction of micro-crack propagation.

Achievement of reliable predictions using the micromechanical model can be attributed to a CP material which is representative of real 316L SS behaviour. The crystallographic work FIP is directly affected by the stabilised cyclic hysteresis loop shape of the CP material model. It has previously been postulated that kinematic hardening may not be necessary in CP modelling due to a natural macroscopically-observed Bauschinger effect reflecting inter-granular interactions [62]. However, as discussed in Section 4.3.1, the Bauschinger effect has been shown to be a combination of both inter- and intra-granular back-stress contributions [61,166]. Comparison of stabilised hysteresis curves in Fig. 4.11 suggests that incorporation of CP kinematic hardening is in fact necessary for accurate representation of cyclic behaviour, at least for 316L SS. Using the Goodman-Basquin prediction of total fatigue life of 7.63×10^8 for the J_2 continuum stent model, crack initiation is predicted to occur early in fatigue life, at approximately 0.52% of the number of cycles to stent fracture. It should be noted that the conventional stress-based Basquin-Goodman approach, used for total life predictions, assume that a crack length on the order of 1 mm constitutes failure [168, 174]. However, such a crack length is not possible before fracture of a stent strut, as stent strut dimensions are significantly smaller than this, suggesting that failure will in fact occur at much lower number of fatigue cycles than predicted here. Basquin constants generated from macro-scale experiments alone are, therefore, not applicable to the prediction of stent fatigue behaviour. Extension of the damage coupling presented above would facilitate more microstructurally representative predictions of number of cycles to failure, via prediction of crack propagation from crack initiation sites.

While some scatter due to microstructural inhomogeneity is predicted using the microstructure-sensitive approach, the full range of responses is unlikely captured
for the number of simulations presented. Random crystallographic orientations and average grain size distributions are employed in the microstructure realizations simulated of the stent sub-model. Therefore, while some scatter, or range of possible responses, is observed, this is unlikely to include the extremes of possible fatigue behaviour. For example, it is clear from comparison of experimental and simulated grain area distributions in Fig. 4.8 that the tail of the experimental distribution is not captured in the realizations simulated. Instead of random generation of the sub-model microstructure, development of extreme realizations which include rogue grain combinations, as discussed in Section 2.3 may give a better indication of the full scatter possible.

Future work should address some limitations in this study, which may have further influence on stent fatigue predictions. It has been shown in previous studies that a length scale effect can be seen in fine-grained materials due to high deformation gradients [60, 157]. Introduction of a length scale effect can result in redistribution of high crystallographic slip at grain boundaries [56]. In the context of stents such an effect would be expected to reduce the cyclic accumulation of the microstructure-sensitive FIPs and thus extend the predicted number of cycles to crack initiation. Strain-gradient CP modelling is employed later in the thesis to investigate length scale effects on fatigue.

Other limitations are related to assumptions used in the modelling of the 3D stent-artery model, which provides fatigue boundary conditions for the 2D unit cell sub-model. An idealised stent-artery geometry is modelled without the presence of plaque or curvature of the artery. End effects seen during the stent deployment process [117] have also been neglected. The use of hyperelastic isotropic constitutive models to represent the material behaviour of the arterial layers is another aspect of the 3D model which could be improved upon, through use of more representative constitutive models [175]. The 3D stent fatigue simulation involved application of pulsatile pressure to the inner surfaces of both the stent
and artery, for modelling convenience. Strictly, pressure should not be applied to the (small) portions of arterial wall covered by the stent. However, additional analyses have established that this additional modelling detail would lead to a small change (decrease) in applied fatigue displacements for the unit cell sub-model and a negligible associated increase in predicted fatigue life (~100 cycles out of about $10^6$ cycles). Another factor which deserves consideration with respect to stent fatigue is the possibility of elevated heart rate and/or elevated blood pressure, either of which can drastically reduce predicted fatigue life. Finally, the 3D stent-artery model does not take into full account the effects of the physiological environment of a stent in-vivo. Corrosion fatigue is an important factor in stent design considerations, especially in relation to the new generation of biodegradable stents being developed [176]. Future work could explore the competing mechanisms of micromechanical fatigue and corrosion fatigue in stent fatigue life design.

4.6. Conclusions

The following can be concluded from this study:

(i) Realistic modelling of stent fatigue requires accurate micromechanical representation of the stent material for both monotonic and cyclic behaviour, to capture deformation during both installation and pulsatile loading. A kinematic-isotropic hardening crystal plasticity material model, calibrated against experimental stent material behaviour, exhibits excellent correlation with a 316L SS $J_2$ continuum material model for (i) tensile behaviour, (ii) evolution of cyclic stress-strain response and (iii) stabilised cyclic hysteresis loop. As indicated by the results, the crystal plasticity material model is able to accurately simulate post-deployment residual stresses in a
stent unit cell sub-model as well as the fatigue behaviour of the stent due to systolic-diastolic loading. Introduction of kinematic hardening into the crystal plasticity model for more accurate representation of hysteresis loop shape also contributed towards the successful use of a crystallographic work parameter for prediction of fatigue micro-crack initiation.

(ii) Use of suitable microstructure-sensitive fatigue indicator parameters is essential for reliable fatigue predictions in micromechanical modelling. Conventional stress-based approaches for predicting HCF failure give inconsistent results, with unacceptably large scatter in total life predictions. The Sines equation for multiaxial fatigue is unable to predict fatigue life due to high residual stresses generated in the deployment process. In contrast, predictions of fatigue micro-crack initiation employing an effective plastic strain FIP and a crystallographic work FIP give realistic scatter. Thus, micromechanical fatigue assessment requires methods based on microstructural parameters. Coupling of a microstructure-sensitive FIP with a damage variable in cycle jumping analyses allowed prediction of the critical crack location for two stent sub-model realizations, given multiple potential fatigue crack initiation sites. The potential of expanding the damage coupling approach for prediction of fatigue micro-crack propagation also exists.

(iii) A methodology is presented here for prediction of fatigue crack initiation in micromechanical models, with the use of stent fatigue as a relevant demonstrator application. The methodology encompasses several aspects of micromechanical modelling, including (i) realistic microstructure geometries, (iii) an appropriate crystal plasticity constitutive model and (ii) microstructure-sensitive FIPs for prediction of crack initiation. Technological advances are constantly driving towards the development of components, with a wide range of applications, with smaller size scales [41]. Thus, the micromechanical methodology proposed here for fatigue assess-
ment can be readily applied to many of these applications.
5. Fatigue Assessment of a Stent Design for a CoCr alloy

5.1. Chapter Summary

Experimental characterisation of a biomedical grade CoCr alloy is presented in this chapter, including both microscopy and mechanical testing. The micromechanical approach developed in the previous chapter for fatigue assessment of a 316L stainless steel stent is applied for the CoCr alloy, more typically used in modern stents. Measured damage evolution for low cycle fatigue test data allows identification of number of cycles to fatigue crack initiation (FCI), corresponding to a critical damage level, as compared with total life. Fatigue indicator parameters (FIPs) within the micromechanical framework are calibrated against the data, for the prediction of microstructure-sensitive FCI. As for the 316L stent of Chapter 4, predictions of FCI are compared with traditional Basquin-Goodman total life predictions for the stent sub-model, revealing more realistic scatter of data for the microstructure-based FIP approach. Comparison of stent predictions with performance of the 316L stent from the previous study exposes the generic design as over-conservative for the CoCr alloy. In response, use of the micromechanical framework to modify the stent design for the CoCr alloy is demonstrated, improving design efficiency.
5. Fatigue Assessment of a Stent Design for a CoCr alloy

5.2. Introduction

The L605 CoCr alloy is a popular material used in a broad range of applications with fatigue loading, including biomedical implants [9], gas turbine components and bearings [177]. In such applications, the development of reliable and accurate methods for fatigue life prediction is a necessary design requirement. L605 fatigue life data and cyclic stress-strain behaviour are essential inputs for development of successful fatigue assessment techniques. This allows the capture of energy dissipation and stresses and strains reached cyclically in the material, which has direct impact on the life of a component. Microstructural characteristics, such as grain size and precipitates, can have a significant role in the fatigue performance of L605 and, hence, must also be included in predictive modelling techniques. A limited number of experimental characterisation studies have been reported for this alloy. Stress-life data has been published for notched L605 specimens in a study on the use of ultrasonic methods for detecting cracks in fatigued specimens [178]; however, no information on the cyclic behaviour of the material is provided. Other studies provide high cycle fatigue (HCF) stress-life data and crack growth data for the L605 alloy [26,179], but again, do not report cyclic stress-strain data. Microstructural studies on L605 primarily focus on microstructural evolution under applied heat treatments. Teague et al. [180] carried out a series of aging treatments to look at the effects of resulting precipitation on tensile behaviour, reporting that aging above 800°C produced incoherent precipitates, decreasing yield strength, while aging below 800°C resulted in precipitation of coherent precipitates, strengthening the material. Other studies focused on L605 in stent applications, looking at the effect of annealing temperatures on precipitation [181], changes in grain size and tensile properties under different combinations of cold working and annealing [182] and stent surface enhancement via an electrochemical process [183].
5. Fatigue Assessment of a Stent Design for a CoCr alloy

The primary objective of this study is the development of a micromechanical approach to L605 fatigue assessment. The L605 stent is an ideal application for this approach, as stent struts can be 80 μm in thickness [9, 10], compared to a grain size on the order of 10 μm [123]. Consequently, with often less than ten grains through the strut thickness, the performance of the stent is highly dependent on the inhomogeneous microstructure. This has been verified in previous studies for monotonic behaviour of stent struts, using crystal plasticity (CP) constitutive modelling [5, 39, 99, 101, 121–123]. However, this microstructure-sensitive method demands extension to fatigue performance assessment of stents. Halwani et al. [18] reported two instances of stent fracture in CoCr alloy stents within 24 and 13 months. A clear need exists for improved fatigue analysis in the stent design process. Current industry standards employ basic finite element (FE) models in conjunction with the stress-based Goodman technique, in accordance with FDA requirements [24], to ensure that stent operational life will exceed 10 years. Microstructural effects are ignored, eliminating the possibility of predicting crack formation in slip bands, as has been reported to occur [18]. Attempts have been made in the literature to improve fatigue prediction methods for the stent application, as outlined in Section 2.5 of the Background chapter and in Section 4.2 of the previous chapter. However, approaches tended to use macroscopic material descriptions, unable to account for microstructural inhomogeneity. CP modelling has been employed to assess the fatigue performance of a 316L stent in McGarry et al. [100] and, also, in the study of the previous chapter. McGarry et al. [100] calibrated the CP constitutive model for monotonic behaviour and carried out a simple Goodman analysis, while the methodology was developed further in the previous chapter, where a rigorous cyclic calibration of the material behaviour was carried out, along with microstructure-sensitive predictions of fatigue crack initiation (FCI) as well as Goodman-based total life predictions. The use of multiple microstructural realizations for the stent model produced scatter in predictions, successfully showing the effect of microstructural inhomogeneity.
This work aims to develop a micromechanical framework, which can be used as a tool in the fatigue design and assessment of CoCr alloy stents, for which a clear need has been explicitly expressed in past work [26]. The L605 CoCr alloy, commonly used in current generation cardiovascular stents [9], is experimentally characterised both microstructurally and mechanically, via microscopy, and tensile and low cycle fatigue (LCF) testing, respectively. The experimental data is used in the development of the L605 micromechanical modelling framework, including realistic geometries, based on measured microstructures, and a CP model, calibrated for both monotonic and cyclic behaviour. This framework is then used to assess the fatigue performance of an L605 model for a generic stent design, which is compared to results from Chapter 4 for a 316L stent. A multiscale approach is adopted whereby boundary conditions for the CP sub-model are extracted from a $J_2$ continuum global stent-artery model. In order to assess the design of the stent and the potential for premature failure, microstructure-sensitive FIPs [83, 86] are implemented for the prediction of number of cycles to fatigue crack initiation. Use of the methodology as a design tool is demonstrated, where the chosen L605 stent design is modified to improve design efficiency.

5.3. Experimental Studies

This section outlines experimental work carried out on the L605 CoCr alloy, trade-named HAYNES 25 alloy [177], used in the as-received condition: a hot-rolled bar, solution-annealed at 1230°C, with chemical composition of 20 wt% chromium, 15 wt% tungsten, 10 wt% nickel, 3 wt% iron, 1.5 wt% manganese, 0.4 wt% silicon, 0.1 wt% carbon and the balance consisting of cobalt. The experimental programme covers both the microstructural and mechanical characterization of the L605 alloy via microscopy, and fatigue and tensile testing, respectively.
5.3.1. Microscopy

Optical microscopy was used to measure the crystallographic grain morphology in the L605 microstructure. The L605 material was supplied in cylindrical bar form. Therefore, microscopy was carried out on both transverse cross-sections (parallel to the cylindrical axis) and longitudinal cross-sections (perpendicular to the cylindrical axis). The microscopy samples were mounted in an epoxy resin. Surface preparation was achieved via manual grinding, across a range of grit sizes, automated polishing, with a range of diamond pastes, finishing with a 0.02 µm polishing suspension, and cleansing in an ultrasonic bath. An etching solution of 100 ml HCl and 5 ml 30% H₂O₂ was used [184].

Sample optical micrographs of the L605 microstructure from both longitudinal and transverse cross-sections can be seen in Fig. 5.1(a) and Fig. 5.1(b), respectively. Individual crystallographic grains are highlighted for illustrative purposes. A Matlab program was developed to extract information on grain area distributions from several optical micrographs for both the longitudinal and transverse views, the results shown in Fig. 5.1(c). An average distribution is also included in Fig. 5.1(c). There is clearly a high correlation between the two orientations, indicating an equiaxed microstructure. Assuming a hexagonal 2D grain shape, the average grain size was found from these distributions to be 32 µm. An ASTM grain size of 5 was observed for the microstructure.

SEM imaging was also applied to the etched samples. A scanning electron micrograph of the L605 microstructure can be seen in Fig. 5.2(a); precipitates appear as light-coloured spots and some grain boundaries appear as light-coloured lines. This contrast between L605 matrix and precipitate material allowed image processing to be carried out using a Matlab code, developed for the extraction of information on precipitate area distributions, including average precipitate area
Fatigue Assessment of a Stent Design for a CoCr alloy

Figure 5.1: Optical microscopy images of the L605 alloy, showing (a) longitudinal and (b) transverse views of the bar and (c) grain area distributions for the two views.

Figure 5.2: a) SEM image of the L605 alloy microstructure and (b) particle area distribution within the L605 microstructure; the inset histogram continues the distribution for grain areas above $1 \mu m^2$.

and frequency of occurrence within the matrix, as shown in Fig. 5.2(b). A precipitate area ratio of 0.52% was observed. As highlighted in Fig. 5.2(a), precipitates appear both at grain boundaries and within the matrix, with no evident preferential location.

Energy dispersive x-ray (EDX) analysis was used in conjunction with SEM imaging to identify the composition of precipitates within the L605 matrix. Table 5.1 provides EDX data for two sample spectrums, one of which corresponds to the L605 matrix and the other of which corresponds to a precipitate. The weight percentage of elements dominant in each spectrum are shown. Reasonably good
Table 5.1: EDX readings for chemical composition in a particle and within the L605 matrix.

<table>
<thead>
<tr>
<th>Element</th>
<th>Weight (%)</th>
<th>% change in weight %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Matrix</td>
<td>Particle</td>
</tr>
<tr>
<td>Co</td>
<td>46.31</td>
<td>15.22</td>
</tr>
<tr>
<td>Cr</td>
<td>20.74</td>
<td>10.9</td>
</tr>
<tr>
<td>W</td>
<td>17.21</td>
<td>63.04</td>
</tr>
<tr>
<td>Ni</td>
<td>11.13</td>
<td>3.46</td>
</tr>
<tr>
<td>C</td>
<td>4.61</td>
<td>7.37</td>
</tr>
</tbody>
</table>

agreement exists between the readings shown for the L605 matrix and the manufacturer specifications, provided at the start of Section 5.3; the carbon content in the EDX reading appears high, due to carbon contamination on the surface of the SEM specimen, and peaks for some of the elements listed are too small to be detected. The final column of Table 5.1 provides the percentage change in weight percentage of each element when comparing the precipitate to the matrix. The data shows that the precipitates have significantly increased weight percentages of tungsten and carbon, while cobalt, chromium and nickel contents have decreased.

5.3.2. Mechanical Testing

Monotonic tensile and fully reversed LCF tests are employed to characterise the monotonic and cyclic plastic behaviour of the alloy. Macroscopic plasticity is achieved in LCF tests (as opposed to HCF tests, which evoke macroscopically elastic behaviour), thus generating cyclic hysteresis loops which can be reliably used for the calibration of cyclic plasticity constitutive behaviour. In HCF, the macroscopically elastic behaviour results in a predictable increment in strain for a given increment in stress and, therefore, load control can be used. However, in LCF, the material is brought past macroscopic yield, after which the stress-
strain relationship becomes non-linear and an increment in stress can result in a significantly increased increment in strain; thus, strain control is preferable for LCF tests, as is used here. The fatigue specimen has a dogbone design, based on ASTM standards [185] and shown in Fig. 5.3, consisting of a large diameter at the ends for gripping and two tapers down to a uniform cross-section in the gauge region. A light interferometer was used to ensure that the final surface roughness (Ra) in the gauge section of specimens was below 0.2 µm. All tests were carried out at room temperature on an Instron 8500 servo hydraulic system with hydraulic grips and V-shaped jaws. The tensile test was carried out on one specimen, using displacement control at a rate of $1 \times 10^{-3}$ mm/s per mm gauge length, and a video extensometer was used to measure the strain in the gauge region of the specimen. In order to characterise the LCF behaviour of the material, strain-controlled tests were carried out at four different strain ranges with a cyclic strain ratio $R_\varepsilon = \varepsilon_{\text{min}}/\varepsilon_{\text{max}}$ of -1. An extensometer with knife-edged probes was attached to the gauge region to measure, and hence control, strain. LCF tests at the lowest strain range were carried out at strain rates of 0.001 s$^{-1}$ and 0.01 s$^{-1}$. The cyclic stress-strain response of the CoCr alloy demonstrated rate independence at these rates; therefore, the higher strain rate of 0.01 s$^{-1}$ was used for all other LCF tests.

The measured tensile behaviour of the L605 alloy is shown in Fig. 5.4(a). An
5. Fatigue Assessment of a Stent Design for a CoCr alloy

Figure 5.4: Tensile curve for the L605 alloy compared with a biomedical grade 316 LVM [39] and (b) the fractured tensile specimen.

... elongation to failure of over 60% is measured, the 0.2% offset yield strength is 514 MPa, the ultimate tensile strength (UTS) for the material is 1075 MPa and Young’s modulus is measured to be 224 GPa. Tensile fracture occurred along a 45° crack path, as seen in Fig. 5.4(b). While localised necking at the crack site is not observed, a large amount of surface roughening along the entire gauge length is evident. Comparing with a biomedical grade 316L SS [39], as shown in Fig. 5.4(a), the L605 CoCr alloy displays superior tensile behaviour both in terms of strength and ductility, as reported by others [8,118,176].

Fig. 5.5(a) shows the measured evolution of the cyclic stress range for LCF tests at ±0.5%, ±0.8%, ±1.0% and ±1.2% controlled cyclic strain. The material exhibits some initial hardening, followed by slight softening within the first 100 or so cycles. Thereafter, a stabilised stress range is exhibited, until a sudden drop in stress range, corresponding to termination of the test due to a 30% load drop in tension being reached. This can be taken as failure. Fig. 5.5(b) shows a more detailed evolution of stress-strain hysteresis loops for ±1% applied strain range; cycle 4087 is the last cycle before failure.

Cracked specimens are shown in Fig. 5.6 for the ±0.5%, ±0.8% and ±1.0% strain...
5. Fatigue Assessment of a Stent Design for a CoCr alloy

Figure 5.5: (a) Cyclic stress range evolution corresponding to LCF total strain ranges and (b) experimental stress-strain hysteresis loops after various number of cycles for the ±1% strain range.

Table 5.2: Fitted Coffin-Manson constants for the L605 alloy.

<p>| | |</p>
<table>
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<tbody>
<tr>
<td>$C_1$</td>
<td>1.49</td>
</tr>
<tr>
<td>$\gamma_1$</td>
<td>1.77</td>
</tr>
</tbody>
</table>

ranges; 180° circumferential cracks are visible on these specimens, while a more jagged crack is evident on the specimen corresponding to the ±1.2% strain range of Fig. 5.7(a), which fractured into two pieces. Two types of fracture surface are observed in Fig. 5.7(b) and (c), corresponding to fatigue cracking and a final tensile overload, respectively. The plastic strain-life curve corresponding to these L605 fatigue tests is shown in Fig. 5.8, including identification of the Coffin-Manson relationship for total life, $N_f$, as a function of plastic strain range, $\Delta \epsilon_p$:

$$N_f = \left( \frac{\Delta \epsilon_p}{C_1} \right)^{-\gamma_1} \quad (5.1)$$

and the identified values of the $C_1$ and $\gamma_1$ constants are given in Table 5.2.
Figure 5.6: Post-test LCF specimens for the ±0.5%, ±0.8% and ±1.0% strain ranges, with crack highlighted in each case.

Figure 5.7: (a) Post-test LCF specimen for the ±1.2% strain range, (b) fatigue striations in location of initial crack and (c) static fracture surface.
5. Fatigue Assessment of a Stent Design for a CoCr alloy

5.4. Computational Framework

5.4.1. Constitutive Models

As for the 316L study of the previous chapter, both $J_2$ plasticity and CP constitutive models are used in this study for the same functions as before, with the exception of the target response being defined by experimental data for the L605 alloy. Eqs. 3.16 – 3.21 define the non-linear isotropic and kinematic hardening $J_2$ formulation used, where it was found that three kinematic back-stresses, $x_i$ in Eq. 3.17, are required to capture the non-linear monotonic and cyclic micro-plasticity response of the CoCr alloy.

The power-law CP formulation defined in Section 3.4.1 is used for the micromechanical simulations in this study. The L605 matrix has a face-centred cubic (fcc) crystal structure [180] and, therefore, twelve $\{111\} \langle 110 \rangle$ slip systems are modelled. Anisotropic cubic elasticity (Eq. 3.23), consistent with the fcc L605 crystal structure, is used, where a Poisson’s ratio of 0.31 and crystal anisotropy of 0.506 [186], combined with the Young’s modulus identified in Section 5.3.2,
5. Fatigue Assessment of a Stent Design for a CoCr alloy

gives rise to the cubic elastic constants $C_{11} = 310.5$ GPa, $C_{12} = 139.5$ GPa and $C_{44} = 82$ GPa. Two kinematic back-stresses, $x_i^\alpha$ of Eq. 3.35, are required to simulate the experimental monotonic and cyclic response.

5.4.2. Finite Element Microstructure Model

A micromechanical finite element model of the measured microstructure is developed for the identification of the micro-scale behaviour of the L605 material under cyclic and tensile loading. A customized Matlab code is developed for generation of the 3D microstructures via superposition of a 3D Voronoi tessellation on a voxel mesh. In order to ensure that the grain volume distribution of the resulting polycrystal accurately simulates the experimental distribution, 2D grains were idealised as hexagons and 3D grains as rhombic-dodecahedrons (as seen in Fig. 5.9). The resulting relationship between grain volume (3D) and grain area (2D) is then given as follows:

$$V = \frac{1}{\sqrt{2}} \left( \frac{2A}{\sqrt{3}} \right)^{\frac{3}{2}}$$

where the common dimension $d$ is the 2D to 3D link. This equation facilitates calculation of experimental grain volume distribution from the measured grain area distribution. A number of polycrystal model microstructures were generated to iteratively achieve correlation between polycrystal grain volume distribution and experimental distribution.

A key challenge for micro-scale modelling of the microscopy images of Figs. 5.1(a), 5.1(b) and 5.2(a) is representation of precipitates in the final polycrystal model. As the average precipitate volume is smaller than the volume of a standard element in the mesh, a seven-element unit was used to replace a normal element in the mesh, as shown in Fig. 5.10, where a precipitate element lies at
the centre of the unit, surrounded by six matrix elements. The microscopy observations indicate no preferred location of precipitates along grain boundaries or within the matrix. Hence, the precipitate-matrix unit is inserted randomly into the FE mesh to give the experimentally observed volume fraction of precipitates. The final microstructure model is shown in Fig. 5.10; it has cubic dimensions of $(120 \, \mu m)^3$ and contains 28 crystallographic grains, with 3723 20-noded brick elements. Periodic displacement boundary conditions are applied to simulate macroscopic behaviour. Due to the computational expense associated with crystal plasticity modelling and the 3D nature of the micromechanical model, it is prohibitively expensive to simulate a sufficiently large number of grains to achieve a definitive representative volume element (RVE). However, it has been shown previously by Jiang et al. [187], that it is possible to predict a response for an inhomogeneous material which lies between the lower and upper bounds of the macroscopic response, using periodic displacement boundary conditions applied to a unit cell microstructure model which is smaller than a definitive RVE.

5.4.3. Constitutive Model Calibration

The CP and $J_2$ continuum responses are calibrated against both the experimental tensile response and the first thirteen cycles of loading for each applied LCF strain range. In the case of the $J_2$ continuum model, the approach of Lemaître
and Chaboche [168] is used for the initial estimation of constants. A least squares objective function, similar to Eq. 4.3 of the previous chapter, is implemented for identification of the optimised constants, as follows:

$$F(x_k) = \sum_{j=1}^{n} \sum_{i=1}^{m} \left[ (\sigma_{i}^{exp})_{j} - (\sigma_{i}^{sim})_{j} \right]^2$$

(5.3)

where $n$ and $m$ represent the number of strain ranges and a pre-determined number of stress-strain data points throughout the cyclic loading history, respectively, and $\sigma_{i}^{exp}$ and $\sigma_{i}^{sim}$ are the experimentally measured and simulated macroscopic stresses, respectively, at pre-determined sample strains. This minimisation function was used for calibration of both the CP and $J_2$ continuum constants.

For the CP model, the isotropic hardening function $g^\alpha$ and the back-stress $x_1^\alpha$ are found to be sufficient for accurate calibration of the cyclic response, or small strain regime. It was found, however, that an additional back-stress $x_2^\alpha$ was required to also achieve satisfactory calibration of the tensile response, or large strain regime, while using one set of CP constants for both tensile and cyclic responses. Similarly for the $J_2$ continuum model, the isotropic hardening parameter $r$ and the back-stresses $x_1$ and $x_2$ are used to calibrate for cyclic behaviour.
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Figure 5.11: Comparison of the $J_2$ continuum and CP tensile curves with the L605 experimental data; the large-strain range is calibrated using the additional back-stress terms and the small-strain range (before dotted line) is calibrated using initial back-stress terms.

while the third back-stress $x_3$ is used for capturing the large-strain L605 tensile response. Calibration of the constitutive models against both cyclic and tensile data is important in applications of high initial plastic deformation, which induces high residual or mean stresses, followed by fatigue, such as for a stent where crimping, crimp recoil, deployment and recoil incur plastic deformation, followed by systolic-diastolic pulsatile loading.

The calibrated tensile (monotonic) responses of the $J_2$ and CP constitutive models are compared with the experimental data in Fig. 5.11. A comparison of predicted stabilised hysteresis loops with the experiments in Fig. 5.12 shows correlation of model and measured data. Both models successfully capture the evolution from monotonic to stabilised cyclic hysteresis loops. The optimised constants for the $J_2$ continuum and CP constitutive models are provided in Tables 5.3 and 5.4, respectively.
Figure 5.12: Comparison of $J_2$ continuum and CP stabilised hysteresis loops with the L605 experimental data for different applied strain ranges.

5.4.4. FCI Predictions

A key objective of the present work is the assessment, including calibration and validation, of a micro-scale method for FCI prediction in L605. This is particularly important for stent applications, primarily due to the scale of stent struts relative to microstructural features such as grain size and precipitates. A number of microstructure-sensitive FIPs have been developed to predict location and number of cycles to FCI for a range of materials, leading ultimately to failure [29, 86, 188]. It has been shown that an effective plastic strain FIP, which sums strain due to crystallographic slip over all slip systems, allowed prediction across both LCF and HCF regimes from calibration against one LCF test data.
Table 5.3: Calibrated $J_2$ continuum constants for the L605 alloy.

<table>
<thead>
<tr>
<th>$k$</th>
<th>230 MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q$</td>
<td>60 MPa</td>
</tr>
<tr>
<td>$b$</td>
<td>9</td>
</tr>
<tr>
<td>$c_1$</td>
<td>240 MPa</td>
</tr>
<tr>
<td>$\gamma_1$</td>
<td>1846</td>
</tr>
<tr>
<td>$c_2$</td>
<td>50 GPa</td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>250</td>
</tr>
<tr>
<td>$c_3$</td>
<td>2.7 GPa</td>
</tr>
<tr>
<td>$\gamma_3$</td>
<td>0.55</td>
</tr>
</tbody>
</table>

Table 5.4: Calibrated CP constants for the L605 alloy.

<table>
<thead>
<tr>
<th>$g_0$</th>
<th>100 MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_\infty$</td>
<td>130 MPa</td>
</tr>
<tr>
<td>$h_0$</td>
<td>100 MPa</td>
</tr>
<tr>
<td>$C_{kin1}$</td>
<td>80 GPa</td>
</tr>
<tr>
<td>$D_{kin1}$</td>
<td>750</td>
</tr>
<tr>
<td>$C_{kin2}$</td>
<td>1.25 GPa</td>
</tr>
<tr>
<td>$D_{kin2}$</td>
<td>0.001</td>
</tr>
</tbody>
</table>

point [83]; a similar approach will be adopted here. The same FIP has been successfully used to predict the FCI location and initial crack path for a case of experimentally-observed FCI in a nickel-base alloy [62]. As in the previous chapter for 316L, two candidate microstructure-sensitive FIPs are examined. The first is the previously mentioned accumulated effective plastic strain parameter [83], $p$, defined by Eq. 4.1. Use of $p$ for prediction of number of cycles to FCI has been successfully validated for a nickel-base alloy [83] and a 316L SS [84]. The second microstructure-sensitive FIP is the accumulated crystallographic work parameter [86], $W$, which sums energy dissipation over all crystallographic slip systems, defined in the previous chapter by Eq. 4.2.

Crack initiation is predicted to occur when critical values of the FIPs, $p_{crit}$ and $W_{crit}$, are reached. Unit cell LCF simulations for the experimentally applied strain ranges are employed for the identification of $p_{crit}$ and $W_{crit}$ using the micromechanical unit cell of Fig. 5.10. A mesh sensitivity study for LCF loading of polycrystal geometry of Fig. 5.10, described in Appendix A.2, demonstrates an acceptably converged solution for the mesh density used, both in terms of macroscopic stress-strain response and FIP prediction. In order to account for scatter in the microstructure-sensitive predictions, five realizations of random crystallographic orientation are applied to the cubic polycrystal for the four strain...
ranges. A high probability of FCI at the free surface exists in the LCF and HCF regimes \[28, 58\]. While periodic boundary conditions are commonly used for comparing unit cell and RVE responses with macroscopic material behaviour, the possibility of free surface FCI is thereby precluded. Therefore the boundary conditions applied to the polycrystal model are designed to replicate a unit at the free surface of a fatigue specimen, whereby one surface is free, a plane boundary condition is applied to the opposite surface and the four remaining surfaces are constrained by periodic boundary conditions. This facilitates the possibility of surface FCI in the identification of \( p_{\text{crit}} \) and \( W_{\text{crit}} \).

The \( p \) and \( W \) FIPs predict number of cycles to FCI; however the experimental L605 tests provide total life fatigue data. Therefore, a damage approach is employed here for the back-calculation of an approximate \( N_i \) for each experimentally applied strain range. The damage evolution equation used is a function of the experimental \( N_f \) \[64, 189\]:

\[
D = 1 - \left[ 1 - \left( \frac{N}{N_f} \right)^{\frac{1}{\alpha-\beta}} \right]^{\frac{1}{\alpha-\beta}}
\]  

(5.4)

where \( \alpha \) and \( \beta \) are constants, identified to give the best fit across all strain ranges. Fig. 5.13(a) shows a comparison of damage curves from Eq. 5.4 with experimental damage, evaluated as \( D = 1 - \frac{\sigma}{\sigma_{\text{max}}} \), where \( \sigma_{\text{max}} \) is the maximum peak tensile stress for a given LCF test. \( N_i \) is assumed to occur experimentally at a critical damage, \( D_c \), as marked in Fig. 5.13(a). A value of 0.0125 is chosen for \( D_c \), based on a circumferential crack with depth equal to the standard element size initiating at the free surface in a unit cell. The resulting \( N_i \) data points are shown along with experimental \( N_f \) data in Fig. 5.13(b). \( p_{\text{crit}} \), and similarly \( W_{\text{crit}} \), are calibrated using data for a single strain range via the simple relation \( p_{\text{crit}} = \frac{N}{p_{\text{cyc}}} \), where \( p_{\text{cyc}} \) is the effective plastic strain accumulated over a stabilised cycle of loading, averaged over the five simulations for that single strain range.
Figure 5.13: (a) Comparison of curves for experimental data and the damage evolution relation and (b) predictions of $N_i$ using $p_{\text{crit}}$ and $W_{\text{crit}}$ in comparison with $N_i$ data back-calculated from experimental $N_f$ data via use of the damage evolution relation.

$p_{\text{crit}}$ and $W_{\text{crit}}$ have been identified as 439.9 and $15.63 \times 10^4$ MJ m$^{-3}$, respectively, using $N_i$ for the ±0.5% strain range. Reasonable agreement is observed when these critical FIP values are used to predict number of cycles to FCI for the other three strain ranges, as shown in Fig. 5.13(b).
5.5. Stent Fatigue Application

The focus application of the present biomedical grade L605 alloy is the design of cardiovascular stents. A key objective of this study is the development of a multi-scale fatigue methodology for such stents. As a demonstration, this methodology is applied to a generic stent geometry, based on the NIR stent, used in Chapter 4, allowing comparison with results for the 316L SS stent material. As for the previous study, a combination of a global 3D macroscopic stent-artery FE model using $J_2$ cyclic plasticity and a 2D micromechanical CP FE model for the smallest repeating unit in the generic geometry is adopted. The load history includes simulation of crimp, deployment and systolic-diastolic fatigue of the stent; the fatigue boundary conditions for the 2D sub-model are driven by the 3D global model. The global stent model is set up as in the previous chapter, consisting of a single ring of the stent and a three-layered artery, as shown in Fig.5.14(a), where a schematic of the change in stent diameter throughout the loading history is provided in Fig. 5.14(b). Cyclic pressure during the fatigue step is applied to the inner surface of the artery only. The cyclic change in stent diameter is extracted from the 3D global model and converted geometrically to a cyclic displacement applied to the micromechanical sub-model.

The geometry used in the micromechanical sub-model represents the smallest repeating unit in the stent, converted into a 2D geometry, shown in Fig. 5.14(c). 2D Voronoi Tessellation is employed via a custom-written Matlab code to generate a random crystallographic grain structure representative of that seen in annealed L605 tubes used in stent manufacture [123]. Once a representative microstructure morphology with high statistical correlation to the experimental morphology is iteratively achieved, automatic meshing is applied, followed by selective manual repair meshing to remove distorted elements. Automatic gener-
5. Fatigue Assessment of a Stent Design for a CoCr alloy

Figure 5.14: (a) 3D global stent artery model, (b) schematic of change in stent diameter during applied loading history and (c) 2D micromechanical sub-model with 5-element unit facilitating the inclusion of precipitates.

The dispersion of precipitates in the mesh was achieved via a Fortran program, to achieve a volume fraction of precipitates consistent with that of L605 stent tubing [182]. The average element in the stent sub-model mesh has larger area than the average precipitate in the L605 microstructure. To accommodate this, a 5-element unit, shown in Fig. 5.14(c), is used to randomly replace existing elements in the mesh, similar to the 7-element unit used for the 3D polycrystal. This allows the occurrence of precipitates at the free surface and along grain boundaries. The measured area fraction of precipitate is achieved within the generated microstructure. The final sub-model contains 1753 crystallographic grains, 52798 4-noded, reduced integration, generalised plane strain elements and includes precipitates with areas in the range of 0.03 – 0.78 µm$^2$, corresponding to an experimentally observed precipitate area range of 0.01 – 0.74 µm$^2$. While a 2D geometry is
used for the stent sub-model, the micromechanical analyses carried out can be considered quasi-3D due to (i) the 3D nature of the CP constitutive model, allowing slip in three dimensions, and (ii) use of generalised plane strain elements, allowing uniform strain in the third dimension. Seven realizations of the stent sub-model microstructure are generated via assigning different sets of random crystallographic orientations to the grain morphology developed, allowing simulation of typical inhomogeneities observed in real stent microstructures. For comparative purposes a separate sub-model analysis is carried out using the $J_2$ constitutive model, but without the precipitates, as the $J_2$ constitutive model was calibrated against the macroscopic behaviour of the alloy, i.e. including the effects of precipitates.

As for the previous study, the loading steps of Fig. 5.14(b) are applied in the sub-model via displacement of a master node on the lower strut in Fig. 5.14(c). Boundary conditions are applied to maintain periodicity of the sub-model in the global stent structure; a more detailed description is provided in the previous chapter.

Two approaches are adopted for the fatigue assessment of the stent sub-model. The first is a microstructure-sensitive approach for the prediction of number of cycles to FCI, $N_t$, in the CP sub-model analyses via use of the $p$ and $W$ FIPs, as for the 316L study. Repeated here for clarity, the number of cycles to FCI is calculated by:

$$N_t = \frac{p_{crit} - p_{recoil}}{p_{cyc}}; \quad N_t = \frac{W_{crit} - W_{recoil}}{W_{cyc}}$$

(5.5)

where $p_{recoil}$ and $W_{recoil}$ are values of the FIPs accumulated post-recoil, taking into account initial plastic deformation during the stent installation process.

The second method, used here for comparative purposes, is the industry standard approach for predicting the number of cycles to fatigue failure, $N_f$. This total life
approach uses a combination of the Basquin HCF equation and the Goodman equation for mean stress effects, typically used in stent design practices under the recommendation of the US Food and Drug Administration (FDA) [24]. The combined equation is represented as follows:

\[ N_f = \left( \frac{\Delta \sigma}{C_2 \left( 1 - \frac{\sigma_m}{\sigma_{TS}} \right)} \right)^{-\gamma_2} \quad \text{(5.6)} \]

where \( \Delta \sigma \) and \( \sigma_m \) are the maximum principal stress range and mean maximum principal stress, respectively, for a stabilised cycle of loading, \( \sigma_{TS} \) is the ultimate tensile strength of the L605 CoCr alloy and \( C_2 \) and \( \gamma_2 \) are Basquin constants calculated from HCF data for the L605 alloy [26].

### 5.5.1. Results

Table 5.5 shows the microstructure-sensitive FCI predictions for the L605 stent for all 7 microstructure realizations and for both \( p_{crit} \) and \( W_{crit} \). The table also shows the Basquin-Goodman predictions for total life. As the latter is traditionally applied to macro-scale results, which do not account for peaks due to microstructural inhomogeneities, a grain volume-averaging technique, described in more detail in the previous study, is applied to \( \Delta \sigma \) and \( \sigma_m \), used in Eq. 5.6, for the CP models. For comparative purposes these stress values are averaged over the average grain volume for the \( J_2 \) continuum sub-model. An average Basquin-Goodman total life of 6.43\times10^{14} cycles with standard deviation (SD) of 1.58\times10^{15} is predicted for the CP sub-models, compared with a total life of 2.45\times10^{16} cycles for the \( J_2 \) sub-model.

The \( p_{crit} \) method predicts an average \( N_i \) of 2.71\times10^7 cycles (SD = 1.36\times10^7) and the \( W_{crit} \) method predicts an average \( N_i \) of 3.48\times10^7 cycles (SD = 2.48\times10^7).
Table 5.5: $N_f$ and $N_i$ predictions for the CP stent unit cell simulations.

<table>
<thead>
<tr>
<th>Realization</th>
<th>$N_i(p_{crit})$</th>
<th>$N_i(W_{crit})$</th>
<th>$N_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$3.98 \times 10^7$</td>
<td>$3.90 \times 10^7$</td>
<td>$1.16 \times 10^{12}$</td>
</tr>
<tr>
<td>2</td>
<td>$3.95 \times 10^6$</td>
<td>$2.35 \times 10^6$</td>
<td>$4.07 \times 10^{12}$</td>
</tr>
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<td>$7.73 \times 10^7$</td>
<td>$7.09 \times 10^{11}$</td>
</tr>
<tr>
<td>4</td>
<td>$2.20 \times 10^7$</td>
<td>$3.12 \times 10^7$</td>
<td>$6.37 \times 10^8$</td>
</tr>
<tr>
<td>5</td>
<td>$2.19 \times 10^7$</td>
<td>$1.20 \times 10^7$</td>
<td>$2.73 \times 10^{14}$</td>
</tr>
<tr>
<td>6</td>
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<td>$3.11 \times 10^7$</td>
<td>$1.18 \times 10^8$</td>
</tr>
<tr>
<td>7</td>
<td>$4.00 \times 10^7$</td>
<td>$5.10 \times 10^7$</td>
<td>$4.22 \times 10^{15}$</td>
</tr>
</tbody>
</table>

All Realizations

<table>
<thead>
<tr>
<th></th>
<th>Average</th>
<th>$N_i(p_{crit})$</th>
<th>$N_i(W_{crit})$</th>
<th>$N_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$2.71 \times 10^7$</td>
<td>$3.48 \times 10^7$</td>
<td>$6.43 \times 10^{14}$</td>
</tr>
<tr>
<td>SD</td>
<td></td>
<td>$1.36 \times 10^7$</td>
<td>$2.48 \times 10^7$</td>
<td>$1.58 \times 10^{15}$</td>
</tr>
</tbody>
</table>

Figure 5.15: (a) Predicted site of fatigue failure for the $J_2$ continuum sub-model and (b) predicted sites of fatigue crack initiation for the CP sub-models.

The predicted locations of microstructure-sensitive FCI for both FIPs and all microstructure realizations are shown in Fig. 5.15(b). Clearly, FCI is predicted to have a high probability of occurring along the inner radius of the top strut, the same location at which failure is predicted to occur for the $J_2$ continuum sub-model, as shown in Fig. 5.15(a).
5.6. Discussion

5.6.1. Experiments

Quite a broad range of particle areas is observed embedded in the L605 matrix, as seen from Fig. 5.2(b). Precipitate size can have significant influence on the fatigue performance of a material; fine precipitates that are coherent with the matrix, and can be sheared by mobile dislocations, strengthen the material behaviour and cause increased hardening, whereas coarse precipitates, with incoherent precipitate-matrix interface that cannot be overcome by mobile dislocations, act as stress concentrators and may offer free surfaces conducive to crack initiation [190, 191]. The effects of both types of precipitates on tensile behaviour have been observed experimentally for L605 [180]. Future work should investigate the influence of precipitate size on fatigue behaviour to provide insight into desirable microstructures for stent materials. Previous studies on L605 have also found the precipitates to have a tungsten-rich composition [180–182].

Teague et al. [180] identified precipitates in the as-received L605 material as $M_6C$ and $M_{23}C_6$, where M represents metallic elements, such as tungsten. Based on the analysis of the present study, it is possible to confirm that the precipitates are hard carbide particles and an elastic modulus is assigned accordingly in the simulations as 714 GPa [192].

The fracture surface of the ±1.2% strain specimen in Fig. 5.7(a) shows signs of a 45° crack at the left side of the specimen gauge length, followed by a flatter surface to the right. In Fig. 5.7(b) fatigue crack fronts are seen at the edge of the shear crack, while a static fracture surface is seen in Fig. 5.7(c). This indicates that initial crack growth occurred along a 45° crack path, followed by sudden static failure upon final fracture.
5. Fatigue Assessment of a Stent Design for a CoCr alloy

It is assumed for this study that the behaviour of the L605 matrix is unaffected by changes to microstructural features, such as grain size and precipitates. Ensuing from this assumption, the L605 tensile and cyclic data of Section 5.3.2 can be used to calibrate L605 matrix behaviour across all grain sizes and for different precipitate sizes and distributions. For an effective calibration of the matrix behaviour, however, features such as grain size, precipitate size and frequency of precipitates, as is provided in Section 5.3.1, must be included in the geometry of the calibration model. This approach neglects the initial and evolving dislocation distributions in the L605 matrix, which are influenced by grain size and precipitates. While grain size and precipitate effects are not the focus of the current study, their influence on L605 fatigue behaviour will be investigated later in the thesis.

5.6.2. CoCr Computational Framework

Accurate calibration of the $J_2$ and CP cyclic and monotonic plasticity models against the measured responses in Figs. 5.11 and 5.12 is critical to the particular elastic-plastic loading history of stent deployment and in-service life prediction. Tensile calibration allows the capture of stent deployment behaviour, during which the stent undergoes a large amount of plastic deformation, which in turn affects the residual stress distribution for mean stress effects on fatigue life. The additional back-stress terms are critical to the accuracy of the tensile calibration in the large-strain region of Fig. 5.11 for the micro and macro-scales, respectively. Omission of these terms gives errors of up to 55% in macroscopic tensile stresses. Such a response would result in gross underestimation of the amount of strain hardening and, thus, stress magnitudes achieved during stent deployment. Under-prediction of deployment stresses would result in reduced elastic recovery predicted during recoil and, thus, an increase in predicted residual stresses during
stent fatigue.

The damage evolution law of Eq. 5.4 provides a method for back-calculation of \( N_i \) from experimental \( N_f \) data. However, it can be seen from Fig. 5.13(b) that using the critical FIP values, \( p_{\text{crit}} \) and \( W_{\text{crit}} \), identified for the \( \pm 0.5\% \) strain range, the majority of \( N_i \) predictions for the \( \pm 1.2\% \) strain range are longer than the experimentally observed number of cycles to failure. In Fig. 5.13(a), the poorest correlation exists between the experimental and calculated damage evolution curves for the \( \pm 1.2\% \) strain range, particularly at \( D = D_c \). In fact the experimental damage curve for the \( \pm 1.2\% \) strain range indicates that FCI occurs almost immediately before fatigue failure, as is predicted using the CP simulations of Fig. 5.13(b). It should also be noted that use of the damage evolution law of Eq. 5.4 to calculate \( N_i \) at a constant critical damage \( D_c \) results in a constant ratio of \( \frac{N_i}{N_f} \) across all strain ranges. A previous study, which describes use of an ultrasonic method for detection of cracks between the range of 30 – 110 \( \mu \text{m} \) in notched L605 fatigue specimens [178], reported that the \( \frac{N_i}{N_f} \) ratio increases with decreasing fatigue life, for tests with total fatigue lives in the \( 10^2 – 10^5 \) cycles regime. This supports the CP predictions of Fig. 5.13(b) for the higher strain ranges, where \( N_i \) is predicted at larger numbers of cycles than is predicted by the damage evolution law.

5.6.3. Stent Fatigue Simulations

The FDA recommends that stents are designed to have a minimum operational life of 10 years or approximately \( 4 \times 10^8 \) cycles. Both the traditional \( J_2 \) continuum approach and the average CP sub-model response predict total stent fatigue life several orders of magnitude greater than the FDA minimum requirement, for the L605 alloy. In the previous chapter, CP analyses for the 316L SS stent predicted an average fatigue life of \( 7.27 \times 10^8 \) cycles, compared to an average total life of
5. Fatigue Assessment of a Stent Design for a CoCr alloy

6.43×10^{14} cycles for the L605 CP sub-models. The contrast in performance of the two materials illustrates that, while the generic stent design is suitable for the 316L SS material, it is a highly conservative design for the L605 alloy. Therefore, the stent geometry could be modified, for the L605 alloy, to improve design efficiency. To investigate this, additional L605 analyses were carried out for a modified stent geometry, where the stent strut cross-section was reduced by 20 µm in each dimension. The results are compared in Fig. 5.16 with predictions for the original stent geometry and with 316L predictions from the previous chapter. The bar chart of Fig. 5.16 shows the average predictions for CP sub-model analyses, where error bars mark the range of data and FDA minimum required \( N_f \) is shown. At 1.28×10^{12} cycles, the average total life predicted for the L605 thin strut geometry is two orders of magnitude lower than for the original geometry. However, this total life remains several orders of magnitude higher than the FDA recommended minimum total life, indicating that the thin strut design remains over-conservative. Therefore, according to the predictions of Fig. 5.16, a further reduction in strut cross-sectional area could be adopted for the L605 stent geometry, while still attaining acceptable fatigue performance. Thinner struts are highly desirable in stent geometries due to increased flexibility and reduced restenosis rates \([9]\). It is important to note, however, that the analyses carried out in this study do not investigate strut necking during the installation process, which may also limit the stent design \([39,101,121]\).

FCI is predicted to occur early in operational life for both the original and thinner strut designs, anywhere from a few weeks to more than one year after installation of the stent. For all cases represented in Fig. 5.16, a significantly narrower scatter band is seen for \( N_i \) predictions, compared with stress-based Basquin-Goodman total life predictions. This indicates that the microstructure-sensitive FIP approach is a more reliable method for stent fatigue assessment. Returning to a comparison between L605 and 316L, a broader range in \( N_i \) predictions is seen for
5. Fatigue Assessment of a Stent Design for a CoCr alloy

Figure 5.16: Averages and scatter in total life and FCI predictions for the L605 thin strut and normal strut sub-models and for a 316L normal strut sub-model.

the L605 alloy. Precipitates in the L605 matrix are likely to be the source of this increased scatter, as they introduce additional microstructural inhomogeneity, absent in the 316L microstructure. Additional L605 sub-model analyses for one case has shown that omission of precipitates results in increased number of cycles to FCI, but reduced total life. This in fact agrees with experimental observations that precipitates often promote crack initiation [193,194], but increase resistance to crack growth by obstructing the crack path [195, 196]. It is also anticipated that the introduction of strain-gradient effects, i.e. increased hardening in regions with a high gradient of plastic deformation, into the CP constitutive model would increase the influence of precipitates on the lives predicted. Such a constitutive model can capture the grain size effect [159], i.e. the superior fatigue performance of finer-grained materials, and also the increased hardening experienced by matrix material surrounding precipitates [157]. The influence of strain-gradient effects on stent fatigue performance will be investigated later in the thesis.

As in the previous chapter, it is unlikely that the full range of responses is captured by the microstructure-sensitive predictions here; the sub-model grain mor-
phology was generated to have strong correlation to the average experimentally observed grain area distribution and crystallographic orientations were assigned randomly. Informed stent fatigue design would require improved capture of scatter, to ensure a design is not over-conservative and, more importantly, that in-vivo fatigue fracture is not a risk. Extreme combinations of microstructure must instead be modelled to achieve this. For example, the notably lower number of cycles to fatigue crack initiation for Realization 2 in Table 5.5 can be attributed to microstructural inhomogeneity. This particular realization by chance contains a grain geometry/orientation combination at the inner free surface of the hinge which triggers increased deformation. It is likely that other realizations with more extreme combinations could result in lower predictions again of $N_i$.

From Fig. 5.15 (b), the locations of FCI predictions, while occurring in multiple regions, clearly highlight a critical region for crack initiation in the notch area, along the inner radius of the top strut. While predictions using $p$ and $W$ do not take into account compressive stress effects (i.e. a crack-inhibiting environment), the prediction of this critical region is corroborated by the $J_2$ continuum $N_f$ prediction (Fig. 5.15 (a)), which does take into account compressive stress effects. Beam bending theory also supports the prediction of FCI in this notch region. The upper strut can be viewed as a beam with one end fixed in the hinge region, which has experienced a large upwards load at its ‘free’ end. Therefore, the upper strut is expected to experience cyclic compression on its outer radius and cyclic tension on its inner radius, which is conducive to cracking. If the $J_2$ continuum model was calibrated for cyclic behaviour only, i.e. neglecting the large-strain monotonic hardening, the predicted location of $N_f$ would be along the outer radius of the lower strut. Simple beam bending theory indicates that this region experiences cyclic compression, which is not conducive to cracking. This illustrates the importance of accurate calibration of constitutive models against both monotonic and cyclic plasticity responses.
Fig. 5.17 has been constructed to assess the effect of crystallographic orientation on FCI predictions. The maximum Schmid factors with respect to the $y$-direction (the direction of loading applied to the lower sub-model strut) are plotted for every grain in the original L605 stent sub-model, across all seven crystallographic orientation realizations. Maximum Schmid factors for grains in which FCI is predicted to occur are clearly marked. The graph generally shows a trend for FCI to occur in grains with high maximum Schmid factors. Interestingly, the most noticeable outlier in this trend (the $p_{crit}$ prediction for Realization 6) is the only case for which FCI is predicted to occur in a grain along the outer radius of the lower strut, a region in which $x$-direction loading is likely to be significant, compared with $y$-direction loading. Therefore, the maximum Schmid factor relative to the principal loading direction for this grain may be higher than shown and, consequently, may be in line with the general trend.

A 2D generalised plane strain stent sub-model is employed, for demonstrative purposes, in the current chapter. The 2D constraint is expected to give a stiffer response compared with a 3D representation. However, it is likely that the uni-
form out-of-plane strain, enforced by the generalised plane strain condition, results in increased strain in some grains, while others experience reduced deformation. Another notable shortcoming of the 2D approach is the inability to simulate out-of-plane loading (radial loading for the stent application), which may affect the lives predicted. Clearly, an important next step, albeit computationally onerous, is the development of a 3D micromechanical stent sub-model. Limited comparisons are provided in the literature between computational methods for assessing stent performance and experimental data. Those that do carry out comparisons are generally concerned with monotonic loading of the stent only [99, 116] or patient-specific cases [126, 171]. Therefore, experimental validation of the micromechanical methodology for assessment of stent fatigue design is a key objective, which is investigated in a later study in the thesis.

5.7. Conclusions

A micromechanical framework for the fatigue behaviour of a biomedical grade CoCr alloy has been presented, including realistic microstructure geometries, a crystal plasticity constitutive model with experimentally observed cyclic and monotonic hardening behaviour and in-built functionality to predict microstructure-sensitive fatigue crack initiation. The micromechanical framework has been applied to the fatigue assessment of a generic stent platform to demonstrate microstructure-driven design capability, resulting in efficient CoCr stent design. This work has successfully illustrated the microstructure-sensitive nature of stent fatigue, including dependence of fatigue crack initiation site on crystallographic orientation and scatter in number of cycles predicted to fatigue crack initiation due to different microstructure realizations, thus reaffirming the need for microstructure-sensitive approaches in stent fatigue design.
6. Modelling Crack Initiation for Four-Point Bending Fatigue

6.1. Chapter Summary

While the previous studies were concerned with application of a micromechanical framework to stent fatigue, in this chapter the focus is diverted towards the factors contributing to fatigue crack initiation (FCI). FCI in polycrystal ferritic steel is investigated through experimental observation of multiple large-grained, notched, four-point bend tests. Physically-based crystal plasticity (CP) finite element (FE) techniques are combined with explicit microstructural representation of the same specimens to assess fatigue indicator parameters, together with the roles of elastic anisotropy and length scale effects in slip development, and hence in crack initiation.

6.2. Introduction

As discussed in Chapter 2 of this thesis, FCI and the initial stages of crack propagation are strongly influenced by the inhomogeneous stress field in the local
microstructure and less so by the far-field stress state. Microstructure-based fatigue indicator parameters, such as slip, can be identified as drivers for crack formation and, thus, can be used to predict FCI sites [29]. Various attributes in the microstructure are thought to influence the accumulation of these fatigue indicator parameters (FIPs), including, but not limited to (i) elastic anisotropy, due to local crystallographic orientations, (ii) the natural anisotropy of crystal slip in different crystal structures, (iii) length scale effects, due to evolution of geometrically necessary dislocation (GND) density and (iv) hardening, due to statistically stored dislocation (SSD) accumulation.

The high cycle fatigue (HCF) regime can be defined by the degree of heterogeneity of the polycrystal plastic slip field [197]. While HCF loading triggers a seemingly elastic response at the macro-scale, micro-plasticity occurs in isolated regions (e.g. grains which are favourably oriented for slip), surrounded by dominantly elastic regions. This differs from the low cycle fatigue regime, where widespread slip results in a macroscopically elastic-plastic response. The concept of statistical volume elements (SVEs) has facilitated the analysis of many microstructure realizations for investigating FCI behaviour in the HCF regime. For example, Przybyla and co-workers [57, 58, 198] use SVEs to develop probability functions for extreme values of FIPs, which are correlated with the occurrence of different microstructural attributes (e.g. grain crystallographic orientation combinations) to assess their influence on FCI. Morrisey et al. [199] use CP modelling to investigate the effect of cyclic stress ratio on micro-slip, reporting a transition in behaviour between high and low stress ratios, where the onset of local plastic ratchetting was predicted with increasing cyclic stress ratio. Sauzay and Gilormini [200] investigated the influence of the free surface on persistent slip band (PSB) formation for HCF, predicting an increase in plastic slip towards the surface compared with the bulk material. A study by Sauzay and Jourdan [201] examined the role of elastic anisotropy in a free surface grain, demonstrating the
effect of orientation of neighbouring grains on the resolved shear stresses and normal stresses, which develop during HCF. Cheong and Busso [54] demonstrate the effects of lattice misorientations on polycrystal plastic strain field distribution for monotonic loading, while Cheong et al. [202] employed CP modelling to successfully capture the experimentally-observed effect of grain orientation on accumulated plastic strain for HCF of an aluminium test sample. Studies by Zikry and co-workers [203–205] demonstrate the effect of crystallographic orientation on dislocation accumulation and strain distributions at the grain boundaries, using CP FE methods. Studies by Dunne and co-workers [206, 207] have successfully used CP modelling to explain the occurrence of facet fatigue, cold-dwell crack initiation in hcp titanium polycrystals, in terms of rogue grain combinations and material rate sensitivity.

Wilkinson et al. [208] and Ahmed and Wilkinson [209] have employed electron channelling contrast imaging (ECCI) to experimentally investigate PSB formation in fatigued single crystal specimens of OFHC copper. The experimental observations confirmed PSBs to be a precursor to FCI, for the single crystal case investigated. The effective plastic strain FIP \( p \), used in the previous chapters, sums cumulative slip over all slip planes. A study by Dunne et al. [62] successfully demonstrated use of \( p \) for the identification of FCI sites in a directionally solidified, two-dimensional fcc polycrystal for a nickel alloy polycrystal.

In this chapter, the factors influencing FCI are investigated for four-point bending fatigue of ferritic steel via comparison of experimental observations for nine notched specimens with CP simulations, including explicit representation of the grain morphology and crystallographic orientations measured in the notch region for each specimen. The effect of elastic anisotropy on the development of stress fields and distributions of crystallographic slip and the effective plastic strain FIP is assessed in detail and compared with micrographs of the experimental FCI site for one specimen, while the influence of length-scale effects on the predicted FCI
site is investigated for another specimen. The FCI predictive abilities of effective plastic strain, including measures accumulated over the entire analysis and over a single cycle, and crystallographic slip on dominant slip systems are assessed for all nine specimens, while the correlation between dominant slip direction and experimentally observed initial crack propagation direction are also investigated. In the next section, the crystal plasticity formulation, including length scale effects, is described, which is followed by a description of the experimental four-point bend test programme, development of the notched FE models, and the results of detailed investigation of FIPs via comparison with experiments.

6.3. Crystal Plasticity Constitutive Model

A physically-based CP formulation, with the optional feature of GND density evolution is employed in this study. The small strain kinematics implementation of Section 3.4.2 is used, where the flow rule, repeated here for clarity, is given by:

\[ \dot{\gamma}^\alpha = \rho_{SSD} b^2 \nu \exp \left( -\frac{\Delta H}{kT} \right) \sinh \left( \frac{\left| \tau^\alpha \right| - \tau_c - r}{kT} \frac{\nu b^2}{\rho_{SSD} + \rho_{GND}} \right) \text{sgn}(\tau^\alpha) \]  

(6.1)

The material under consideration in this study is SUS 430LX ferritic steel, supplied by Nippon Steel Corporation, which has a body-centred cubic (bcc) crystal structure. Crystal structures of type bcc in general have forty eight slip systems in total, but the twenty four \{123\} \langle 111 \rangle slip systems in iron do not operate extensively at room temperature [210,211]. Therefore, only twenty four slip systems have been implemented into the CP constitutive model; the twelve \{110\} \langle 111 \rangle and twelve \{112\} \langle 111 \rangle slip system types.

As outlined in Chapter 3, the physically-based CP formulation is implemented within a user-element subroutine (UEL) in Abaqus to allow calculation of the spa-
tial gradients of the plastic deformation gradient at element Gauss integration points, which are required for calculating the evolution of GND density, \( \rho_{GND} \). An eight-noded, reduced integration element is defined, where out-of-plane crystallographic slip is allowed in the model, but within an overall constraint of plane strain, i.e. an equal and opposite out-of-plane elastic strain is imposed. Length scale effects can be included or otherwise in the constitutive model simply by excluding the evolution of \( \rho_{GND} \).

In another study, 3D simulation results from the generic CP formulation used here have been compared against electron backscatter diffraction (EBSD) analysis for loading of a single crystal with an embedded carbide particle [59]. The results show good correlation between CP simulations and EBSD measurements for both the strain field and the lattice rotations in the crystal local to the carbide particle, thus providing verification of the validity of the material model.

### 6.3.1. Identification of Constants

Physically-based values of \( \rho_{SSD} \), \( b \) and \( \nu \) are used in the model, provided in Table 6.1. The frequency of dislocation jumps \( \nu \) is chosen to be two orders of magnitude smaller than the Debye frequency which is determined from the Debye temperature and the Boltzman and Planck constants as \( 1 \times 10^{13} \, \text{s}^{-1} \) [212]. The jump frequency is accordingly taken to be \( 1.0 \times 10^{11} \, \text{s}^{-1} \). The Helmholtz free energy, \( \Delta H \), is assigned a value of \( 2.605 \times 10^{-20} \) J to minimise the strain rate sensitivity of the material response, which is reasonable for the room temperature deformation of steel at quasi-static strain rates. The reference strain, \( \gamma_0 \), is simply chosen to be a representative 0.001. Simple shear tests have been carried out by the Nippon Steel Corporation on two SUS 430LX steel specimens for calibration of the remaining CP constants. Shear specimen dimensions are provided in Fig. 6.1(a), where the specimen is gripped in the unshaded region.
and the gauge region is shaded. Images of the sheared specimens can be seen in Fig. 6.1(b). Calibration of CP constitutive model constants for critical resolved shear stress, $\tau_c$, and isotropic hardening evolution, $h$, has been carried out using the shear test data [213]. The model geometry, shown in Fig. 6.1(c), consisted of a 2D oligocrystal containing 27 arbitrarily orientated grains, with average grain size equal to that measured for the material of 1856 µm. The shear tests carried out experimentally were simulated using this RVE geometry in conjunction with the generalised plane strain UEL of Section 6.3 for describing CP constitutive behaviour. Constants were identified from comparison of the shear stress-shear strain curves from the experiments and simulations, as shown in Fig. 6.1(d). The shear stress-shear strain behaviour for a CP simulation without the isotropic hardening parameter, $r$, is also shown in Fig. 6.1(d). Error bars have been included for the FE curve with hardening, representing standard deviations of the shear stress RVE response for multiple texture realisations. An optimisation algorithm was employed which enabled the critical resolved shear stress and hardening coefficients to be determined by means of minimising the squares of differences between the polycrystal computed and experimental macro-level shear stresses over the strain history. Identified values of the material constants and physical properties used are provided in Table 6.1. The calibrated CP constitutive model has been established to give rate insensitive behaviour below a threshold plastic slip rate of 0.08 s$^{-1}$, which is greater than slip rates being applied in this study.

Anisotropic (cubic) elasticity (Eq. 3.23) is used for the bulk of the analyses carried out. However, for one specimen, analyses are carried out for both isotropic (Eq. 3.22) and anisotropic elasticity. A Young’s modulus of 206 GPa and Poisson’s ratio of 0.3 are used to represent isotropic elasticity. For anisotropic elasticity, the cubic constants $C_{11} = 277$ GPa, $C_{12} = 119$ GPa and $C_{44} = 168$ GPa are used to populate the local elastic stiffness matrix. The evolution of $\rho_{GND}$ is excluded.
Table 6.1: Material properties for the ferritic steel SUS 430LX constitutive model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_{SSD}$</td>
<td>$1 \times 10^{10} \text{ m}^2$</td>
</tr>
<tr>
<td>$b$</td>
<td>$2.5 \times 10^{-10} \text{ m}$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>$1.0 \times 10^{11} \text{ s}^{-1}$</td>
</tr>
<tr>
<td>$\Delta H$</td>
<td>$2.605 \times 10^{-20} \text{ J}$</td>
</tr>
<tr>
<td>$k$</td>
<td>$1.381 \times 10^{-23} \text{ JK}^{-1}$</td>
</tr>
<tr>
<td>$T$</td>
<td>293 K</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>$1.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>$\tau_c$</td>
<td>85 MPa</td>
</tr>
<tr>
<td>$q$</td>
<td>170 MPa</td>
</tr>
<tr>
<td>$h$</td>
<td>10</td>
</tr>
</tbody>
</table>

for the bulk of the analyses (i.e. no length scale effects). However, once again, simulations are carried out for one specimen with and without length scale effects in order to assess whether such effects play a role in the prediction of FCI.

In the following section, the experimental programme is outlined for four-point bending tests carried out on notched specimens with fully characterised microstructures local to the notches, and the identification of FCI. This is followed by presentation of the experimental and computational analyses.

6.4. Four-Point Bending Fatigue

6.4.1. Experimental Procedure

Four-point bending fatigue tests have been carried out by the Nippon Steel Corporation on nine ferritic steel notched specimens. Each specimen therefore has a quite substantially different combination of grain morphology and crystallographic orientations local to the specimen notches, thereby generating quite different local, microstructural stress states. An in-line servo-hydraulic loading rig
Figure 6.1: (a) Shear test specimen geometry with dimensions, (b) images of two different sheared specimens at different shear strains, (c) meshed polycrystal RVE used for calibration and (d) shear stress-shear strain response measured for the two specimens compared with crystal FE simulation results.

was used to generate cyclic loading conditions. Specimen geometry and location of the four-point bending supports are shown in Fig. 6.2. Loads of magnitude 500 N each were applied cyclically at the two central lower supports (as shown in Fig. 6.2) with a cyclic load ratio $R = 0$. Specimens were tested until failure or until $2.5 \times 10^6$ cycles, if failure had not occurred before this point. The locations of crack initiation sites and subsequent crack path, which always occurs local to the notches, have been recorded for each specimen using scanning electron microscopy (SEM). The geometry and crystallographic orientation of each grain at the surface in the notch region were identified for each specimen via the combined use of SEM and electron backscattered diffraction (EBSD) imaging. An example is shown in the inset of Fig. 6.2, in which the large grain size relative to the notch can be seen, such that the assumption of a prismatic grain structure (in a manner similar to directional solidification) becomes reasonable. The Nippon
6. Modelling Crack Initiation for Four-Point Bending Fatigue

Figure 6.2: Specimen dimensions for four-point bending fatigue tests, including notch region, with explicit polycrystal representation of the notched region shown schematically in the inset.

Steel Corporation, who carried out the fatigue tests, as mentioned above, also supplied the material and carried out the notch microstructure characterisation.

6.4.2. Finite Element Models and Analyses

Separate FE models were previously developed for each of the nine notched, polycrystal specimens (by virtue of each microstructure being different) [213] and CP analyses of the four-point bending fatigue tests are carried out here for all nine specimens. An average of 35,000 elements is used for each model, with a highly refined mesh employed in the notch region at an average of 661 elements per grain. A previous mesh sensitivity study showed the convergence of CP simulations of the formation of shear bands in thin polycrystalline struts with
an average of 98 elements or more per grain [119]. According to this, the mesh density used in the notch region of the models presented here is sufficient for the purposes of prediction of crack initiation sites. An example of a meshed notch region for one specimen is shown in Fig. 6.3. In this particular specimen, it can be seen that a triple point exists within the notch region and directly on the free surface. The loading applied is HCF in nature in that it is anticipated that the bulk material response remains elastic. As a result, the CP model is employed only for that region local to the notch, where slip is expected to initiate, and it is only in this region that the grain morphology and crystallography are explicitly represented within the finite element geometric model. Outside of this region, the material is expected to deform elastically only. The boundary conditions and loading applied can be seen in Fig. 6.3; nodes at A and D are fixed in the $x$- and $y$-directions and cyclic loads of 500 N are applied in the $y$-direction at nodes B and C. As illustrated in the loading history provided in Fig. 6.3, 5.5 cycles are generally applied for each simulation, except for one additional case with more cycles described below.

### 6.5. Results

The CP finite element analysis results are used to assess the importance of the following in capturing details of FCI:

(i) cyclic loading as opposed to monotonic loading,

(ii) inclusion of anisotropic elasticity,

(iii) inclusion of length scale effects,

(iv) effective plastic strain and
6. Modelling Crack Initiation for Four-Point Bending Fatigue

Figure 6.3: Boundary conditions applied to the crystal FE four-point bending model, with \( R = 0 \) cyclic loading history applied at points B and C, together with a magnified view of the crystal finite element mesh in the notch region.

(v) independent accumulated slip system activity.

Two fatigue indicator parameters are used for analysing results, namely (i) the effective plastic strain accumulated over the entire analysis, \( p \), and (ii) the effective plastic strain accumulated over a single cycle of the analysis, \( p_{cyc} \):

\[
\dot{p} = \left( \frac{2}{3} \mathbf{L}^p : \mathbf{L}^p \right)^{1/2} ; \quad p = \int_{0}^{t_{\text{analysis}}} \dot{p} dt ; \quad p_{cyc} = \int_{t_1}^{t_2} \dot{p} dt \quad (6.2)
\]

where \( t_{\text{analysis}} \) refers to the full analysis time, and \( t_1 \) and \( t_2 \) denote the time at the start and end, respectively, of the final cycle. \( p \) and \( p_{cyc} \) are assessed for their ability to predict the crack initiation sites for each specimen and the contribution of accumulated slip on individual slip systems, \( \gamma^\alpha \), towards these predictions is investigated. In addition, the effectiveness of using direction of dominant slip systems to predict the initial crack direction in experiments is assessed.
6.5.1. Effective Strain and Independent Slip Activity

Fig. 6.4 shows various accumulated plastic strain field plots after monotonic (to peak cycle load) and cyclic loading for an analysis carried out for Specimen 1. Length scale effects are not included for this simulation and anisotropic elasticity is employed. The crack initiation site and crack path in the notch region of Specimen 1 are shown clearly in Fig. 6.4(a), along with the FE mesh in the notch region. In this specimen, the key microstructural feature appears to be the grain boundary terminating at the notch root. For the first comparison in Fig. 6.4(b), field plots of effective plastic strain, $p$, are shown after monotonic (to peak cycle load) and cyclic loading (after 5.5 cycles). Fig. 6.4(a) shows that crack initiation occurs at the grain boundary at the notch free surface, but that this does not unambiguously match the locations of maximum predicted effective plastic strain in Fig 6.4(b) for the case of the first-half loading cycle (although the experimentally observed crack initiation site is predicted to be a local effective plastic strain hot spot). However, once more cycles have been imposed, the slip localisation is more pronounced, as shown in the cyclic loading field plot in Fig 6.4(b), in which the peak effective plastic strain clearly marks the observed initiation site.

Figs. 6.4(c)–(e) show field plots of accumulated slip on three individual slip systems. Recalling Eq. 6.2 and the definition of the plastic velocity gradient $L^p$ in Eq. 3.28, slip on individual slip systems make a direct contribution to the effective plastic strain parameter, $p$. The first set of accumulated slip distributions (Fig. 6.4(c)) belong to the slip system with the highest peak slip, which is of type $\{112\} \langle 111 \rangle$. The ambiguity of crack initiation site seen in the plot for $p$ after monotonic loading is clearly attributable to the slip distribution for this dominant slip system, which shows two regions of high slip. Activity on the second slip system (Fig. 6.4(d)), also of type $\{112\} \langle 111 \rangle$, contributes further to
Figure 6.4: (a) Images of crack path for Specimen 1 along with the FE mesh in the notch region, together with predicted field variations for Specimen 1 of (b) effective plastic strain, $p$, and (c)–(e) accumulated plastic slip, $\gamma^\alpha$, on differing slip systems. Plots are provided for full load after monotonic loading and full load after cyclic loading as indicated.
the difficulty of identifying a crack initiation site by generating increased strain at the second peak location at the notch surface in the distribution of $p$ after monotonic loading. After cyclic loading, a noticeable change is visible in the slip distribution for the dominant slip system (Fig. 6.4(c)), which is responsible for the more substantive distribution of $p$. Recalling Eq. 3.60, this results from the isotropic hardening in the material model which is assumed to contribute to all active systems in equal measure. The slip distribution for the second slip system (Fig. 6.4(d)) appears qualitatively unchanged after cyclic loading and, therefore, does not explain the change in slip distribution for the dominant slip system. However, a third slip system, also of type $\{112\} \langle 111 \rangle$, shown in Fig. 6.4(e), experiences a significant change in its distribution between monotonic and cyclic loading. After monotonic loading, the slip peak on this system is subsurface and the magnitude of slip is negligible compared to the other two slip systems. After cyclic loading, however, the peak of the third slip system shifts to the observed site of crack initiation and is of a magnitude comparable to the first two slip systems. In addition, it contributes high slip at a location which overlaps with a similarly high magnitude resulting from the first slip system, thus generating the highest effective plastic strain at the site of crack initiation shown in Fig. 6.4(b).

Fig. 6.4 provides a clear example of the shift which can occur in deformation distributions within the first few cycles of loading. Changes in accumulated slip distributions, $\gamma^\alpha$, on dominant slip systems directly impact the distribution of effective plastic strain, $p$, and hence predictions of crack initiation sites (if effective plastic strain is used as an FIP). Simulations for other specimens also exhibit considerable changes (sometimes from one side of the notch to the other) in distributions within the first few cycles. This highlights the necessity of examining cyclic loading in simulations.
6.5.2. Effect of Elastic Anisotropy

We next consider a second specimen and the effects of elastic anisotropy. FE analyses are carried out for Specimen 2 using both isotropic and anisotropic elasticity. For both simulations, length scale effects are not included. Fig. 6.5(a) shows the experimentally observed FCI site and crack path for Specimen 2, and also includes the FE mesh used in the notch region for the same specimen. In this specimen, it is interesting that the entire notch root is made up of one grain, if small in size relative to the others in the notch region. Predicted field plots of axial (bending) stress from the crystal FE analyses with isotropic and anisotropic elasticity are provided in Figs. 6.5(b) and 6.5(c) after initial yielding and cyclic loading, respectively. Elastic anisotropy is expected to have a significant effect initially after yielding as the stress distribution is strongly affected by orientation mismatch at the grain boundaries. However, as loading continues, it is expected that the influence of elastic anisotropy reduces as the amount of plastic deformation increases. The axial stress distributions, provided in Fig. 6.5 for Specimen 2, support this. Initially, after yielding (Fig. 6.5(b)), while the stress distribution for the case of isotropic elasticity appears unaffected by the grain boundary, a discontinuous distribution is visible in the region of the grain boundary for the case of anisotropic elasticity. A higher peak stress can be seen in the distribution for the case of anisotropic elasticity. After cyclic loading (Fig. 6.5(c)), similar axial stress distributions are seen for the two models, with the anisotropic elasticity prediction showing a slightly more localised subsurface peak. Both stress distributions appear to be affected by the grain boundary, but this is due to orientation mismatch effects on crystallographic slip, rather than on elastic behaviour.

Fig. 6.6 shows effective plastic strain, $p$, and accumulated slip, $\gamma^\alpha$, comparisons between the same models used in Fig. 6.5. Initially, after yielding (Fig. 6.6(a)), plots of effective plastic strain, $p$, for the simulations with isotropic and
Figure 6.5: (a) Images of crack path for Specimen 2 along with the crystal FE mesh in the notch region, and axial stress FE model predictions with isotropic and anisotropic elasticity (b) initially after yielding and (c) at full load after cyclic loading.

anisotropic elasticity (at the same point in the loading history) are quite different. Firstly, the peak in effective plastic strain is visible to the right of the notch for the isotropic elasticity model, whereas for the anisotropic elasticity model, the peak effective plastic strain occurs to the left of the notch, at the experimentally observed crack initiation site. Secondly, the peak value of effective plastic strain for the isotropic elasticity model is significantly higher than that for the anisotropic elasticity model, suggesting that yielding occurs sooner in the former model. After cyclic loading (Fig. 6.6(b)), once again the effective plastic
strain, \( p \), distributions for the two models are quite different. The peak \( p \) for the isotropic elasticity model is at the opposite side of the notch to the experimentally observed crack initiation site, whereas the anisotropic model appears to predict correctly the crack initiation site with a peak \( p \) which is much more localised. The distribution of \( p \) for the anisotropic elasticity model is discontinuous at the grain boundary as opposed to the smoother distribution exhibited by the isotropic elasticity model. Differences in \( p \) distributions initially after yielding can be directly attributed to differences in the axial stress distributions. However, after cyclic loading the axial stress distributions of the two models are quite similar and, therefore, are not responsible for differences in \( p \) distributions. Effective plastic strain distribution plots for the model with anisotropic elasticity show a clear correlation between the sites of peak \( p \) in the early stage (Fig. 6.6(a)) and in the fully developed distribution (Fig. 6.6(b)). This suggests that the effective plastic strain distributions which develop initially after yielding are the cause of differences in the more fully developed \( p \) distributions.

Different slip systems were found to exhibit the highest peak slip for the two models. Slip distributions are shown for these dominant slip systems, both of type \{\( \{112\} \langle 111 \rangle \), for each model after cyclic loading in Fig. 6.6(c). It is clear that these dominant slip systems are responsible for the trends in effective plastic strain distributions for the respective models. An image of the experimental crack path has been superimposed on the accumulated slip distributions for both in the region of the observed crack initiation site (Fig. 6.6(c)). It can be seen clearly that the dominant slip system for the anisotropic elasticity model correctly predicts the FCI site, whilst the dominant slip system for the isotropic elasticity model is unsuccessful in this respect.
Figure 6.6: Field variations for Specimen 2 from crystal FE models with isotropic and anisotropic elasticity of (a) effective plastic strain, $p$, initially after yielding, (b) effective plastic strain, $p$, at full load after cyclic loading and (c) accumulated plastic slip, $\gamma^\alpha$, on the slip system with the highest slip for each model at full load after cyclic loading.

6.5.3. Length Scale Effects

CP finite element analyses were also carried out for Specimen 2 both including and excluding the evolution of GNDs, $\rho_{GND}$; that is, with and without length scale effects included. Anisotropic elasticity is used for these simulations. Recalling the crystal constitutive model slip rule in Eq. 6.1, the hardening effect due
to the build-up of GNDs is negligible until $\rho_{GND}$ is at least the same order of magnitude as $\rho_{SSD}$, which is taken in these analyses to be constant and equal to $1 \times 10^{10}$ m$^{-2}$. Therefore, differences between the models with and without length scale effects remain small at initial yielding when $\rho_{GND}$ is small. However, a comparison between the effective plastic strain distributions for the two models after cyclic loading is provided in Fig. 6.7(a). The distribution without length scale effects is the same as that shown for anisotropic elasticity in Fig. 6.6(b), although different scales are used. The introduction of length scale effects appears to inhibit the build-up of the highest peak of effective plastic strain, $p$, at the notch surface, while leaving the distribution largely unchanged at all other locations. Fig. 6.7(b) shows the predicted distribution of density of GNDs, $\rho_{GND}$, after cyclic loading for the model with length scale effects. The peak in this distribution is of order $1 \times 10^{11}$ m$^{-2}$, and observable hardening effects due to evolving densities of GNDs are therefore to be expected, causing a reduction in plastic strain. The reduced peak magnitudes in the effective plastic strain distribution, with inclusion of length scale effects, may impact on the cyclically accumulated values and, hence, on the number of cycles predicted to FCI. It is interesting to note that the development of GND density is highly localised and that the primary distribution of GND density can be seen to correspond precisely with the site of FCI. This raises the possible hypothesis that a differential diagnosis of location of FCI based on FIPs would likely include effective plastic strain and density of GNDs, with the most likely initiation site at that point where peaks in both quantities coincide.

6.5.4. Accumulated vs Cyclic Plastic Strain

For all of the nine experimental specimens, crystal finite element simulations have been carried out using anisotropic elasticity and without length scale effects. Two
parameters are assessed as possible FIPs for prediction of the locations of FCI sites. The first is the effective plastic strain parameter, \( p \), at full load after cyclic loading and the second is the effective plastic strain accumulated in the final cycle of loading only, \( p_{cyc} \). Crack initiation sites are predicted at peaks in plots of \( p \) and \( p_{cyc} \) for each specimen. A dimensionless parameter \( x/d \) is employed to quantify the proximity of the FE predicted crack initiation site to the observed crack initiation site, where \( d \) is the average grain size and \( x \) is the distance between predicted and observed crack initiation sites. Table 6.2 provides values of \( x/d \) for each specimen simulation using the discrete maximum values from predicted distribution plots of \( p \) and \( p_{cyc} \). The peak value of \( p \) is found to coincide precisely with the experimentally observed crack initiation site for four out of nine specimens (\( x/d = 0 \)). For four other specimens, predictions of crack initiation site are on the correct side of the notch, but slightly to one side of the crack initiation site. The value of \( x/d \) is highest (i.e. worst) for Specimen 6, the only specimen out of nine for which the site of the peak effective plastic strain is predicted on the wrong side of the notch with respect to the crack initiation site. Examples of
Table 6.2: Proximity \((x/d)\) of predicted FCI sites to experimentally observed crack initiation sites. Predictions using discrete and volume-averaged peak values of effective plastic strain, \(p\), and cyclic effective plastic strain, \(p_{cyc}\), are shown.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Discrete</th>
<th>Averaged</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(p)</td>
<td>(p)</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>0.11</td>
<td>0.13</td>
</tr>
<tr>
<td>4</td>
<td>0.07</td>
<td>0.05</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>0.27</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>0.03</td>
<td>0.08</td>
</tr>
<tr>
<td>9</td>
<td>0.05</td>
<td>0.03</td>
</tr>
</tbody>
</table>

Figure 6.8: Field variations of effective plastic strain, \(p\), with superimposed images of experimentally observed crack initiation and growth for (a) Specimen 7, (b) Specimen 8 and (c) Specimen 6. Experimental and crystal FE predicted sites of FCI are highlighted.

effective plastic strain, \(p\), distributions for specimens for which the FCI site is (i) correctly predicted by the effective plastic strain peak, (ii) predicted slightly to one side of the observed site and (iii) predicted at the opposite side of the notch to the observed site are shown in Figs. 6.8(a)–(c), respectively, in all of which the experimentally observed crack initiation and growth paths are superimposed. It is notable for Specimen 6 (Fig 6.8(c)) that two localised zones of effective plastic strain are predicted to develop, one of which coincides precisely with the observed crack initiation site. Also, Specimen 6 is one for which a single, large grain exists.
which incorporates the majority of the notch (as shown in Fig 6.8, where grain boundaries are depicted by solid black lines). However, returning to Table 6.2, it can be seen that for use of the cyclic accumulation of effective plastic strain, \( p_{cyc} \), while most predicted peak locations change only slightly or not at all, the peak \( p_{cyc} \) location (and so the crack initiation site) is now accurately predicted for Specimen 6. To demonstrate this, Fig. 6.9(a) shows the accumulation of effective plastic strain, \( p \), with increasing number of cycles at two points A and B at the notch surface for Specimen 6 (locations marked in Fig. 6.8(c)), where A corresponds to the crack initiation site predicted using \( p \) and B corresponds to the experimentally observed initiation site. It can be seen from the graph that during the five cycles analysed, the effective plastic strain, \( p \), remains higher at point A than at point B, but that the rate of accumulation of \( p \) is in fact larger at point B than at point A. This is due to a larger cyclic effective plastic strain, \( p_{cyc} \), at point B than at point A (as marked in Fig. 6.9(a)). Fig 6.9(b) shows the field plot of cyclic effective plastic strain, \( p_{cyc} \), for Specimen 6, which provides an accurate prediction of the observed crack initiation site. Therefore, if increased number of cycles were applied in the simulation, the effective plastic strain distribution would show the peak \( p \) at point B. A smaller graph, resulting from an extended simulation with further cycling for Specimen 6, has been inset into the graph of Fig. 6.9(a) to illustrate this. It can be seen from this additional graph that the effective plastic strain at point B exceeds that at point A after 7 cycles of loading. Consequently, quite a different prediction of the crack initiation site can result by using the effective plastic strain, \( p \), as opposed to the cyclic effective plastic strain, \( p_{cyc} \). Therefore, while distributions after only a small number of cycles are being used here to predict crack initiation in the HCF regime, the \( p_{cyc} \) parameter provides an indicator as to whether a change can be expected in effective plastic strain distribution for a specimen. For the majority of the specimens analysed the most significant changes in \( p \) distributions occur within the 5.5 cycles simulated, and differences between predictions using \( p \) and \( p_{cyc} \) are
Figure 6.9: (a) Plot of effective plastic strain, $p$, against number of cycles for two points at the notch surface for Specimen 6 and (b) distribution of cyclic effective plastic strain, $p_{cyc}$, for crystal FE simulation of Specimen 6, with the experimental and predicted sites of FCI indicated.

not significantly different. For these cases it is reasonable to use either parameter for predicting crack initiation. However, for cases in which stabilisation of the $p$ distribution has not yet been reached (e.g. Specimen 6) the $p_{cyc}$ parameter is more appropriate. It can be seen from Fig. 6.9(a) that high $p_{cyc}$ at the predicted crack initiation site contributes to a ratchetting effect which may cause redistribution of the stress and strain fields local to the predicted crack initiation site. However, it is anticipated that any changes in stress and strain fields will only serve to increase deformation at the predicted crack initiation site, rather than result in a change in prediction of location of crack initiation site.

Aside from the possible change in qualitative information, Fig. 6.9(a) also highlights the importance of cycling from a quantitative perspective. Values of $p_{cyc}$ have been used in previous studies to predict the number of cycles to FCI, in conjunction with an identified critical value of $p$ [83]. From the graph in Fig. 6.9(a) it can be seen that cyclic loading is required in order to allow the stabilisation of $p_{cyc}$. Material hardening results in a reduction of $p_{cyc}$ in the first few cycles of loading. If $p_{cyc}$ values are extracted from the first cycle of loading, resulting predictions of cycles to crack initiation will be conservative.
Returning to the field distribution of effective plastic strain, \( p \), for Specimen 6 provided in Fig. 6.8(c), as mentioned previously, two localised zones of effective plastic strain are visible at the notch surface and, while the peak effective plastic strain occurs to the left of the notch at cycle 5.5, it appears that a larger volume of material is subject to high plastic strain to the right of the notch. In response to this observation, a volume-averaging approach is assessed in predictions of crack initiation sites, whereby values of \( p \) and \( p_{\text{cyc}} \) are averaged over a volume of material of fixed diameter, in this case 0.1\( d \). Using this approach, crack initiation is predicted at a site in a region of high plastic strain, rather than at discrete points of high plastic strain. The proximity of predictions, \( x/d \), using volume-averaged values of \( p \) and \( p_{\text{cyc}} \), are provided in Table 6.2. From the values provided, it can be seen that use of volume-averaged values generally result in predictions of the crack initiation sites with high proximity (i.e. low \( x/d \)) to the observed initiation sites. However, while use of volume-averaged values of \( p \) results in improved prediction of the crack initiation site for Specimen 6, compared with use of discrete values of \( p \), incorrect predictions of the crack initiation site (i.e. high \( x/d \)) are visible for other specimens using both volume-averaged values of \( p \) and \( p_{\text{cyc}} \).

6.5.5. Dominant Slip System Activity

Slip on individual slip systems, \( \gamma^\alpha \), contributes directly towards the effective plastic strain distribution, \( p \). An illustration of this for Specimen 1 (experimental images in Fig. 6.4) can be seen in Fig. 6.10. A field plot of the effective plastic strain after cyclic loading is provided in Fig. 6.10(a), while Fig. 6.10(b) shows plots of the accumulated slip, \( \gamma^\alpha \), on the five most dominant slip systems. Each of the five slip systems can be seen to contribute to different regions of the effective plastic strain distribution. The most dominant slip system can be
clearly identified, due to a peak accumulated slip significantly higher than on other slip systems. This dominant slip system also coincides with the experimentally observed crack initiation site. Therefore, it seems reasonable to take into consideration the accumulated slip on dominant slip systems as a possible FIP for predicting crack initiation.

In this study the dominant slip system is defined as the slip system with the highest magnitude of accumulated slip after cyclic loading. Values of $x/d$ found using distribution plots of the accumulated slip on the dominant slip system, $\gamma_\alpha$, are provided for each specimen in Table 6.3. Information on the dominant slip system type for each analysis is also provided. The $\{112\langle111\rangle$ type slip systems appear as the dominant systems for more specimens than $\{110\langle111\rangle$ slip systems. Predictions of crack initiation site using the accumulated slip on the
Table 6.3: Dominant slip system types and proximity of predictions of FCI sites, using discrete values of accumulated plastic slip on the dominant slip system, to experimentally observed crack initiation sites.

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Dominant slip system type</th>
<th>$x/d$ using discrete $\gamma^a$ values</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>${112} \langle 111 \rangle$</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>${112} \langle 111 \rangle$</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>${112} \langle 111 \rangle$</td>
<td>0.11</td>
</tr>
<tr>
<td>4</td>
<td>${110} \langle 111 \rangle$</td>
<td>0.07</td>
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dominant slip system follow the same trend as predictions using effective plastic strain, $p$, suggesting that the dominant system tends to be responsible for the highest peak in the effective plastic strain distribution. Once again, it is anticipated that cyclic accumulation of slip is a more reliable parameter for making predictions, for the same reasons as mentioned for effective plastic strain distributions in Section 6.5.4. Plots of accumulated slip for the dominant slip system in cases where the crack initiation site is accurately predicted are provided in Fig. 6.11. Images of the experimentally observed crack are also provided for comparative purposes. The slip plane and direction corresponding to the dominant systems are also provided, through the use of an oriented bcc unit cell, in which the slip plane is marked in grey and the slip direction is marked in red. Comparing with the experimental images, the initial crack direction predicted for Specimen 7 (Fig. 6.11(d)) does appear to have some correlation to the experiment, as the crack grows along a grain boundary to meet a triple point close to the notch surface. However, it is apparent that the initial crack directions are generally not parallel to the predicted dominant slip directions. Therefore, while high plastic slip on dominant slip systems may promote crack initiation, this study shows no evidence that a crack grows along a slip system with high
6. Modelling Crack Initiation for Four-Point Bending Fatigue

It should be noted, however, that rotation of the crystallographic orientations is not included in the CP constitutive model implemented for this study. Strain distributions shown for this study do not exhibit particularly high levels of plastic strain. However, they are shown for up to 5.5 cycles of loading. As mentioned in Section 6.4, loading applied to the specimens in this study is HCF in nature, which involves numbers of cycles on the order of magnitude of $10^6$. Due to the load-controlled loading applied, with a ratio of $R = 0$, it is anticipated that ratchetting occurs in the notch region of the specimens. The plots of $p$ against cycles of loading for points at the notch in Specimen 6 (Fig. 6.9(a)) support this clearly via the presence of ratchetting. Ratchetting can cause the incremental build-up of plastic strain to a high magnitude with the application of many cycles, which may have some highly local effect on the crystallographic orientations within the notch region. Also, while the analyses carried out have been shown to be effective in prediction of experimentally observed FCI sites, explicit modelling of crack initiation and crack growth have not been included. As such, the analyses do not capture the redistribution of the stress and strain fields due to crack initiation and crack growth, nor the resulting change in crystallographic orientations and dominant slip systems. Therefore, this study does not show evidence of cracks growing along dominant slip directions. However, it may be that these slip directions are not properly represented during FCI in the small deformation simulations carried out here. Also, these simulations do not capture a possible change in dominant slip system due to the event of crack initiation itself.

6.6. Discussion and Conclusions

Detailed comparisons have been presented between the results of four-point bend tests carried out on large-grained polycrystal ferritic notched steel specimens and
directly corresponding CP finite element model representations of the same specimens. The CP model, incorporating elastic isotropy or anisotropy as specified, together with plastic length scale effects, has been calibrated against averaged behaviour of polycrystal specimens tested in shear. Details of polycrystal morphology and crystallographic orientations have been explicitly obtained for nine different specimens by means of EBSD, and corresponding crystal finite element specimen representations developed.

Elastic anisotropy has been demonstrated to play a pivotal role in the distribution and magnitude of polycrystal slip relative to observed crack initiation site in
the context of constrained cyclic micro-plasticity. It has also been shown to change the level and distribution of micro-stress hence leading to the substantially differing slip distributions. This is of particular importance in constrained micro-plasticity, which is of most significance in the context of HCF crack initiation.

The impact of length scale effects on the magnitudes and distributions of effective plastic strain (at least under conditions of constrained micro-plasticity relevant to HCF, but over a small number of cycles) and accumulated slip, were small. However, over many cycles (typical of HCF), such effects could become significant, since small changes in slip development per cycle may become large when accumulated over many cycles, potentially influencing cycles to crack initiation. The crystal model results showed that the location of the peak density of GNDs coincided precisely with that of (i) the peak effective plastic strain, (ii) dominant accumulated plastic slip and (iii) the experimentally observed crack initiation site. Additionally, strain-gradient length scale effects are known to be most influential at fine grain sizes [214], whereas the ferritic steel presented here has a coarse-grain structure. A closer look will be taken later in the thesis at strain-gradient effects for finer-grain structures for the L605 CoCr alloy.

The distributions of micro-plasticity within the polycrystal specimens were found to change quite significantly between first yield and after multiple cycles. As a result, the changes in location of peak plastic strain and accumulated crystallographic slip with cycling can be profound and need to be considered when appraising FIPs. In the experiments and model specimen analyses carried out, the non-zero mean loading imposed resulted in considerable, but highly localised ratchetting, and this was found to be the major driver for the changing locations, during cycling, of the sites of peak plastic strain and accumulated slip. A significant consequence is that effective plastic strain per cycle was found to be a better indicator of FCI than peak effective plastic strain, particularly when measured after just a few cycles, as is the case for FE simulations. In nine in-
dependently tested and analysed polycrystal specimens, cyclic effective plastic strain and slip system peak accumulated slip were found to be good indicators of FCI sites. Slip on dominant slip systems has not been shown to be a good indicator of subsequent (micro-structurally short) crack growth path; however, incorporation of a damage model, such as that presented in Chapter 4, and/or micro-crack growth model is required to fully assess the usefulness of this FIP for crack path prediction.

Clearly, a number of candidate constitutive formulations, some arguably more physically-based than others (e.g. [54,55]) could have been adopted in the framework presented here. One specific example relates to the isotropic hardening formulation adopted in Eq. 3.60, which could be replaced by a similar, slightly more complex formulation, based on dislocation density evolution. In fact, additional parallel analyses investigating such a hardening model have shown that, while this would potentially affect predicted numbers of cycles to crack initiation, the predicted initiation sites would be the same.

The experiments carried out by the Nippon Steel Corporation for this material presented a rare opportunity to investigate the ability of the micromechanical framework, in particular the microstructure-sensitive indicator parameters, to predict the site of FCI for explicit microstructures, via direct comparison between simulations and experiments. While there is often a limitation on the sample size of microstructure which can be modelled with CP, it was possible here to model the full notch region for each specimen due to the coarse-grained material tested and, thus, the small number of grains in the notch region. CP modelling of the same region for a fine-grained stent material would be difficult. However, while the experiments and simulations presented in this chapter are not for a stent material, the conclusions of this study apply to the micromechanical framework for any material, including existing and potential future stent materials. Regarding relevance of the loading history adopted here to stent fatigue,
bending is experienced in the hinge or connecting link of a stent, where crack initiation is likely to occur according to experimental observations (e.g. [18]) and the results of Chapters 4 and 5. A region of tension is also a likely location for the initiation of a crack which could cause fracture, due to promotion of crack opening. The four-point bending tests simulated in this chapter have a cyclic load ratio of $R = P_{\text{min}}/P_{\text{max}} = 0$ and are, therefore, macroscopically tension bending tests. The fatigue loading applied in this study is, therefore, similar to that experienced by an at risk region of the stent.

The work presented in this chapter has provided validation of the qualitative FCI (i.e. FCI site location) predictive abilities of the cyclic effective plastic strain parameter, used in Chapters 4 and 5 for stent fatigue assessment. The need for anisotropic elasticity for FCI prediction in HCF, as used in the stent analyses of the previous chapters, has also been reaffirmed. While inclusion of strain-gradient effects is shown to have little influence on FCI site prediction for the large-grained material presented in this chapter, accumulation of GND density at the experimentally-observed site of FCI suggests that strain-gradient effects could have a significant influence on FCI behaviour for finer-grained materials, for which GND densities are higher. This will be investigated further in the next chapter for the CoCr alloy presented in Chapter 5.
7. Strain-Gradient Modelling of the Grain Size Effect

7.1. Chapter Summary

In this chapter, a strain-gradient crystal plasticity framework, based on physical dislocation mechanisms, is developed for simulation of the experimentally-observed grain size effect on low cycle fatigue (LCF) behaviour of the CoCr alloy presented in Chapter 5. Finite element models of the measured microstructure are presented for both as-received and heat-treated CoCr material, with significantly different grain sizes. Candidate crystallographic slip based parameters are assessed for prediction of fatigue crack initiation. The measured beneficial effects of fine grain size on both cyclic stress-strain response and crack initiation life are predicted. As forecast in the previous chapter, the build-up of geometrically necessary dislocations due to strain-gradients, leading to grain-size dependent material hardening, is shown to play a key role.
7.2. Introduction

It has been well established thus far in the thesis that fatigue damage and fatigue crack initiation (FCI) in metals are sensitive to microstructure [28, 29]. Experimental evidence indicates that grain size is a key microstructural feature affecting fatigue performance. Morrison and Moosbrugger [3], for example, presented an experimental study on the fatigue of coarse- and fine-grain polycrystalline nickel, reporting larger stress amplitudes and longer fatigue lives for the fine grain material under strain-controlled plasticity conditions. While fine-grain materials are FCI-resistant, coarse grains have been shown to give an increased threshold stress intensity factor range and, thus, improved resistance to fatigue crack growth [215,216]. Consequently, numerous industrial applications take advantage of the grain size effect, with components designed to have fine-grain surfaces, where FCI is more likely to occur [28], and coarse-grain interiors, for example, to resist crack growth. In the case of micro-scale components, for which microstructural features are comparable in size to component sectional dimensions, such as stents or micro-electro-mechanical devices, FCI typically dominates fatigue life and, therefore, a fine-grain structure is desirable throughout the load-carrying sections [41].

FCI is known to originate within persistent slip bands (PSBs), formed due to the build-up of mobile dislocations during irreversible cyclic slip [29,32]. This study aims to demonstrate that the key physical basis of the grain size effect in fatigue lies in the development of immobile geometrically necessary dislocations (GNDs) to accommodate curvature of the crystal lattice in response to plastic strain-gradients, which hinder the movement of mobile dislocations. Littlewood and Wilkinson [46] presented an electron back-scatter diffraction study on cyclically deformed Ti-6Al-4V in which lattice rotation was measured and used to iden-
Strain-Gradient Modelling of the Grain Size Effect

tify GND distributions via a cross-correlation technique. The study provided experimental evidence of high GND densities in regions of large strain gradients near grain boundaries and within grains. Finer-grain microstructures produce higher gradients of plastic strain and, thus, associated regions of increased GND densities. As a result, these regions experience increased cyclic hardening and, therefore, exhibit reduced plastic slip, improving fatigue performance. As described in Section 2.3.1 of the Background chapter, other size effects can equally influence the fatigue behaviour of metals, where size effects can be categorised [45] into strain-gradient effects, intrinsic size effects, statistical size effects and surface constraint size effects. CP modelling is a useful tool for modelling size effects. For example, Grogan et al. [123] investigated statistical size effects on the performance of stents via a CP approach and developed a series of equations ensuring safe stent design, including a relationship between grain size, strut length and maximum strain. Geers et al. [45] used CP modelling to investigate surface constraint effects, demonstrating that the behaviour of material at an interface or along a free surface can significantly affect the behaviour of a thin specimen.

Nye [217] and later Ashby [218] proposed the storage of GNDs as the mechanism by which strain gradients are accommodated in the crystal lattice. Fleck et al. [214] developed a strain gradient plasticity theory based on dislocation mechanisms, describing the storage of GNDs as a result of strain-gradients, and applied it to torsion of circular section wire. Macroscopic continuum models have since been developed to deal with the presence of strain gradient effects. For example, one study homogenised the behaviour of a weld steel material in finite element (FE) fatigue analyses by assigning strength to homogenisation units based on the empirical Hall-Petch relation and a statistical grain size distribution [219], to circumvent the explicit modelling of strain-gradients in different-sized grains. Taking this a step further, a crystal plasticity (CP) formulation, describing plastic slip on individual slip systems in the crystal lattice, has also been developed.
to include a Hall-Petch term with a threshold stress for fretting fatigue of Ti-6Al-4V [79, 80, 220]. However, more accurate and realistic predictive models require a more fundamental, physically-based approach, based on GND evaluation, to capture length scale and, hence grain (and other microstructure) size effects. Various strain-gradient CP formulations, including the work of Fleck et al. [214], have been developed [53, 55, 59, 60, 221, 222], via inclusion of hardening mechanisms based on the evolution of GND density. One such CP formulation has been used by Cheong et al. [60] to predict the grain size effect on monotonic stress-strain response for copper polycrystals. Ma et al. [55] applied a similar approach to predict the stress field during shearing of an aluminium single crystal, while Dunne and co-workers [59] successfully predicted the measured GND density field near a carbide particle in a nickel single crystal. However, evidence has yet to be presented on strain-gradient CP modelling of the experimentally observed grain size effect on fatigue behaviour.

A key objective of this study is the assessment of fatigue performance, via prediction of fatigue life. Available fatigue indicator parameters (FIPs) for FCI prediction have been discussed in the previous results chapters and in Section 2.4.2 of the Background chapter. It has been thoroughly established that microstructure-sensitive approaches are required for FCI prediction. Acknowledgement of the role of dislocation mechanisms in FCI can be seen in some existing approaches. Mura [88] proposed a model for FCI based on the stability of dislocation structures in a PSB, evaluated via an energy balance in a mathematical model for the evolution of dislocation structures. Sangid and co-workers [95–97] adopted a detailed physically-based energy balance approach for FCI in a slip band spanning a grain, including terms to account for applied stress-field, work hardening, formation of dislocation dipole structures, dislocation nucleation at grain boundaries, penetration of grain boundaries by dislocations, and interruption of lattice staking sequence in the matrix and precipitates. Strain-gradient CP modelling
inherently accounts for certain dislocation mechanisms, by virtue of the dislocation based CP constitutive equations. Microstructure-sensitive FIPs such as the effective crystallographic slip parameter presented by Manonukul and Dunne [83], can be coupled with strain-gradient CP modelling for the prediction of FCI. The effective plastic strain parameter, $p$, has been successfully used to predict numbers of cycles to FCI across both low and high cycle fatigue regimes, for various cyclic loading ratios and temperatures [83]. The applicability of this FIP has been further validated in Chapter 6, where strong correlation was demonstrated between distributions of the effective crystallographic slip FIP and experimentally observed crack initiation sites for ferritic steel notched specimens. The study also revealed a strong correlation between computationally predicted peaks of GND density and experimental FCI sites, suggesting that GND density itself could be employed as an FIP. The crystallographic work parameter $W$ is another FIP developed for use with CP models [86], which addresses the need for stress-strain criteria.

In this study, a physically-based strain-gradient CP methodology is developed and is shown to successfully predict the effect of grain size on both the cyclic stress-strain (hysteresis) and fatigue crack initiation behaviour of a biomedical grade CoCr alloy. LCF test data is presented for both fine-grain (as-received) and coarse-grain (heat-treated) test specimens of the material, to quantify the effect of grain size on cyclic stress-strain curves and initiation life. The strain-gradient constitutive formulation of [59] is modified through the inclusion of statistically-stored dislocation (accumulation and annihilation) evolution equations. The measured grain morphology statistics are implemented in unit cell FE models of the coarse- and fine-grain materials and combined with the constitutive model for comparison with the measured hysteresis and FCI behaviour, in relation to grain size and stress range effects.
7.3. Experiments

The material tested is the L605 CoCr alloy, trade-named HAYNES 25 alloy [177], for which data was also presented in Chapter 5. The material was received as a hot-rolled bar, solution-annealed at 1230°C, with chemical composition of 20 wt% chromium, 15 wt% tungsten, 10 wt% nickel, 3 wt% iron, 1.5 wt% manganese, 0.4 wt% silicon, 0.1 wt% carbon and the balance consisting of cobalt. The test programme for this study included (i) heat-treatment of the alloy to increase the grain size, (ii) microstructural characterisation via microscopy of the as-received and heat-treated material and (iii) mechanical testing of the two material conditions to measure the effect of microstructure on the fatigue behaviour. Some microscopy and mechanical testing of the as-received material were reported in Chapter 5, but are presented here also for comparison.

7.3.1. Heat-Treatment and Microscopy

Heat-treatment of the L605 material was employed to effect a sizeable increase in grain size. The initial iterative heat-treatment tests were based on solution annealing temperatures suggested for the L605 alloy [223]. Based on the observed changes in grain size, a final heat-treatment protocol was implemented; this corresponds to annealing at a 1250°C for 2.5 hours.

Optical microscopy was carried out for both as-received and heat-treated material, using an etching solution of 100 ml HCl and 5 ml 30% H₂O₂, to discern information on grain size and grain area distributions. Optical micrographs of the as-received and heat-treated material can be seen in Fig. 7.1(a); the average grain sizes were found to be 32 µm (as previously reported in Chapter 5) and 243 µm, respectively. Twin boundaries are visible in both microstructures, formed
7. Strain-Gradient Modelling of the Grain Size Effect during the annealing process. Microscopy images of both transverse and longitudinal cross-sections of the as-received and heat-treated bar portions revealed no discernible difference in grain structure and, thus, an equiaxed microstructure was inferred for the two conditions. Scanning electron microscopy (SEM) was used to investigate particles in the L605 matrix, including energy dispersive x-ray (EDX) spectroscopy for identification of particle composition, and crystallographic texture, via electron backscatter diffraction (EBSD), carried out at the Materials and Surface Science Institute in University of Limerick, for the two material conditions. As reported in Chapter 5, the as-received material contained precipitates with high tungsten and carbon content (relative to the L605 matrix) with a total area fraction of 0.52%. Microscopy of the heat-treated material yielded no signs of precipitates. This is in agreement with a previous study on L605 precipitates [181], which reported that almost no precipitates were visible after heat-treating at temperatures above 1200°C. EBSD orientation maps, provided in Fig. 7.1(b) for both the as-received and heat-treated material conditions, for views parallel and perpendicular to the central axis of the cylindrical CoCr bar, indicate the absence of crystallographic texture (i.e. random crystallographic orientations) for the two material conditions.

7.3.2. Mechanical Testing

As in Chapter 5, experimental LCF stress-strain hysteresis loops are needed for the calibration of the cyclic plasticity CP constants. The fatigue test program consisted of strain-controlled LCF tests on the as-received and heat-treated materials at strain ranges ±0.5% and ±1.0%. The specimen design followed ASTM standards [185] for strain-controlled fatigue; the test rig employed is an Instron 8500 servo hydraulic system with hydraulic grips and V-shaped jaws at a strain rate of 1.0% s⁻¹. The test was stopped in each case when a 30% drop in maximum
7. Strain-Gradient Modelling of the Grain Size Effect

Figure 7.1: (a) Optical micrographs of the as-received material and heat-treated material conditions and (b) EBSD orientation maps for the two material conditions along views both parallel and perpendicular to the central axis of the CoCr bar.

load was observed following stabilisation of initial cyclic hardening.

7.4. Computational Framework

This section describes the development of the FE model, including both strain-gradient CP constitutive formulation and microstructure geometry, used to simulate the LCF tests of Section 7.3 for the as-received and heat-treated materials.
7. Strain-Gradient Modelling of the Grain Size Effect

7.4.1. Crystal Plasticity Constitutive Model

The large deformation implementation for strain-gradient CP of Section 3.4.2 is adopted for this study. Further details on the implementation of the formulation to that provided in Chapter 3 can be found in Dunne et al. [59] and Kiwanuka [158]. The equations used in the formulation describe the movement of mobile dislocations, or dislocation glide, through the crystal lattice, with the application of stress. Hardening occurs due to the presence of immobile dislocations, including both statistically-stored dislocations (SSDs) and GNDs, which behave as obstacles in the path of mobile dislocations. The presence of GNDs introduces the strain-gradient effect into the model, as shown below. The schematic of Fig. 7.2 shows the mechanism proposed here to explain the role of the development of GNDs in causing a grain size effect on fatigue behaviour. This schematic is necessarily a simplistic 2D representation of a complex 3D crystallographic phenomena. An arbitrary grain in a polycrystal is hypothesised to experience a spatial gradient in plastic deformation due, for example, to the orientation and geometry of adjacent grains, as illustrated in Fig 7.2(a). In this case, the plastic deformation in the $x$-direction (signified by the $xx$ component of the plastic deformation gradient, $F_p$) at A is greater than at B, i.e. a gradient in $F_p^{xx}$ forms in the $y$-direction. A simplified view of the hypothesised deformed crystal lattice within this grain is provided in Fig. 7.2(b). Dislocations of a particular sign must be stored in order to accommodate the curvature in the lattice, consistent with the gradient in plastic deformation. Therefore, these dislocations are geometrically necessary (i.e. GNDs). While the lattice also experiences stretch and additional rotation under applied and/or residual stress, these forms of deformation are elastic. From Fig. 7.2(b), the density of GNDs is dependent on the length of the lattice, $L$, over which the gradient in plastic deformation exists, as the same number of GNDs are required for a given change in plastic deformation, regardless of the distance over which the change takes place. Two grains under
7. Strain-Gradient Modelling of the Grain Size Effect

Figure 7.2: Schematic of (a) development of spatial gradient of plastic strain in a grain due to the orientation of surrounding grains, (b) formation of a GND in the crystal lattice and (c) storage of different GND densities in grains of different size.

the same applied loading field, in an identical scaled microstructure morphology, will develop GND densities dependent on their respective grain sizes, $d_1$ and $d_2$, as shown in Fig. 7.2(c). The same number of GNDs must form along the $d_2$ dimension of the finer grain as along the $d_1$ dimension of the coarser grain. Hence, GND densities are higher in finer-grain materials, resulting in increased hardening, and thus, reduced cyclic plasticity.

The flow rule for the CP formulation, repeated here for clarity, is given by:

$$
\dot{\gamma}^\alpha = \rho_{SSD,m} b^2 \nu \exp \left( -\frac{\Delta H}{kT} \right) \sinh \left( \frac{(|\tau^\alpha| - \tau_c) \gamma_0 b^2}{kT} \right) \frac{1}{\sum_\alpha \left( \rho_{SSD,i}^\alpha + \rho_{GND}^\alpha \right) \sgn(\tau^\alpha)}
$$

(7.1)
where the L605 alloy has a face-centred cubic (fcc) crystal structure [180] and, thus, the twelve \{111\}⟨110⟩ slip systems are modelled. Cubic elastic constants, defined in Chapter 5, are used to construct the elastic stiffness matrix (Eq. 3.23) owing to the fcc structure of the L605 lattice. As the calculation of GND densities is dependent on spatial gradients of deformation (Eq. 3.69), the CP equations are implemented in a user-element subroutine (UEL) for a 20-noded, brick, reduced integration element, to provide access to the necessary element information, as outlined in Chapter 3.

The temperature, \( T \), is set at room temperature (293 K) for the CP simulations, while, similar to the previous chapter, the frequency, \( \nu \), is set at \( 1.0 \times 10^{11} \text{ s}^{-1} \), chosen to be two orders of magnitude smaller than the Debye frequency [212]. The mobile SSD density, \( \rho_{SSD,m} \), and the initial immobile SSD density, \( \rho_{SSD,i0} \), are both taken to be \( 5 \times 10^{10} \text{ m}^{-2} \), based on the data presented in [214]. The critical resolved shear stress, \( \tau_c \), calculated by dividing the yield stress of the material (reported in Chapter 5) by the Taylor factor for an fcc crystal, is taken as 173.5 MPa. The reference strain is taken as a constant at 0.001. The constant, \( c \), used in Eq. 3.70, is set at 0.01, within the range suggested by Ohashi et al. [224], while the critical annihilation distance, \( y_c \), is taken to be \( 2. \times 10^{-9} \text{ m} \), similar to that reported by Essmann and Mughrabi [225]. The Helmholtz free energy, \( \Delta H \), is identified via comparison of the cyclic micromechanical FE analyses with experiments. For simulation of tests at room temperature, as in this study, thermal activation is unlikely to be important, so that in fact the rate-sensitivity (relating to \( \Delta H \)) in the model is negligibly small.

As stated in the introduction, a key aspect of the present work is the prediction of numbers of cycles to crack initiation, \( N_i \), and the effect of grain size on this. Microstructure-sensitive FIPs are implemented for this purpose in the UEL, based on variables in the CP formulation. The importance of scale compatibility between constitutive model and FIP based-predictive methods for CP modelling...
has been discussed in Chapters 4 and 5. Manomukul and Dunne’s [83] effective crystallographic slip parameter, \( p \), (Eq. 4.1) is used again here. \( p \) has been related to the formation of PSBs in fatigue [29]. This FIP has been used to predict experimentally-observed locations of FCI in Chapter 6, while in the present study an attempt is made to correlate this parameter with crack initiation life within the context of a physically-based length scale dependent CP constitutive framework. The crystallographic work parameter of Korsunsky et al. [86], \( W \), (Eq. 4.2) is also investigated here. This energy-based parameter takes into account different aspects of work carried out at a crystallographic level, defined by the terms of Eq. 7.1. This includes plastic work done by the applied stress field, due to \( \tau^\alpha \), work hardening with increase in density of GNDs and immobile SSDs, and activation energy for unpinning of mobile dislocations. Both components of the crystallographic work parameter are affected by GND density; slip rate is directly influenced in accordance with Eq. 7.1, decreasing with increasing GND density due to increased microstructural barriers to slip, and slip system shear stress increases with GND density as increased energy is required to overcome barriers. Calculation of \( p \) and \( W \) are defined in Eqs. 4.1 and 4.2 of Chapter 4, respectively. In the present work, as for previous studies in Chapters 4 and 5, crack initiation is considered to correspond to critical values of the FIPs, \( p_{crit} \) and \( W_{crit} \), being reached. Cyclic values of the FIPs (i.e. accumulated over a single stabilised cycle) are used to assess when these critical values are reached, i.e. \( N_i = \frac{W_{crit}}{W_{cyc}} \) (similar for \( p \)).

7.4.2. Finite Element Microstructure Geometry

Microscopy data acquired in Section 7.3 was used for the generation of realistic polycrystal models for the micromechanical FE analyses. Recalling from Chapter 5, approximation of 2D and 3D grains as a hexagon and rhombic-
dodecahedron, respectively, facilitates the conversion from experimental grain area distributions to grain volume distributions, where a common dimension \( d \), shown in Fig. 7.3 (a), is used to convert between the grain area and volume. The FE model developed in Chapter 5 for the as-received L605 material, including precipitate representation, is used again here. This model was then scaled to obtain the heat-treated microstructure geometry according to average grain volumes of the two material conditions, i.e. \( \frac{(V_p)_{\text{coarse}}}{(V_p)_{\text{fine}}} = \frac{(V_g)_{\text{coarse}}}{(V_g)_{\text{fine}}} \), where \( V_p \) and \( V_g \)
represent FE polycrystal and average grain volumes, respectively. Comparison of the experimental and sample FE model grain volume distributions can be seen in Figs. 7.3(b) and (c) for the as-received and heat-treated materials, respectively. The FE geometry for the as-received material can be seen in Fig. 7.3(d), along with the seven-element unit with a precipitate at its centre, which slots into the space of a regular element in the mesh. The precipitates are assumed to be tungsten carbides, based on the EDX observations, and are accordingly assigned a high Young’s modulus of 714 GPa [192]. SEM did not reveal precipitates in the heat-treated material and, thus precipitates are excluded for the heat-treated material geometry. Twin boundaries have not been included in the polycrystal FE geometries for this study.

Each FE polycrystal comprised 28 crystallographic grains. The mesh for the heat-treated condition consisted of 3375 (15$^3$) 20-noded brick elements with polycrystal dimensions of (866µm)$^3$. Replacement of normal elements with the seven-element unit for the as-received condition resulted in a mesh composed of 3723 elements (see Fig. 7.3(d)), with polycrystal dimensions of (120µm)$^3$. The final mesh used here employs an average of 120 elements per grain; results from a strain-gradient CP mesh sensitivity study by Cheong et al. [60] indicated that macroscopic polycrystal response showed little sensitivity to mesh refinement above 8 elements per grain for grain sizes greater than 30 µm. Also, a mesh sensitivity study for the polycrystal morphology of Fig. 7.3 (d) for the strain-gradient CP formulation used here, described in Appendix A.2, demonstrates a reasonably converged solution for the mesh density used, both in terms of macroscopic stress-strain response and FIP prediction. Periodic displacement boundary conditions were applied to the polycrystal to simulate macroscopic behaviour. Due to the prohibitively large computational expense associated with cyclic 3D strain-gradient CP FE analyses, a definitive representative volume element (RVE) has not been used here. However, it has been shown [187] that periodic displacement boundary
conditions applied to a volume element smaller than an RVE provide a response between the upper and lower limits of the macroscopic response of that material.

The polycrystal FE analyses used the strain-gradient CP constitutive model to simulate LCF loading of the as-received and heat-treated materials at the two experimental strain ranges of ±0.5% and ±1.0%, until stabilisation of the cyclic stress-strain response. In order to predict microstructure-induced results, three realisations of random crystallographic orientation distributions, as represented by the inverse pole figures of Fig. 7.3(e), are presented for each strain range and material condition. Assignment of random orientations corresponds to a lack of crystallographic texture, corroborated by the EBSD maps of Fig. 7.1(b).

7.5. Results

7.5.1. LCF Testing

The fine grain (as-received) material was found to exhibit superior fatigue behaviour for both applied LCF strain ranges. The stress range history of the two materials can be seen in Fig. 7.4, where cyclic stress amplitudes ($\Delta\sigma/2$) of the fine grain material are approximately 100 MPa greater than that of the coarse grain (heat-treated) material across both applied strain ranges.

The measured total and plastic strain-life data is shown in Figs. 7.5 (a) and (b), respectively, including additional results from the previous study on the L605 alloy for the as-received material at applied strain ranges of ±0.8% and ±1.2%. A Coffin-Manson fit for the as-received material is also provided in Fig. 7.5(b). The total strain data of Fig. 7.5(a) shows that the coarse grain (heat-treated) material exhibits lower fatigue life. However the fine and coarse
7. Strain-Gradient Modelling of the Grain Size Effect

Figure 7.4: Experimental stress range histories for LCF tests.

\[ \frac{\Delta \sigma}{2} \text{(MPa)} \]
\[ \text{Cycles} \]

Figure 7.5: (a) Total strain-life data, and (b) plastic strain-life data for the LCF tests, with fitted Coffin-Manson curve. Plastic strain range, \( \Delta \varepsilon_p \), is calculated as a function of total strain range \( \Delta \varepsilon \), stress range, \( \Delta \sigma \), and Young’s modulus, \( E \): \( \Delta \varepsilon_p = \Delta \varepsilon - \Delta \sigma / E \).

Grain material data points appear to fall on the same Coffin-Manson curve. This demonstrates increased hardness and reduced cyclic plasticity of the fine grain material condition, and suggests that the material exhibits the same relationship between plastic strain and fatigue life for the two grain sizes.

7.5.2. Micromechanical Simulations

The polycrystal FE simulations are used to identify the Helmholtz free energy, \( \Delta H \), for the strain-gradient CP constitutive model, via comparison of the pre-
dicted and measured responses, for the as-received material, using a least squares objective function. All other material parameters are based on physical considerations, as described in Section 7.4. The complete set of constitutive constants used in the strain-gradient CP formulation is provided in Table 7.1.

GND density distributions from the CP LCF simulations are presented for a sample microstructure realisation in Fig. 7.6, for both grain sizes, for the two strain ranges. Clearly, significantly higher $\rho_{GND}$ values are predicted for the fine grain cases. The average $\rho_{GND}$ distribution is an order of magnitude higher for the fine grain material. A comparison of the predicted and experimental stabilised stress-strain hysteresis loops for one microstructure realisation (one random crystallographic orientation set) is shown in Fig. 7.7; excellent agreement is achieved generally. Cyclic stress range data for experiments and simulations is compared in Fig. 7.8, including results for all three microstructure realisations. Significantly lower stress ranges are clearly predicted for the coarse grain material.

The measured evolution of cyclic maximum stress response is used here to compute the evolution of fatigue damage and, hence, identify the experimental num-

---

**Table 7.1:** Strain-gradient CP constants.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$</td>
<td>$1.381 \times 10^{-23}$ JK$^{-1}$</td>
</tr>
<tr>
<td>$T$</td>
<td>293 K</td>
</tr>
<tr>
<td>$b$</td>
<td>$2.56 \times 10^{-10}$ m</td>
</tr>
<tr>
<td>$\nu$</td>
<td>$1.0 \times 10^{11}$ s$^{-1}$</td>
</tr>
<tr>
<td>$\rho_{SSD,m}$</td>
<td>$5 \times 10^{10}$ m$^2$</td>
</tr>
<tr>
<td>$\rho_{SSD,i\alpha}$</td>
<td>$5 \times 10^{10}$ m$^2$</td>
</tr>
<tr>
<td>$\tau_c$</td>
<td>173.5 MPa</td>
</tr>
<tr>
<td>$\gamma_0$</td>
<td>$1.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>$y_c$</td>
<td>$2 \times 10^{-9}$ m</td>
</tr>
<tr>
<td>$c$</td>
<td>0.01</td>
</tr>
<tr>
<td>$\Delta H$</td>
<td>$2.85 \times 10^{-20}$ J</td>
</tr>
</tbody>
</table>
7. Strain-Gradient Modelling of the Grain Size Effect

Figure 7.6: Distributions of GND density, $\rho_{GND}$, in a cut-away view of the model for one microstructure realization, with crystallographic structure shown at the bottom left for the as-received model.

The number of cycles to FCI, $N_i$. $N_i$ is considered to occur at a critical damage $D_c$. A high probability exists of FCI occurring at the free surface for the LCF regime [28,58]. Therefore, as in Chapter 5, $D_c$ is selected based on the ratio of cross-sectional area of the specimen compromised by initiation of a crack with depth equal to the standard element size (from the FE polycrystal models) in each repeated unit at the free surface of the fatigue specimen. This leads to a value for $D_c$ of 0.0125. Experimental damage curves are thus computed for each test, as shown in Fig. 7.9, using the relation $D = 1 - \frac{\sigma}{\sigma_{max}}$, based on the effective stress damage concept [226], where $\sigma$ is the cyclic maximum stress and $\sigma_{max}$ is the maximum value of $\sigma$ for each test. The critical values of the FIPs, $W_{crit}$ and $p_{crit}$, are calibrated against $N_i$ for the fine grain material at the ±1.0% strain range, where $W_{crit} = W_{cyc}N_i$ (similar for $p_{crit}$). Maximum cyclic values of the microstructure-sensitive FIPs, $W_{cyc}$ and $p_{cyc}$, are extracted from the microme-
Figure 7.7: Comparison of experimental and simulated stabilised hysteresis loops for one simulated microstructure realization.

Mechanical LCF simulations. The resulting identified values for $W_{\text{crit}}$ and $p_{\text{crit}}$ are $9.19 \times 10^4$ MJ m$^{-3}$ and 164.3, respectively. Predictions of $N_i$ for the other grain size-strain range combinations using these critical values, along with the calibrated case, are shown in Fig. 7.10. $W$ and $p$ both clearly capture the decrease in $N_i$ for the coarse-grain material (red symbols) for a given applied total strain range. $W$ predicts significantly more accurately than $p$ for all validation cases.
7. Strain-Gradient Modelling of the Grain Size Effect

Figure 7.8: Comparison of experimental cyclic stress-strain curves with FE simulations for three microstructure realizations. Filled symbols indicate experimental data, while open symbols mark micromechanical simulations.

Figure 7.9: Experimental damage accumulation curves for the LCF tests.

7.6. Discussion

The as-received, fine-grain material exhibits superior fatigue performance than the heat-treated material. The coarse-grain, heat-treated material exhibits lower stress ranges and shorter lives for a given applied strain range, as seen in Figs. 7.4 and 7.5(a), respectively. Interestingly, data points for the coarse- and fine-grain materials essentially lie on the same Coffin-Manson line, as shown in Fig. 7.5(b).
It can be postulated that this is due to the increased hardening and thus reduced cyclic plasticity, experienced by the fine-grain material due to the presence of GNDs. In contrast with this, Morrison and Moosbrugger [3] reported differing Coffin-Manson curves for fine and coarse grain nickel (with similar grain sizes to those used here). However, data points reported in the LCF region investigated here showed little difference in Coffin-Manson trend. The work of Morrison and Moosbrugger suggests that with further testing towards the HCF regime the Coffin-Manson curves of the fine and coarse grain materials will begin to diverge.

The cyclic hysteresis loops of Fig. 7.7 clearly show the ability of the strain-gradient micromechanical framework to capture the grain size effect in fatigue. A decrease in stress range is seen with increase in grain size in Figs. 7.7 and 7.8. The increased hardening of the fine grain material can be explained by the increased build-up of GNDs. The differences in GND densities of Fig. 7.6, due to grain size, corroborates the mechanism of GND formation due to spatial strain gradients proposed in Fig. 7.2. The authors are not aware of any published measurements of GND density for the present material, particularly after cyclic loading; however, Littlewood and Wilkinson [46] have measured GND densities.
in Ti-6Al-4V following cyclic loading, and showed that the range was between $10^{10}$ and $10^{16} \text{ m}^{-2}$. The predicted values of Fig 7.6. lie within this range. The influence of hardening due to GNDs on fatigue behaviour is dependent on the relative densities of GNDs and immobile SSDs, as given by Eq. 3.66. For the coarse grain simulations, the ratio of GND to immobile SSD average densities ranges from 0.35 to 1; for the fine grain simulations, the range is from 2.5 to 4.1. This indicates that while a further decrease in grain size will result in a greater influence of GNDs, as expected, on the other hand, an increase in grain size will result in negligible further deterioration in fatigue performance. This is due to GND densities dropping further below immobile SSD densities and, thus, becoming negligible. To corroborate this, analyses have been carried out using one microstructure realization at the ±5% strain range for two additional grain sizes. The macroscopic hysteresis loops and $N_i$ predictions for all four grain sizes are compared in Figs. 7.11 (a) and (b), respectively. While a decrease in grain size below that of the as-received material clearly induces increased hardening in hysteresis loops and an increase in predicted $N_i$, the trends of Figs. 7.11 (a) and (b) indicate that coarsening of the grain size beyond that of the heat-treated material will have little influence on either hysteresis loops or predicted $N_i$. This is consistent with the findings of Fleck et al. [214], who showed that strain-gradient effects are most influential in polycrystals for grain sizes of below 20 µm.

Although both microstructure-sensitive FIPs successfully predict the trend of fatigue performance for the two material conditions (Fig. 7.10), i.e. higher $N_i$ for the fine grain material, the crystallographic work parameter, $W$, is significantly more accurate. This is corroborated by the approach of Sangid and co-workers [95–97], which predicts crack initiation in a PSB spanning a grain based on minimisation of a summation of energy terms, describing work carried out in the formation of the slip band and extrusions at the intersection with
the grain boundary. The $W$ parameter used in this work does not operate on the assumption of a PSB spanning a grain, but predicts FCI at the point of maximum crystallographic work. However, courtesy of the slip rule in Eq. 3.66, it incorporates components of energy similar to terms used in the approach of Sangid and co-workers, such as the applied stress field, work hardening due to immobile dislocation build-up and unpinning of immobile dislocations for glide. Other energetic mechanisms are omitted by the FIP, including dislocation activity explicitly at the grain boundary (i.e. dislocation nucleation and formation of extrusions) and the interruption of lattice stacking sequence by mobile dislocations during slip. The Sangid model is a more detailed one, including atomistic simulations for quantifying grain boundary energy terms, based on the analysis of a single slip band in each grain. It is expected that some of the additional terms may have less influence in the CP approach used here, where the highly organised dislocation dipole structures of a PSB and the PSB-grain boundary interface are not explicitly modelled.

While it may be postulated that the data of Fig. 7.5(b) indicates that the Coffin-Manson relation can predict total fatigue life for a material across multiple grain sizes, it is important to note that a Coffin-Manson life prediction (for non-laboratory conditions) is dependent on the predicted cyclic plastic strain.
range and, thus, the constitutive model. The strain-gradient model presented here can clearly be used effectively for multiple grain sizes in conjunction with the Coffin-Manson relation. However, use of this approach with a definitive RVE polycrystal would not produce scatter in life predictions, as this is a bulk material prediction. In contrast, microstructure-sensitive FIPs offer the benefit of capturing localised effects, where FCI is predicted to occur at peaks in FIP distributions, present due to microstructural inhomogeneity. Hence, the combination of microstructure-sensitive constitutive model and microstructure-sensitive FIPs facilitates capture of scatter in life predictions and provides a statistical basis for fatigue design.

It can be seen from the as-received models in Fig. 7.6 that peaks in $\rho_{GND}$ distributions often occur near precipitates. To investigate the effect of precipitates on fatigue performance, a polycrystal model for one microstructure realisation of the as-received material without precipitates was analysed for the two strain ranges. The results indicate that precipitates have a negligible effect on macroscopic hysteresis behaviour of the as-received material. Changes in predictions of $N_i$ upon removal of precipitates for the two FIPs and the two strain ranges are provided in Table 7.2. For $p_{cyc}$, the predicted effect of precipitate removal on $N_i$ is small, less than 3%, and does not show a consistent increase or decrease. $N_i$ is predicted to increase for both strain ranges using $W_{cyc}$, with a maximum increase of nearly 13% predicted. The higher $N_i$ values lie within the range (scatter-band) of predictions for the three microstructural realisations of the as-received model with precipitates. Nonetheless, as $W_{cyc}$ predictions were found to give better correlation with the measured data in Fig. 7.10, results from these additional simulations predict a bigger difference between fatigue performance of the as-received and heat-treated conditions (recall that the heat-treated case is assumed to not have precipitates) and, thus, an even larger effect of grain size on FCI life.
Table 7.2: Percentage change in $N_i$ predictions for one microstructure realisation of the fine grain model, upon removal of precipitates.

<table>
<thead>
<tr>
<th>$N_i$ using $W_{cyc}$</th>
<th>$N_i$ using $p_{cyc}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta \varepsilon = \pm0.5%$</td>
<td>$\Delta \varepsilon = \pm0.5%$</td>
</tr>
<tr>
<td>+3.56%</td>
<td>-2.05%</td>
</tr>
<tr>
<td>$\Delta \varepsilon = \pm1.0%$</td>
<td>$\Delta \varepsilon = \pm1.0%$</td>
</tr>
<tr>
<td>+12.89%</td>
<td>+1.26%</td>
</tr>
</tbody>
</table>

This work does not address all types of size effects in fatigue, e.g. some mechanisms relating to intrinsic size effects. For example, a size effect due to build-up of dislocations at grain boundaries is not captured. For the bulk material behaviour presented here, statistical size effects and surface constraint effects are not considered to be important. However, such effects may become important for micro-scale applications. Twin boundaries observed in both the as-received and heat-treated microstructures have not been modelled in this study. Simulations of polycrystals with a high frequency of twin boundaries by Sangid and co-workers [95,97], using the energy balance approach for FCI in PSBs, provided strong evidence of FCI occurring in grains with twin boundaries. More recent work presented CP FE simulations investigating the effect of twin boundaries on predicted FIP values [82]. While this work showed that inclusion of twin boundaries in polycrystal simulations results in an increase in frequency of high FIP values in the vicinity of twin boundaries, the range of maximum FIP values observed appeared largely unaffected. Therefore, while it is anticipated that the inclusion of twin boundaries would generally act to reduce predicted crack initiation lives, it is expected that changes in $N_i$ predictions would be small and predictions for both grain sizes would be equally affected without a change in trend of fatigue behaviour. Alternate candidate constitutive models exist in the literature which could improve hysteresis loop shapes, such as physically-based kinematic hardening formulations, e.g. see [159,221,227]. Also, while the mesh used in this work is sufficiently refined to capture the macroscopic behaviour of a polycrystal [60], further mesh refinement would undoubtedly affect local FCI predictions. However, the purpose of this study was to demonstrate the key role
of strain-gradients and GNDs in explaining the grain size effect on fatigue.

The micromechanical framework presented here is directly relevant to analysis of micro-scale devices, where fatigue performance is highly microstructure-dependent, for the assessment and design of device geometry and microstructure. Micromechanics has been used to generate a set of design curves for deployment of cardiovascular stents [123], for example. The present framework can facilitate development of a similar set of design rules for the fatigue of stents, as a function of grain size, crystallographic texture, precipitates, geometry etc.

### 7.7. Conclusions

A strain-gradient crystal plasticity methodology has been developed to predict the experimentally-observed effect of grain size on cyclic hysteresis response and fatigue crack initiation life for a CoCr alloy, thus demonstrating the key role played by geometrically necessary dislocations. Computational simulations of experimental LCF tests indicate that, for the CoCr alloy tested, precipitates have negligible effect on hysteresis behaviour and, while, they appear to have an effect on fatigue damage accumulation, leading to crack initiation, it is relatively minor compared to the influence of grain size. A crystallographic work-based parameter was found to be most effective in predicting fatigue crack initiation; this is attributed to the dependence of persistent slip band formation on the dissipation of energy via dislocation activity. The framework presented is applicable to microstructure-sensitive fatigue design of devices and materials. In the context of Chapters 4 and 5, for example, the strain-gradient framework could be used to identify suitable microstructures for a given stent geometry. However, in order to justify application of the micromechanical framework to stent fatigue design, validation of the framework must be extended into the HCF regime; this will be
the focus of the next chapter.
8. High Cycle Fatigue of Micro-Scale Specimens

8.1. Chapter Summary

A study on micromechanical modelling of high cycle fatigue (HCF) tests of L605 CoCr foil micro-specimens is presented in this chapter, providing validation for the application of the micromechanical framework, developed in this body of work, to the assessment of stent fatigue. Manufacture of the foil specimens, including both laser-cutting and electro-polishing is described, along with the development of FE polycrystal models of the foil fatigue specimens, based on microscopy carried out on the L605 CoCr foil. The power-law and strain-gradient crystal plasticity models used in the work of this thesis are both coupled with the generated microstructure morphologies to predict fatigue crack initiation (FCI) under the HCF conditions applied experimentally and predictions are compared with foil stress-life data.
8. High Cycle Fatigue of Micro-Scale Specimens

8.2. Introduction

The issue of premature fracture of stents has come to the fore in recent times due to the evolution of drug-eluting stents e.g. [15,16,18]. Slip bands reported by Halwani et al. [18] at sites of stent fracture support the case for HCF as the probable fracture mechanism. For micro-scale devices, for which dimensions are comparable in size to microstructural features, such as stents, fatigue life is composed only of number of cycles to FCI and microstructurally small crack growth, as specimen cross-section is compromised before later stages of crack growth can occur. Therefore, the dependency of fatigue performance on microstructural attributes is increased for such devices. It follows that microstructure-based approaches, such as the framework developed in this body of work, are needed to truly assess stent fatigue performance. Some studies have attempted to address this need, including the work of Marrey et al. [26] in which an El Haddad type approach, accounting for crack sizes which are below a microstructural threshold, was applied to fracture mechanics calculations for a CoCr alloy stent, facilitating prediction of the minimum size of an initial flaw in a stent strut which could cause failure. Another example is the work of Barrera et al. [134] in which the Dang Van criterion was adopted for prediction of fatigue performance of a 316L SS stent, using shear and hydrostatic stresses evaluated at the mesoscopic level. While these approaches are shown in the respective studies to be useful tools, experimental validation of the methodologies has not been carried out. Patient-specific modelling, such as presented by Schievano et al. [126], can offer a means of validation via direct comparison between models and deformed stents, extracted from real patient vessel geometries. However, the procurement of the required data is difficult and this approach may be less applicable to the initial stages of stent fatigue design, prior to approval for in vivo operation by the relevant regulating organisation. Representative testing can be used for experimental validation of models
8. High Cycle Fatigue of Micro-Scale Specimens

at the design stage. Wiersma et al. [132, 133] applied the theory of critical distances to prediction of the HCF behaviour of 316L stent material and validated predictions via comparison against HCF tests on micro-specimens with features representative of stents. Pelton et al. [137] demonstrated that a subcomponent micro-specimen exhibited similar fatigue behaviour to a full stent, effectively endorsing the concept of a representative test as a simplified experiment against which predictive models can be calibrated and/or validated.

As emphasised previously in the thesis, prediction of HCF behaviour requires the use of microstructure-sensitive methods. Microstructure-sensitive fatigue indicator parameters (FIPs) coupled with CP modelling represents one such approach. Studies by Przybyla and McDowell [57, 58] used such an approach to investigate the influence of different attributes on the development of extreme values of FIPs, considered to be drivers of FCI, in HCF. These studies used large numbers of statistical volume elements (SVEs) to develop reliable probability functions for different microstructural attributes, where SVEs are large enough such that an FIP at a point is unaffected by variations in the microstructure at a distance equal to the size of the SVE, but differ from RVEs in that the macroscopic response of SVEs may vary. The work of Chapter 6 demonstrated the use of a CP-based microstructure model, coupled with the effective plastic strain FIP, $p$, for prediction of FCI locations in HCF of ferritic steel, four-point bending specimens. This study did not, however, investigate the ability of the framework to predict number of cycles to FCI. Manonukul and Dunne [83] postulated that the critical value of the effective plastic strain FIP, at which FCI is predicted to occur, is a material constant and have consolidated this concept via prediction of fatigue behaviour for a range of loading conditions, across both low cycle fatigue (LCF) and HCF regimes, including mean stress effects, for a nickel-base alloy.

The study presented here adopts the concept of representative testing for validation of the micromechanical framework developed and applied throughout this
thesis. L605 foil micro-specimens are manufactured and tested under HCF loading conditions, and microscopy is carried out on the foil to aid in generation of realistic cross-section polycrystalline models for the foil specimens. Both the power-law and strain-gradient CP formulations, calibrated against L605 LCF data in Chapters 5 and 7, respectively, are investigated. The effective plastic strain and crystallographic work parameters are used here for the prediction of $N_i$ for HCF behaviour, based on critical FIP values calibrated for LCF behaviour, and predictions are compared with the experimental stress-life data.

8.3. Experiments

The experimental test program for the L605 CoCr alloy foil will be discussed in this section, including microstructural characterisation of the foil and preparation and testing of foil fatigue specimens. The L605 foil used in the study was supplied in $100 \times 100$ mm sheets with thickness of 265 to 270 $\mu$m by Goodfellow Cambridge Limited, with chemical composition of 50 wt% cobalt, 20 wt% chromium, 15 wt% tungsten, 10 wt% nickel, 3 wt% iron and 2 wt% manganese.

8.3.1. Microscopy

Microstructural characterization of the foil was carried out both to determine if heat-treatment is required, to remove any strong texture developed during foil manufacture, and, of course, to aid in FE model development. The existence of texture in the foil would have an effect on mechanical performance. Optical microscopy is first carried out to determine the grain structure in the foil. An etching solution of 100 ml HCl and 5 ml 30% $\text{H}_2\text{O}_2$ is used, as described for the macro-scale CoCr material in Chapters 5 and 7. Optical micrographs of the
foil are shown in Fig. 8.1 (a), where three directions, corresponding to the flat surface and two perpendicular edges, are investigated. A Matlab program was written to extract grain area statistics from the micrographs. As seen from the micrographs of Fig. 8.1 (a) and the grain area distributions of Fig. 8.1 (b), a similar grain morphology is observed for all three directions. Applying a hexagon-based conversion, as in the previous chapters, to each grain measurement, a grain size of 38 $\mu$m is identified for the foil. Additionally, twin boundaries can be observed in the micrographs, indicating that this material was annealed after manufacture.

Scanning electron microscopy (SEM) is employed both for investigation of crystallographic texture and characterization of particles in the microstructure. The electron backscatter diffraction (EBSD) technique is coupled with SEM (carried out at the Materials and Surface Science Institute at the University of Limerick),
Figure 8.2: (a) EBSD orientation maps for the three direction of the L605 foil and (b) SEM image of the L605 microstructure showing precipitates.

to produce the EBSD crystallographic orientation maps, shown in Fig. 8.2 (a), for the three directions of Fig. 8.1. A lack of crystallographic texture is observed, again suggesting that heat treatment has been applied to the foil after manufacture. SEM is also used to identify precipitates in the microstructure, as shown in Fig. 8.2 (b), where energy dispersive x-ray (EDX) analysis is employed to confirm a tungsten rich composition, as for precipitates observed in the as-received L605 bar of Chapter 5. A Matlab program was again written to extract statistics for precipitate area and frequency from micrographs, indicating an average precipitate area of \(1.51 \, \mu m^2\) and area fraction of 0.34%.

8.3.2. Specimen Preparation

Micro-scale foil specimens are manufactured to allow size-consistent testing for comparison with predictions from the micromechanical framework. Microscopy results from the previous section demonstrate the lack of morphological or crystallographic texture in the foil, thus eliminating concerns over directionality in the material itself. Specimen manufacture includes both laser-cutting and electro-polishing (EP). Dimensions for the laser-cut specimen are given in Fig. 8.3 (a)
and (b), where consideration of laser beam spot size and material removal in EP is taken into account. The specimen design, based on the work of Donnelly [228], has a dogbone-type gauge region, with uniform gauge length and tapers at each end to a larger cross-section. A second taper is then used to transition to the gripped cross-section. Support struts are included to allow ease of handling and structural integrity before testing. A laser-cut specimen is shown in Fig. 8.3 (c), in which the support struts are labelled. The laser-cutting was carried out at the National Centre for Laser Applications (NCLA) in NUI Galway on a Trumpf TruMicro 5050 picosecond laser with fundamental wavelength of 1030 nm. 2100 passes at a rate of 0.5 m/s were completed for each specimen using a final wavelength of 343 nm and beam power, repetition rate and pulse energy of 5.6 – 5.7 W, 200 Hz and 120 µJ, respectively. A total of eighteen final specimens were laser-cut.

Electro-polishing (EP) is required to remove the heat-affected zone created during laser-cutting and roughened surfaces from cutting and handling. A number of studies have looked at the electro-polishing of L605 for stent applications, reporting use of various EP solutions, including a hydrofluoric and nitric acid solution [183], phosphoric acid of different concentrations [229], a perchloric and acetic acid solution [230] and a sulfuric and phosphoric acid solution [231]. Various optimal temperatures, EP times and current-voltage settings have also been reported. Three studies report temperatures around 55 °C [183, 230, 231], while another reports more uniform EP rates at 0 °C [229]. An EP approach based on the work of Kaufmann et al. [231] is adopted here. Specimens are first cleaned ultrasonically after laser-cutting, allowing the removal of slag generated during cutting. EP is then applied to each specimen, after which it is rinsed with alcohol and then cleaned ultrasonically in deionised water. The EP solution is comprised of 45% sulfuric acid, 50% phosphoric acid and 5% water. A schematic of the EP setup is provided in Fig. 8.4, where the specimen and a piece of
stainless steel are connected to the anode and cathode of a 1.5 - 10 V/10 A power supply, respectively, and agitation is provided via a magnetic stirrer. EP tests were initially carried out at 55 °C with a current of 1-1.5 A cm⁻², as prescribed in [231]. However, an uncontrolled EP process was observed at these settings with non-uniform material removal resulting in pitting. Therefore, the temperature and current were reduced until a relatively controlled EP process was observed. Final temperature and current settings of 25 °C and 0.66 A cm⁻², respectively, were used, while it was found that an EP time of 10 minutes was required to remove visible surface marring from the laser-cutting process. Optical micrographs of the gauge region of a specimen before and after EP are shown in Fig. 8.5, where a reduction in dimensions and improved surface quality is observed post-EP. After cleaning, gauge cross-section dimensions are measured.
using an optical microscope for each specimen. Average measurements for twelve specimens are provided in Table 8.1; all other specimens were damaged either during the EP process or later in HCF test set-up. For all specimens successfully electro-polished, average flat and edge dimensions of 176 and 208 µm, respectively, were recorded. The ranges in measurements for individual specimen flat and edge dimensions were 18.9 and 14.7 µm, respectively.
8.3.3. HCF Testing

HCF testing is carried out for the polished specimens on the Bose Corporation EnduraTEC® ElectroForce® 3200 Series fatigue tester. Due to the macroscopically elastic nature of HCF, tests are typically load-controlled; strains are small and, thus, the HCF behaviour is considered to be a function of the applied stress history. Load-controlled tests were carried out at a cyclic nominal stress ratio of $R_\sigma = \sigma_{\min}/\sigma_{\max} = 0.1$ for three stress ranges corresponding to maximum stresses of 600, 650 and 700 MPa, where the stress levels were chosen, based on L605 HCF data in [26], forecasted to give a range of lives below $10^7$ cycles. A higher $R_\sigma$ value (up to 0.9) would be more representative of loading conditions for critical points in the L605 micromechanical stent simulations of Chapter 5. However, the low stress ranges which correspond to high $R_\sigma$ values present is-
sues in feedback control for the fragile foil specimens. A cyclic stress ratio of 0.1 is still representative of the loading experienced by many medium risk material points for the simulations of Chapter 5. A full test protocol for HCF tests and sample test parameter sheet is provided in Appendix A.3. Tests include a ramp to maximum load, followed by sinusoidal cyclic loading at 1, 20 and, finally, 50 Hz, where the lower initial frequencies are applied to overcome transient feedback control effects. An upper limit or run-out life of $10^7$ cycles was selected for these tests, to facilitate the completion of the full test programme. As mentioned in the previous section, twelve specimens were successfully tested, comprising four at each stress range, where the loading applied was specific to each specimen, based on the measured gauge cross-section dimensions (i.e. load set to achieve correct stress using specimen specific dimensions of Table 8.1).

8.4. Computational Framework

8.4.1. Polycrystal Generation

FE polycrystal geometries are generated for simulation of the foil fatigue testing via the approach presented in Chapters 5 and 7. In contrast with previous work, the full specimen cross-section is modelled in this study, facilitated by the micro-dimensions involved, using the average cross-section dimensions reported in the previous section and a dimension of 200 µm in the loading direction, as shown in Fig. 8.6. Abaqus is used to generate a voxel mesh and the Matlab program previously developed in Chapter 5 was employed to superimpose 3D Voronoi tessellations on the mesh and, thus, to identify element sets corresponding to grains. A grain volume distribution is generated from the measured grain area statistics of the foil material, based on the approximation of 2D and 3D grains as
Hexagons and rhombic-dodecahedrons, respectively, with a common dimension $d$, as illustrated in Fig. 5.9. Five polycrystal morphologies corresponding to grain volume distributions resembling that of the foil were identified, shown in Fig. 8.6 (labelled as realizations 1 to 5, respectively).

The seven-element unit introduced in Chapter 5 is used again here to represent precipitates in the microstructure. The approximation of the precipitate shape as a circle in 2D and a sphere in 3D allows conversion of area data to volume data. An average precipitate volume is, thus, identified and used to determine dimensions of the precipitate element at the centre of the seven-element unit. A sufficient number of normal elements are then replaced by the unit to achieve the experimentally-measured particle volume fraction. Each polycrystal model contains 19634 reduced-integration, 20-noded, brick elements, corresponding to the same (converged) mesh density used for the 3D polycrystal model of Chapter 5.
8. High Cycle Fatigue of Micro-Scale Specimens

Figure 8.7: Schematic of boundary conditions applied to the FE model, including two surfaces to which periodic boundary conditions (BCs) are applied, to simulate periodicity along the gauge length, and four free surfaces.

(Fig. 5.10) and between 138 to 140 grains. Random crystallographic orientations are assigned, in keeping with the absence of crystallographic texture observed in Fig. 8.2, as evident from the inverse pole figures given for each polycrystal in Fig. 8.6. As the polycrystal models include the full gauge cross-section, periodic displacement boundary conditions are applied on faces perpendicular to the direction of loading only, leaving the remaining four faces unconstrained, representing free surfaces, as illustrated in Fig. 8.7.

8.4.2. Constitutive Models

Both power-law (PL) and strain-gradient (SG) crystal plasticity (CP) constitutive models are used in this chapter. The power-law model is defined by the equations of Section 3.4.1, while the large deformation SG formulation of Section 3.4.2 is used here. These models have been calibrated against LCF data for macro-L605 specimens in Chapters 5 and 7; PL constants are provided in Table 5.4 in Chapter 5 and SG constants are given in Table 7.1 of Chapter 7. Anisotropic elasticity, corresponding to the cubic elastic constants given in
### Table 8.2: Critical values of $W$ and $p$ for the power-law and strain-gradient CP formulations, identified using cyclic values at discrete material points (from **Chapters 5 and 7**) and volume-averaged over individual grains.

<table>
<thead>
<tr>
<th></th>
<th>Power-Law CP</th>
<th>Strain-Gradient CP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$p_{\text{crit}}$</td>
<td>$W_{\text{crit}}$ (MJ m$^{-3}$)</td>
</tr>
<tr>
<td>Discrete</td>
<td>439.9</td>
<td>$15.63 \times 10^4$</td>
</tr>
<tr>
<td>Averaged</td>
<td>200.8</td>
<td>$7.32 \times 10^4$</td>
</tr>
</tbody>
</table>

**Chapter 5**, is employed for both models, consistent with the fcc crystal structure of the L605 alloy. All five polycrystal realizations of Fig. 8.6 are simulated at each stress range applied in the experiments for the PL constitutive model. Due to the computational expense associated with SG CP modelling, only the first realization of Fig. 8.6 is simulated across the three stress ranges for this SG constitutive model. As for the experimental tests, the fatigue simulations are load-controlled, whereby load levels corresponding to the desired nominal stress levels are applied. The model is initially ramped up to the maximum load level, after which twenty cycles of loading between maximum and minimum load levels are applied.

A key objective of the current study is to investigate the predictive ability of microstructure-sensitive FIPs for fatigue performance under different regimes of loading. The effective plastic strain and crystallographic work parameters $p$ and $W$, respectively, are used again here, first defined in Eqs. 4.1 and 4.2, respectively. Critical values of these FIPs have been identified in previous studies for the PL and SG models via comparison of predictions with L605 LCF test data, such that maximum cyclic values of the FIPs, $p_{\text{cyc}}$ and $W_{\text{cyc}}$, can be used to predict the number of cycles to FCI via the relation $N_i = p_{\text{crit}}/p_{\text{cyc}}$ (similar for $W$). These FIPs and previously identified critical values at discrete material points, provided in Table 8.2, are used here for prediction of HCF behaviour, based on the hypothesis that critical FIP values correspond to FCI across both the LCF and HCF regimes, as demonstrated in [83] for a nickel alloy.
8. High Cycle Fatigue of Micro-Scale Specimens

8.5. Results

8.5.1. HCF Tests

Stress-life data for the foil HCF tests is provided in Fig. 8.8, where a single run-out occurred at the lowest stress range. A fit for the Basquin-Goodman relation introduced in Chapter 4 is also shown in Fig. 8.8. The relation is recast here to include cyclic loading ratio $R_\sigma$:

\[
N_f = \left[ \frac{\Delta \sigma}{C_2 \left( 1 - \frac{\Delta \sigma (1+R_\sigma)}{2 \sigma_{YS} (1-R_\sigma)} \right)} \right]^{-\gamma_2}
\]

(8.1)

where the constants $C_2$ and $\gamma_2$ are identified as 2351 MPa and 12.09, respectively. As explained before, combining the Goodman relation with the Basquin relation for HCF allows mean stress effects to be taken into account.

Displacement histories for each test are provided in Fig. 8.9 (a) and load-displacement hysteresis loops for one specimen at each stress range are given in Fig. 8.9 (b). It appears that ratchetting occurs for the first portion of a test where the displacements increase, gradually followed by a plateau corresponding to elastic shakedown and, finally, a sudden failure for the specimens which fractured. Hysteresis loops show a similar trend, where loops for the highest stress level appear marginally wider.

Optical micrographs of each specimen post testing are provided in Fig. 8.10. The fracture region is shown for each specimen, with the exception of the run-out specimen (1) for which a portion of the gauge region is shown. Specimens 5, 6 and 9 show fractures which are located close to the taper at the end of the gauge length, while all other fractures occur within the gauge length. Surface
8. High Cycle Fatigue of Micro-Scale Specimens

Figure 8.8: Stress-life data for HCF tests. A separate marker is used where two data points overlap.

Figure 8.9: (a) Displacement histories for each specimen, divided according to maximum nominal stress and (b) sample load-displacement hysteresis loops for one specimen from each stress range, where ten cycles of loading are shown at each cycle number.
8. High Cycle Fatigue of Micro-Scale Specimens

Figure 8.10: Optical micrographs of specimens after fatigue tests, including a magnified view of a region near the fracture for one specimen.

roughening is visible for every specimen, where roughening appears to increase with stress range. Slip lines are seen clearly in a magnified view of Specimen 9, for example, at the highest stress range.

8.5.2. HCF Simulations

Maximum $p_{cyc}$ and $W_{cyc}$ values are identified from the final cycles of loading in HCF simulations for the PL and SG models. Previously identified $p_{crit}$ and $W_{crit}$ values at discrete material points (Table 8.2) are then used to make predictions.
of number of cycles to FCI, $N_i$, shown in Fig. 8.11 (a). Predicted $N_i$ values are compared here against $N_f$ data. However, for HCF, FCI is expected to dominate fatigue life \[29\]. The relatively sudden change or upturn in displacement histories observed for the foil micro-specimens, shown in Fig. 8.9 (a), supports this. Also, for the micro-scale specimens tested here, only the early stages of crack growth can take place before fracture occurs, owing to the small dimensions involved, removing the contributions of physically small and long crack growth to fatigue life. $N_i$ predictions for the PL model (blue markers) generally lie within the range of the experimental life data. For the SG models (red markers), life is generally under-predicted, particularly for the $W$ FIP, where predictions are lower than experimental data by at least an order of magnitude.

Plots of $p_{cyc}$ and $W_{cyc}$ for one realization of the PL model and for the SG model are shown in Fig. 8.12. Peaks in all distributions occur in elements at the free surface. In some cases peaks occur in corner elements, representing a junction between two free surfaces and a third periodically constrained surface. While this is not unrealistic, some of the peaks in corner elements are much higher in comparison with peaks not located in corner elements. Particularly for $W_{cyc}$ distributions in the SG models, peaks are an order of magnitude higher than expected, as illustrated in a magnified view for the $\sigma_{max} = 600$ MPa case of Fig. 8.12. To remove potential boundary condition effects, a new set of predictions are presented for each model in Fig. 8.11 (b), in which peaks at corner elements are excluded. Only subtle changes in PL predictions (blue markers) are observed, with predictions remaining within range of the experimental data. While $W_{cyc}$ predictions for the SG are shifted towards higher numbers of cycles, SG predictions remain overly conservative.

Predictions presented thus far are based on the assumption of stabilised cyclic FIPs at the final (twentieth) cycle of loading simulated. Upon inspection, plots of $p_{cyc}$ and $W_{cyc}$, reveal a decreasing trend, as expected. However, plots also
Figure 8.11: Comparison of $N_i$ predictions for the PL and SG models with experimental foil life data using cyclic FIPs extracted from the last cycle of loading (a) including and (b) excluding predictions in corner elements and (c) using stabilised cyclic FIP values, estimated from an exponential fit, excluding peaks at corner elements.
reveal that stabilised cyclic values have not yet been reached after the simulated twenty cycles of loading. A two-term exponential curve is, therefore, used here to estimate stabilised cyclic FIP values. For an FIP, $x$, a stabilised cyclic value, $x_{cyc,s}$, can be found by fitting data to the relation:

$$x_{cyc} = x_{cyc,s} + f (x_{cyc,1} - x_{cyc,s}) e^{b_1(N-N_1)} + (1 - f) (x_{cyc,1} - x_{cyc,s}) e^{b_2(N-N_1)}$$  \hspace{1cm} (8.2)$$

as illustrated in Fig. 8.13 (a), where $0 < f < 1$ and $b_1$ and $b_2$ define the rate of decay for each exponential term. Examples of $p_{cyc}$ and $W_{cyc}$ data fitted to the exponential relation for a PL model are illustrated in Figs. 8.13 (b) and (c), respectively. The final plot of Fig. 8.11 in part (c) shows predictions based on stabilised cyclic values, estimated using the exponential relation above. By the
nature of the exponential function, all predictions are shifted to the right. PL predictions have only been marginally affected and still remain in the range of experimental data, a significant improvement is observed in SG predictions here, including the apparent capture of the experimental run-out at the low stress range. However, it should be noted that fits of the exponential relation to data are perhaps not as convincing for the SG models, as illustrated in Fig. 8.14. The SG stabilised values for $W_{cyc}$ estimated using the exponential relation, shown in the individual plots of Fig. 8.14, are unlikely a reflection of true stabilised values, given the data.

A volume-averaging approach is also applied in this study, to provide predictions based on cyclic FIPs averaged over individual grains in the simulated polycrystals, rather than at discrete material points, i.e. the grain with the maximum
volume-averaged cyclic FIP is identified and used to predict $N_i$. Przybyla and McDowell [57,58] also employ grain volume averaging for FIPs in CP polycrystal models to generate probability functions for the occurrence of extreme FIP values, thought to be drivers of FCI. It can be postulated that the FIP distribution over an entire grain contributes to the probability of slip band formation and, thus, FCI in that grain. Critical FIPs, at which FCI is predicted to occur, have previously been calibrated based on peaks at discrete material points, however. Therefore, calibration of $p_{crit}$ and $W_{crit}$ for the PL and SG L605 models, based on grain-averaged $p_{cyc}$ and $W_{cyc}$ values, has been carried out using simulations and experimental data presented in Chapters 5 and 7. The identified critical values based on grain-averaged data are provided in Table 8.2 and the plots in Figs. 8.15 (a) and (b) compare experimental LCF $N_i$ data with predictions based on these critical FIP values, for the PL and SG models, respectively. Calibration of critical FIP values is carried out for both models against one data point, corresponding to the as-received material LCF test at $\pm 1\%$ total strain.

The newly calibrated $p_{crit}$ and $W_{crit}$ values are applied to the prediction of $N_i$ for
8. High Cycle Fatigue of Micro-Scale Specimens

Figure 8.15: Comparison of experimental \( N_i \) data for LCF of the L605 alloy with predictions using \( p_{\text{crit}} \) and \( W_{\text{crit}} \) values based on FIPs volume-averaged over individual grains for (a) the PL and (b) the SG models.

Figure 8.16: Comparison of foil HCF data with \( N_i \) predictions using FIPs volume-averaged over individual grains for the last cycle of loading.

foil simulations in Fig. 8.16, where the maximum grain-averaged \( p_{\text{cyc}} \) and \( W_{\text{cyc}} \) are taken for the final cycle of loading. SG predictions, again, tend towards lower lives. However, predictions for the two constitutive models are close, compared with Figs. 8.11 (a) and (b) where discrete FIP values from the final cycle of loading are used. FCI is predicted to occur in grains at the free surface across all stress levels and for both CP formulations and the critical grain is located at a model corner for only one realization of the PL models at \( \sigma_{\text{max}} = 700 \) MPa, i.e. FCI is predicted to occur away from corner elements for the SG models. While predictions lie in the range of experimental data for the highest stress range, life is under-predicted as the stress range is reduced.
8.6. Discussion

8.6.1. HCF Tests

The experimental fatigue data of Fig. 8.8 shows a clear trend, which follows the Basquin-Goodman relation of Eq. 8.1, where scatter in data is expected due to the dependence on microstructure inhomogeneity in the HCF loading regime and when dealing with micro-scale specimens. Hysteresis loops of Fig. 8.9 (b) clearly show the largely elastic nature of loading. Ratchetting occurs in the earlier part of tests; however, little plasticity is observed in hysteresis loops except, perhaps, for the highest stress range where a small area encompassed by loops is observed, indicating the beginning of widespread plasticity. The optical micrographs of Fig. 8.10 clearly demonstrate the important role of micro-slip in fatigue of the foil specimens. Slip lines are visible in a large number of grains, presumably those which are favourably oriented for slip. An increase in surface roughness and improved visibility of slip lines is observed with increasing stress range, again suggesting a move towards widespread plasticity for the highest stress range. While data points corresponding to fractures which appear at the base of the taper (Specimens 5, 6 and 9) might be brought in to question, fatigue lives for these specimens is consistent with other specimens for which fractures occur within the gauge region.

There are a number of potential factors which influence the fatigue tests reported here. The micro-foil specimens used are quite fragile, hence the need for support struts prior to fatigue testing to facilitate handling and provide structural integrity during specimen preparation. As mentioned in Section 8.3.2, a total of eighteen specimens were laser-cut, while only twelve specimens were successfully brought through preparation and testing steps without incurring unwanted dam-
age. Another challenge in the experimental aspect of this study was the achievement of a level of consistency in foil specimens. Both the laser-cutting and EP processes introduce a degree of non-uniformity into specimen dimensions, as seen from final dimensions in Table 8.1, and surface finish. While various EP tests were carried out prior to EP of final specimens, the EP process was found to be variable, dependent primarily on batch of EP solution and laser-cut surface. The final influential factor involved set-up of tests on the EnduraTEC® system, where feedback control, gripping and alignment presented issues. The protocol of Appendix A.3 was developed to provide a means of overcoming or minimising the effect of these potential sources of error.

8.6.2. Micromechanical Simulations

A number of different approaches have been presented in Section 8.5.2 for post-processing of micromechanical simulation results, used to predict $N_i$ for the foil HCF tests. The PL constitutive model is shown to be more reliable, in terms of capturing experimental life data and FIP output trend. PL predictions are only marginally influenced by exclusion of corner elements and application of the exponential function to give stabilised cyclic FIP values; $N_i$ predictions for PL models lie in the range of experimental data for all cases in Fig. 8.11. Both FIPs perform reasonably well, with $p_{cyc}$ predicting marginally longer lives in general. For predictions based on grain-averaged cyclic values, shown in Fig. 8.16, lives are under-predicted by the PL models for the lower stress ranges. It can be postulated that as stress range reduces and fatigue life climbs higher into the HCF regime, microstructural inhomogeneity and local peaks in slip and strain energy dissipation become more influential on FCI. In contrast, at the higher stress range, the influence of peaks formed in the microstructure diminishes in importance and less-localised or averaged slip and crystallographic work are adequate predictors.
8. High Cycle Fatigue of Micro-Scale Specimens

of FCI. This is also evident from the effectiveness of grain volume-averaged FIPs in predictions of L605 LCF behaviour for both the PL and SG models in Figs. 8.15 (a) and (b), respectively.

It can be seen from Fig. 8.11 (a) that SG $N_i$ predictions are more conservative than PL predictions. This is due to higher FIP peaks in SG models, particularly for $W_{cyc}$, as seen in Fig. 8.12. While omission of corner element predictions in Fig. 8.11 (b) results in reduced cyclic FIP peak values for the SG models, $N_i$ predictions remain conservative. The results of Fig. 8.11 (c), based on stabilised cyclic FIP values identified using an exponential fit, are superficially much improved from the previous plots, showing good correlation with experimental data. However, fits of the exponential relation to cyclic FIP data for the SG models, shown in Fig. 8.14, are questionable for some cases. The exponential fits and stabilised values estimated for $p_{cyc}$ appear reasonable. The same cannot be said for $W_{cyc}$, however. While the exponential fit appears good for $\sigma_{max} = 600$ MPa, the small value estimated for stabilised $W_{cyc}$ is improbable, given the data. Reliable trends cannot be ascertained using the exponential function for $W_{cyc}$ data at $\sigma_{max} = 650$ MPa and $\sigma_{max} = 700$ MPa. Therefore, while the SG models appear to perform well in predictions of Fig. 8.11 (c), including the apparent capture of run-outs, the $W_{cyc}$ predictions in this plot cannot be relied upon. Volume averaging over grains diminishes the effect of unexpectedly high peaks in FIP distributions on FCI prediction for the SG models. However, as evident from Fig. 8.16, predictions based on grain-averaged cyclic FIPs across the applied stress ranges vary little for the SG models. This can be explained via the SG distributions of Fig. 8.12, where only minor variations in bulk FIP distributions are observed across the three stress levels, compared with the PL realization shown.

Recalling Chapter 7, the SG formulation has been calibrated via comparison of the macroscopic response of a polycrystal model against LCF data for as-received and heat-treated L605 specimens. Calibration was carried out against cyclic
data only, with emphasis on capture of the stabilised hysteresis loops, rather than initial yielding, whereas the PL formulation has been calibrated against both tensile and LCF data for the as-received L605 material, as described in Chapter 5. Also, inclusion of back-stress terms in the PL model, versus the absence of a back-stress in the SG formulation, results in hysteresis loop shapes which more closely resemble the experimental behaviour of the CoCr alloy for the PL models. These two factors make the PL model, in this instance, better equipped for HCF predictions. The SG model is also shown to be more sensitive to boundary conditions, evident from the unrealistic peaks in corner elements. The mesh sensitivity studies of Appendix A.2 also suggest that the SG models are more mesh-sensitive than the PL models. However, the importance of SG effects cannot be ignored, particularly where a change in grain size is considered. A grain size of 38 \( \mu m \) is measured here for the L605 foil, which is quite close to the measured grain size for the as-received L605 material of Chapters 5 and 7 (32 \( \mu m \)). Therefore use of the PL model, calibrated for the as-received L605 bar material, is acceptable here, whereas a decrease in grain size could require re-calibration of constants, as demonstrated by the plots of Fig. 7.11.

Predictions of \( N_i \) for the PL model and, in some cases, for the SG model are consistent with experimental life data. However, the micromechanical models presented here are less successful at capturing the full range of life data (i.e. scatter), particularly at the lower stress range. In the plots of Fig. 8.11 the majority of predictions remain in the \( 10^4 \) and \( 10^5 \) cycle regimes, excluding SG predictions based on a stabilised \( W_{cyc} \) estimated from the exponential fit, whereas, one micro-foil specimen of four for the lowest stress range failed in the \( 10^6 \) regime and another specimen reached the \( 10^7 \) run-out limit. As expected, use of volume-averaged cyclic FIP values reduces the capacity to capture scatter further (Fig. 8.16), as predictions are no longer based solely on FIP peaks in the microstructure. It can be postulated that extreme microstructure combinations (e.g. the
“rogue” grain combination modelled in fatigue facet nucleation simulations by Dunne and Rugg [207]) must be modelled in order to capture true scatter. The polycrystal realizations of Fig. 8.6 represent microstructure samples with grain volume distributions with strong correlation to the measured average grain volume distribution for the foil material and, therefore, may not pick up the full influence of microstructural inhomogeneity. It can also be argued that more than the five polycrystal realizations used here is required to truly capture scatter. A study by Przybyla and McDowell [57] show that use of twenty five SVEs is sufficient to investigate the link of potentially influential microstructural attributes with extreme values of FIPs for indication of FCI via probability functions.

Comparison of $N_i$ predictions and experimental $N_f$ data in this study is based on the assumption that crack initiation dominates fatigue life, both due to the HCF regime of loading and the micro-scale of specimens tested. While the displacement histories of Fig. 8.9 appear to corroborate this, indicating a change in load-displacement behaviour only at the end of life, it is probable that microstructurally small crack (MSC) propagation does indeed contribute towards fatigue life. Obrtlík et al. [232] observed a linear increase in crack size below a threshold crack size, followed by an exponential crack propagation stage for notched 316L SS specimens, including a test in the $10^6$ cycles regime. Crack propagation below a threshold crack size is unlikely to influence the bulk displacement response for the foil specimens, while propagation in the exponential stage can be postulated to correspond to the change observed in displacement histories in Fig. 8.9, towards the end of life. The damage coupling approach of Chapter 4 could be extended to simulate crack propagation through the polycrystal model and, thus predict a value for $N_{MSC}$, allowing prediction of total life by $N_f = N_i + N_{MSC}$. Alternatively, a fracture mechanics approach could be adopted for estimating $N_{MSC}^{exp}$, using the El Haddad modification to the Paris relation for crack propagation below a threshold crack size, outlined in Section 2.2.
McCarthy et al. [84] have implemented such an approach for back-calculation of $N_{\text{exp}}^i$ from experimental $N_f$ data, allowing comparison of experimental results against microstructure-sensitive FCI predictions for fretting fatigue.

Some useful observations can be made on preferential sites for FCI in HCF, based on the CP simulations presented here. Aside from the unconstrained free surfaces, predicted FCI sites are also observed to be influenced by precipitates and grain boundaries. Based on predictions excluding corner elements, FCI sites are predicted to occur in elements at grain boundaries for twenty eight out of thirty six cases. Five FCI predictions away from the grain boundary occur in elements adjacent to precipitates, where increased stresses are expected, while the other three correspond to the SG $p_{cyc}$ predictions. This can be attributed to increased material hardening in SG models and, thus, reduced slip at grain boundaries and precipitates due to build-up of geometrically necessary dislocations. FCI is predicted to occur in elements adjacent to precipitates for fifteen out of thirty six cases, where eleven of these cases are for the $W_{cyc}$ parameter. Based on a product of shear stress and plastic slip, the crystallographic work FIP is more susceptible to the influence of increased stresses near precipitates than the purely slip-based $p$ FIP. While peaks in FIP distributions occur in free surface elements for all models, a number of subsurface FCI predictions occur with the exclusion of corner elements. This is consistent with the results of [58], in which an overlap of probability functions for extreme value FIPs for surface and subsurface crack formation indicates that both are likely in HCF. Seven out of nine subsurface FCI sites are predicted using $W_{cyc}$, including the three SG $W_{cyc}$ predictions. All subsurface predictions occur either in an element adjacent to a precipitate, at the grain boundary, or both, demonstrating again the influence of precipitates and grain boundaries as stress-concentrators. An increase in the number of subsurface predictions is observed with a decrease in stress range. This is consistent with observations of increasing probability of FCI due to subsurface mechanisms.
at increased numbers of cycles [28], a trend also predicted by Przybyla et al. [198] using extreme value statistics. However, there are no conclusive trends to show that FCI predictions either subsurface, adjacent to precipitates of at grain boundaries correspond to an increase or decrease in \( N_i \) values, for the study presented here. Twin boundaries observed in the foil microstructure in Figs. 8.1 (a) and 8.2 (a) are not represented in the polycrystal models presented here, as for the macro-scale material studies in Chapters 5 and 7. It is anticipated, based on the study of Castelluccio and McDowell [82] on the effect of twin boundaries on FIP accumulation, that twin boundaries would also be predicted as preferred sites for FCI.

The plot of Fig. 8.17 shows ranges of maximum Schmid factors across all slip systems in the deformed configuration with respect to the direction of applied load across all integration points in each of the micromechanical models. Markers indicate integration points for which FCI is predicted to occur using \( p_{crit} \) and \( W_{crit} \), excluding predictions at corner elements. Maximum Schmid factors at the predicted sites of FCI are generally in the upper half of the full range, with \( W_{crit} \) predictions in particular favouring integration points with higher maximum Schmid factors. However, this is not the case for all predictions and, thus, a concrete link between Schmid factor and FCI location cannot be made.

The micromechanical framework has been successfully applied here for predic-
tion of HCF behaviour of micro-scale specimens of the L605 CoCr alloy and, owing to the microstructure-sensitive nature of the tests and models presented, multiaxiality experienced in individual grains due to the microstructure itself is inherently accounted for. However, further validation is required to investigate performance of the micromechanical framework as a tool in stent fatigue design. The uniform gauge length of the foil specimens tested here and uniaxial loading applied do not capture the macroscopically multiaxial nature of stent fatigue. For example, introduction of a notch into the foil specimen geometry would impose a macroscopically non-uniform stress state on the specimen gauge region, which would be more representative of a hinge in a typical stent geometry. Also, as high mean stresses are common in stents, owing to the high deformation installation procedure, further testing at higher cyclic load ratios than that used here, as highlighted in Section 8.3.3, may provide further insight into mean stress effects on stent fatigue performance. Morrissey et al. [199] report different plastic strain accumulation behaviour at low and high cyclic stress ratios for HCF simulations of Ti-6Al-4V, where distinct regions of plastic strain, compartmentalised within individual grains, were observed for lower stress ratios and plastic strain bands spanning multiple grains were observed for high stress ratios. A similar transition in behaviour could also be captured here with further testing and simulations at higher cyclic stress ratios.

8.7. Conclusions

The HCF behaviour of the L605 CoCr alloy has been successfully characterised via testing of foil micro-specimens. Slip lines observed on the tested specimens reaffirm the need for microstructure-sensitive prediction techniques for HCF of micro-components. An L605 micromechanical framework for the prediction of this behaviour has been developed, using multiple FE microstructure realiza-
tions of the foil specimen cross-section and two CP formulations coupled with microstructure-sensitive FIPs. Predictions of number of cycles to FCI using the power-law CP formulation, based on critical FIP values calibrated for L605 LCF behaviour, are in good agreement with experimental data, validating the micromechanical framework and, specifically, $p_{\text{crit}}$ and $W_{\text{crit}}$ as effective tools for HCF performance assessment. Strain-gradient CP models are sensitive to mixed free surface-periodic boundary conditions applied; however, application of a grain volume-averaging approach allows reasonable predictions of FCI to be made using this strain-gradient constitutive model. Polycrystal simulations allow identification of free surfaces, precipitates and grain boundaries as preferred sites for FCI, while maximum Schmid factor is shown to have a less prominent role.
9. Discussion and Conclusions

9.1. Chapter Summary

This chapter discusses the findings of Chapters 4 to 8 as a collective body of work, with respect to the original aims and objectives set out in Chapter 1. Limitations and gaps of the thesis are discussed, along with potential future research directions to build upon and/or complement the work presented. Overall conclusions for the thesis are provided in the final remarks.

9.2. Discussion of Findings

The primary objective of this body of work, as set out in Chapter 1, is the development of a micromechanical framework for the prediction of fatigue crack initiation (FCI) and this has been the focus of each results chapter presented. The development, calibration and validation of such a framework have been presented in this thesis. Another important output of this work has been the demonstration of the micromechanical framework as a tool for investigation of factors which influence FCI, and for assessment of stent fatigue performance and improvement of stent fatigue design.
Three materials have been investigated in this thesis, including 316L SS in Chapter 4, a ferritic steel in Chapter 6, and the L605 CoCr alloy in Chapters 5, 7 and 8, where 316L SS and the L605 alloy are common stent materials. While four-point bending fatigue experiments, carried out at the Nippon Steel Corporation, are presented for the ferritic steel in Chapter 6, experimental testing in this thesis has focused on the L605 alloy, for which a broad and rigorous test program has been presented. Two as-received forms of the alloy have been used, including a round bar form for macro-scale testing and micromechanical model development and foil material for micro-scale high cycle fatigue (HCF) tests allowing validation of the framework. The heat-treated bar of Chapter 7 can also be considered a third form considered. The microstructure of all three forms of the L605 alloy has been characterised via microscopy, in terms of grain size statistics, precipitate statistics and crystallographic texture. Mechanical testing of the L605 alloy included: (i) tensile testing of the as-received bar material, (ii) low cycle fatigue (LCF) of the as-received and heat-treated bar material and (iii) HCF tests of micro-scale foil specimens. Descriptions of specimen preparation have also been provided, particularly for the foil specimens of Chapter 8, for which a complex process of laser-cutting and electro-polishing was required. The experimental component of this work is key to its success, providing data for (i) generation of microstructure finite element (FE) models, (ii) calibration of constitutive behaviour and microstructure-sensitive predictors and (iii) validation of the micromechanical framework.

The micromechanical framework employed in the studies of this thesis has three components, including a crystal plasticity constitutive model, polycrystalline FE geometries and microstructure-sensitive predictive parameters. While for the four-point bending study of Chapter 6 specific grain morphologies in the notch region of specimens are modelled, all other studies used microstructure realizations designed to be statistically representative of the material being modelled,
9. Discussion and Conclusions

Based on microscopy data, Voronoi tessellation has been successfully utilised to generate both 2D and voxel 3D polycrystalline morphologies. Inclusion of precipitates finer than the typical element size for CoCr FE models has been facilitated via development of novel seven-element and five-element units, first described in Chapter 5, for 3D and 2D models, respectively. The generation and use of multiple FE microstructure morphologies facilitated investigation of the effect of microstructural inhomogeneity and, also, the capture, to some extent, of scatter observed in fatigue behaviour.

Much emphasis has been placed in this thesis on the crystal plasticity (CP) constitutive descriptions used, including both a phenomenological power-law formulation and more physically-based formulations with strain-gradient capability. Calibration of both CP formulations has been carried out via comparison of bulk polycrystal model response with experimentally-observed behaviour for the relevant material. For studies on the L605 alloy, data from the tensile and LCF testing is used. The merits of the power-law model are demonstrated in Chapters 4, 5 and 8, most notably due to the kinematic hardening capability implemented in the study of Chapter 4. Kinematic hardening is demonstrated to be key in capturing initial plastic yield, early cyclic stress-strain behaviour prior to stabilisation and stabilised hysteresis loop shape. The use of multiple kinematic back-stresses is shown in Chapter 5 to facilitate simulation of both cyclic and tensile behaviour for a single set of CP constants, while the work of Chapter 4 demonstrates the necessity of kinematic hardening for representation of the mean stress field which develops prior to stent fatigue, during installation. Another benefit of the power-law model is the reduced sensitivity to boundary conditions, compared with a physically-based CP formulation, as observed in Chapter 8 for predictions of foil HCF behaviour. However, while the power-law formulation does model plastic slip on individual slip systems, the formulation does not capture the dislocation mechanisms which drive and hinder slip. The
physically-based CP models of Chapters 6, 7 and 8 are based on equations describing the plastic slip as a function of mobile dislocation glide, which is impeded by the presence of immobile dislocations, manifested as strain hardening. A key benefit of the physically-based models is the inclusion of geometrically necessary dislocations (GNDs), which form to facilitate spatial gradients in plastic strain. While the influence of GNDs on prediction of FCI site is shown to be minimal for the ferritic steel coarse-grain, four-point bending specimens of Chapter 6, GNDs are shown to accumulate at the experimental site of FCI. For a study on microstructures with finer grain size, however, in Chapter 7, results clearly demonstrate the benefit of strain-gradient capability introduced by GNDs, where the number of cycles to FCI was successfully predicted across two grain sizes, for as-received and heat-treated L605 material, using one set of physically-based CP constants. Using the strain-gradient CP formulation, the physical dimensions of the FE polycrystal geometry alone were sufficient for the effect of grain size on hysteresis behaviour and, thus, indicator parameter accumulation, to be captured. The physically-based models are, however, more sensitive to boundary conditions, as illustrated in Chapter 8, and the benefit of strain-gradient modelling is reduced for analyses on a single grain size. However, other microstructural features, such as precipitates in the L605 matrix as discussed in Chapters 7 and 8, also incur strain-gradient effects which can be captured by the physically-based CP formulations. Elastic anisotropy is another aspect of constitutive behaviour, applicable in both CP formulations, which is shown to be important in modelling of FCI, particularly in HCF. The four-point bending study of Chapter 6, clearly demonstrated, for the specimen investigated, that use of isotropic instead of cubic elasticity, results in prediction of a distinctly different location of FCI. Cubic elasticity is shown to be highly influential on the stress field formed initially after yielding and, therefore, is most important for HCF predictions, including the stent fatigue application, where only localised plasticity takes place due to the inhomogeneous stress distribution.
formed during macroscopically elastic loading.

Fatigue indicator parameters (FIPs) are the third component of the micromechanical framework presented, employed to predict FCI in the polycrystalline models. It is shown early on in Chapters 4 and 5 that consistency between size scale of application, constitutive model and predictive techniques is required. Macroscopic stress-based predictions for the generic stent design modelled, based on the conventional industry approach for stent fatigue assessment, are shown to be incompatible with the microstructure-sensitive model used and exhibit unrealistic scatter, compared with the use of FIPs based on CP variables. Critical values of the effective plastic strain and crystallographic work parameters, $p$ and $W$, have been successfully calibrated for both 316L SS and the L605 alloy, against LCF data. The predictive capabilities of these FIPs have been validated across multiple grain sizes (Chapter 7) and different regimes of loading (Chapter 8). Their ability to capture FCI behaviour in the HCF regime, as demonstrated in Chapter 8, also provides a level of validation for their use in a micromechanical framework for stent fatigue design. The study of Chapter 6 clearly demonstrated the ability of the $p$ parameter to predict experimentally-observed sites of FCI for the specific grain morphologies in the notch region of specimens tested. Specifically, the use of cyclic FIP values in fatigue predictions is validated in this study, where slip on dominant slip systems is also shown to be an effective indicator of FCI.

For four out of five results chapter, two FIPs are investigated and their effectiveness in predicting FCI has been compared. While both parameters show reasonable ability to predict FCI, an argument is made for the crystallographic work parameter in Chapter 7 as the superior of the two FIPs investigated, based on better prediction of number of cycles to FCI across different strain ranges and grain sizes. Also, in Chapter 7, $W$ predictions indicate that precipitates in the microstructure reduce number of cycles to FCI, while predictions using the $p$ pa-
rameter indicate no conclusive effects of precipitates. Due to the inclusion of shear stress in the crystallographic work parameter accumulation, it is better equipped to look at the effects of stress-concentrators on FCI predictions, in comparison with the crystallographic slip parameter, $p$. The energy basis of the $W$ parameter is also considered more in line with newly developed FCI models [95–97], based on an energy balance for dislocation mechanisms within a persistent slip band. Therefore, while the results of Chapter 8 reveal a sensitivity of the $W$ parameter to boundary conditions, once steps are taken to circumvent this sensitivity, it can be postulated that the crystallographic work parameter better captures the dislocation mechanisms leading to slip band formation and thus, FCI.

Crystallographic orientation has also been investigated (to a lesser extent) within this thesis as a potential indicator of FCI and of initial crack direction after FCI. In the study of Chapter 6, while predicted slip on dominant slip systems tended to coincide with the experimentally-observed FCI sites, it was also shown that slip direction on these dominant slip systems does not necessarily dictate the initial crack growth direction. Investigation of the predictive potential of maximum Schmid factors is carried out in Chapters 5 and 8, where predictions of FCI are shown to tend towards sites with a high maximum Schmid factor. However, not all predictions were observed to follow this trend and, therefore, Schmid factor alone is not recommended as an FIP.

The micromechanical framework has been successfully applied to stent fatigue assessment and design, where the need for microstructure-sensitive approaches, in place of the macro-scale Goodman technique currently used in industry, is clearly outlined in Chapters 1 and 2. Chapters 4 and 5 describe the development of a microstructure sub-model of a repeatable unit in a generic stent design for both 316L SS and the L605 CoCr alloy, respectively, where sub-model boundary conditions were identified by virtue of a global $J_2$ stent-artery model. The micromechanical approach allows microstructural inhomogeneity to be captured,
where multiple possible sites for FCI are identified. This is contrasted with a $J_2$ sub-model where only one failure location is predicted. As mentioned previously in this section, the importance of size scale consistency in fatigue prediction methods is also highlighted in these studies. Further analysis for two 316L SS microstructure realizations for the stent sub-model in Chapter 4 demonstrated the potential for the micromechanical framework to be coupled with a damage-based cycle jumping approach to facilitate extended fatigue simulations, allowing investigation of evolving FIP distributions over large numbers of cycles. Additional analyses in the CoCr study of Chapter 5 also demonstrated use of the micromechanical framework for re-design of the generic stent geometry, which was shown to be over-conservative for the CoCr alloy. The studies clearly demonstrate the potential for micromechanical modelling as a tool in stent fatigue design. However, CP modelling may not be considered within the medical devices industry to be a viable tool in place of existing approaches due to the significant computational expense, resulting in long runtimes and the associated constraint to focus only on sub-models of the full stent design. However, there is significant potential for use of the micromechanical framework as a tool for generating a set of microstructure-sensitive design rules for stent fatigue design. Work by Grogan et al. [123], for example, on the micromechanical modelling of statistical size effects in monotonic loading of stent struts included development of a series of design curves, relating relative strut dimensions and grain size to the strain at maximum supported load, which can be used in the safe design of stents for deployment. A similar approach could be developed for stent fatigue design. The work of this thesis has clearly demonstrated the capacity of the micromechanical framework to generate curves relating number of cycles for FCI to strut dimensions, hinge radius, grain size, precipitate content etc. As such, the micromechanical framework could be employed in the design of suitable materials and microstructures, as discussed by McDowell [233], (including processing steps to give different grain morphologies, crystallographic texture and precipitate profile) for stent fatigue,
as well as providing guidelines on relative strut dimensions, curvature etc.

9.3. Future Work

Interesting future research directions arise from the work presented here, relating to microstructure-sensitive fatigue behaviour and the prediction of that behaviour. While some simple limitations of the work may require further investigation, such as the need for bigger models, finer meshes and simulation of more fatigue cycles to ensure stabilisation, there are multiple opportunities for building upon the results presented.

Much scope exists for improving experimental validation of the micromechanical framework presented, particularly when considering application to stent fatigue. While the framework is applied here for LCF and HCF loading, testing which induces multiaxial stress states at the macro-scale has not been carried out. Such tests, along with testing at different cyclic loading ratios, would allow validation of the framework for loading conditions more representative of those experienced by a stent hinge in the body. The effect of corrosion due to biological surroundings on mechanical fatigue performance of the stent material is another aspect which should be experimentally investigated. In terms of FCI prediction, further use could be made of electron backscatter diffraction imaging to allow a more thorough investigation of the effect of crystallographic texture on fatigue performance and to confirm that the reorientation of grains predicted by CP models is accurate. The work of You et al. [99], applied such a technique for a 316L stent strut, where inverse pole figure readings for each grain before and after monotonic loading were measured and compared with CP predictions. Additional studies on post-fatigue fractography could also provide valuable information on FCI sites and the microstructural features which appear to influence the location of those
9. Discussion and Conclusions

sites. The difficulty here lies in the ability to stop testing at a point where FCI has occurred with minimal crack growth, as a complete fracture can destroy features which would aid in identifying FCI site. Ultrasonic techniques can be used, e.g. [178] to detect cracks on the micron scale and, thus, could be used to decide on fatigue test termination. Another potential experimental study, which could further validate the micromechanical framework, but also provide important information for the design of microstructures for stent fatigue, is the investigation of the effect of precipitates on HCF fatigue performance. Teague et al. [180] carried out such a study for tensile loading, reporting the effects of precipitation under different aging treatments. A relatively simple approach was adopted in this thesis for representation of precipitates observed in the microstructure, whereby precipitates were included in models as hard particles and, for the 3D models, using one size only, based on average measurements. This ensured that the effect of precipitates on macroscopic behaviour and FCI location are accounted for, to some degree. However, a parametric study on precipitate composition, size distribution and frequency within the microstructure for varying types of precipitates would be beneficial. Additionally, fatigue tests on CoCr alloy material with a finer grain structure than the as-received L605 material of Chapters 5 and 7 would be beneficial for the further validation of the strain-gradient micromechanical framework presented in this thesis; as the trend of Fig. 7.11 in Chapter 7 suggests, a larger influence of GND density on fatigue behaviour is expected at a finer grain size.

Within the micromechanical framework itself, there is scope for improvement of the CP constitutive formulations and further investigation of FIPs. While the strain-gradient capability of the physically-based CP formulations is shown to be useful in prediction of grain size effects, one of the key drawbacks of these formulations, as they are presented here, is the lack of a kinematic back-stress. Modification of the current physically-based formulations to include a dislocation
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density-based kinematic back-stress, e.g. [159, 221, 227], would improve hysteresis behaviour and allow improved capture of initial yielding, thus rendering the formulations more suitable for stent fatigue modelling. While the effective plastic strain and crystallographic work parameters are shown to be good predictors of FCI, there is certainly scope to investigate further FIPs. For example, the work of Sangid et al. [95–97] indicates that an FIP based on the energy associated with dislocation mechanisms should be used. A crystallographic adaptation of the Fatemi-Socie parameter described in Chapter 2 could also be investigated, where the non-local maximum shear strain could be replaced with crystallographic slip on the dominant slip system, paired with stress normal to the dominant slip plane. The $p$ and $W$ FIPs are scalars and, thus, do not have an associated direction, whereas the Fatemi-Socie parameter either in the form of Eq. 2.13 or as described above, is based on a critical plane, thus introducing a directionality into FCI predictions and providing scope for prediction of microstructurally small crack growth. From this viewpoint, slip on individual slip systems could also be further investigated for FIP potential.

While the micromechanical framework developed in this thesis has shown some ability to capture scatter in HCF, the results of Chapter 8 indicate that the full range of responses is not predicted. Future computational studies for HCF applications should, therefore, include simulations of increased numbers of microstructure realisations, including realizations with extreme microstructural attributes and rogue grain combinations, as well as realisations with strong correlation to the average microstructure, as simulated in this work, in order to give improved prediction of fatigue scatter.

As mentioned in the previous section, much scope exists for furthering the micromechanical framework in stent fatigue modelling. A focus has been placed on the L605 CoCr alloy in this work; however, once experimental microscopy and mechanical data is acquired, the micromechanical framework here can be
adapted for any material which exhibits similar plastic behaviour and, thus, used to develop material-specific design rules.

9.4. Conclusions

This work has resulted in numerous useful findings and observations relating to experimental testing of the L605 CoCr alloy and the micromechanical framework, summarised below:

- Physically-based strain-gradient modelling, including geometrically necessary dislocation evolution, based on microstructural characterisation via microscopy for coarse and fine-grain L605 material, has been demonstrated to be necessary for the successful prediction of the experimentally observed grain size effect on fatigue.

- Microstructure-sensitive fatigue indicator parameters, effective plastic strain, \( p \), and crystallographic work, \( W \), are shown to be effective tools for prediction of fatigue crack initiation; critical parameter values have been validated as indicators of crack initiation across both LCF and HCF loading regimes and across different grain sizes, and accumulation of \( p \) has been shown to coincide with experimentally observed fatigue crack initiation sites.

- Kinematic hardening has been established as a key element in crystal plasticity constitutive models for the capture of initial cyclic stress-strain behaviour and stabilised hysteresis loop shape, and, as a result, is shown to be necessary for capturing mean stress effects in stent fatigue analyses.

- Elastic anisotropy has been demonstrated to play a key role in development of the polycrystal stress field in high cycle fatigue, influencing predictions
of experimentally-observed fatigue crack initiation, and is, thus, important for microstructure-sensitive predictions and, hence, stent fatigue analyses.

- Overall results, including validation of the framework presented for application in high cycle fatigue, indicate that the current industry design practices for stent fatigue analysis should be modified to include microstructure-sensitive design rules, with emphasis on careful characterisation of the microstructure and an understanding of the effect on fatigue performance of each microstructural feature observed.
A. Appendices

A.1. Kinematic Hardening Implementation

The original power-law crystal plasticity (CP) implementation of Huang [148], described in Section 3.4.1 of this thesis, has been modified to include kinematic hardening. A description is provided here of implementation of kinematic hardening for one back-stress, where the steps shown have also been extended to include additional back-stresses.

The power-law CP formulation is implemented numerically in a CP UMAT using the following time integration scheme for the calculation of the plastic slip increment, $\Delta \gamma^\alpha$, on a slip system:

$$
\Delta \gamma^\alpha = (1 - \theta) \Delta \dot{\gamma}^\alpha_t + \theta \Delta \dot{\gamma}^\alpha_{t+\Delta t}(\Delta \gamma^\alpha) \tag{A.1}
$$

where subscripts $t$ and $t + \Delta t$ indicate values at the start and end of a time increment respectively and $\theta$ is defined to be a constant between 0 and 1. A $\theta$ value of 0 constitutes forward Euler integration while a value of 1 invokes backward Euler integration; a $\theta$ value of 0.5 is used for the studies of this thesis, consistent with recommendations from previous work [234]. From Eq. A.1 it can be seen that the plastic slip rate at the end of the time increment is dependent on
the plastic slip increment. In order to achieve an implicit solution it is necessary to solve iteratively for the plastic slip increment using a Newton-Raphson approach. The Newton-Raphson function and its derivative with respect to the plastic slip increment are defined respectively by:

\[ f(\Delta \gamma^\alpha) = \Delta \gamma^\alpha - (1 - \theta) \Delta t \dot{\gamma}^\alpha_t - \theta \Delta t \dot{\gamma}^\alpha_{t+\Delta t}(\Delta \gamma^\alpha) \] (A.2)

\[ f'(\Delta \gamma^\alpha) = 1 - \theta \Delta t \frac{\partial}{\partial \Delta \gamma^\alpha} \left[ \dot{\gamma}^\alpha_{t+\Delta t}(\Delta \gamma^\alpha) \right] \] (A.3)

The partial derivative in Eq. A.3 is defined by:

\[ \frac{\partial}{\partial \Delta \tau^\alpha} \left[ \dot{\gamma}^\alpha_{t+\Delta t}(\Delta \gamma^\alpha) \right] = \Delta t \frac{\partial^2 \sigma^\alpha}{\partial \Delta \gamma^\alpha} \] (A.4)

and recalling the flow rule for the power-law formulation in Eq. 3.37:

\[ \dot{\gamma}^\alpha_{t+\Delta t}(\Delta \gamma^\alpha) = \dot{\gamma}^\alpha_t \text{sgn} \left( \left( \tau^\alpha + \Delta \tau^\alpha \right) - \left( x^\alpha + \Delta x^\alpha \right) \right) \left\{ \frac{\left( \tau^\alpha + \Delta \tau^\alpha \right) - \left( x^\alpha + \Delta x^\alpha \right)}{g^\alpha + \Delta g^\alpha} \right\}^n \] (A.5)

where \( \Delta \tau^\alpha \), \( \Delta g^\alpha \) and \( \Delta x^\alpha \) are functions of \( \Delta \gamma^\alpha \). The partial derivatives of \( \Delta \tau^\alpha \) and \( \Delta g^\alpha \) with respect to \( \Delta \gamma^\alpha \) remain unchanged with the introduction of kinematic hardening; however, all other terms on the right hand side of Eq. A.4 need to be determined. The partial derivatives in Eq. A.4 of \( \dot{\gamma}^\alpha_{t+\Delta t} \) with respect to the \( \Delta \tau^\alpha \), \( \Delta g^\alpha \) and \( \Delta x^\alpha \) are derived from Eq. A.5 to be:

\[ \frac{\partial}{\partial \Delta \tau^\alpha} \dot{\gamma}^\alpha_{t+\Delta t} = \dot{\gamma}^\alpha_t \text{sgn} \left( \left( \tau^\alpha + \Delta \tau^\alpha \right) - \left( x^\alpha + \Delta x^\alpha \right) \right) \left\{ \frac{\left( \tau^\alpha + \Delta \tau^\alpha \right) - \left( x^\alpha + \Delta x^\alpha \right)}{g^\alpha + \Delta g^\alpha} \right\}^{n-1} \frac{1}{g^\alpha + \Delta g^\alpha} \] (A.6)

\[ \frac{\partial}{\partial \Delta g^\alpha} \dot{\gamma}^\alpha_{t+\Delta t} = -\dot{\gamma}^\alpha_t \text{sgn} \left( \left( \tau^\alpha + \Delta \tau^\alpha \right) - \left( x^\alpha + \Delta x^\alpha \right) \right) \left\{ \frac{\left( \tau^\alpha + \Delta \tau^\alpha \right) - \left( x^\alpha + \Delta x^\alpha \right)}{g^\alpha + \Delta g^\alpha} \right\}^{n-1} \frac{\tau^\alpha + \Delta \tau^\alpha - x^\alpha - \Delta x^\alpha}{(g^\alpha + \Delta g^\alpha)^2} \] (A.7)

\[ \frac{\partial}{\partial \Delta x^\alpha} \dot{\gamma}^\alpha_{t+\Delta t} = -\dot{\gamma}^\alpha_t \text{sgn} \left( \left( \tau^\alpha + \Delta \tau^\alpha \right) - \left( x^\alpha + \Delta x^\alpha \right) \right) \left\{ \frac{\left( \tau^\alpha + \Delta \tau^\alpha \right) - \left( x^\alpha + \Delta x^\alpha \right)}{g^\alpha + \Delta g^\alpha} \right\}^{n-1} \frac{1}{g^\alpha + \Delta g^\alpha} \] (A.8)

From the Armstrong-Frederick relation for the kinematic back-stress in Eq. 3.36:
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Figure A.1: Flowchart showing details of implementation of non-linear kinematic hardening formulation in crystal plasticity UMAT.

\[
\Delta x^\alpha = C_{\text{kin}} \Delta \gamma^\alpha - D_{\text{kin}} x^\alpha |\Delta \gamma^\alpha| \tag{A.9}
\]

which is used to derive the partial derivative:

\[
\frac{\partial \Delta x^\alpha}{\partial \Delta \gamma^\alpha} = C_{\text{kin}} - D_{\text{kin}} x^\alpha \text{sgn}(\Delta \gamma^\alpha) \tag{A.10}
\]

A flowchart is provided in Fig. A.1 in which the algorithm used for the iterative calculation of the plastic slip increment is demonstrated.
A.2. Mesh Sensitivity Studies

Results of three mesh sensitivity studies carried out within the work of this thesis are provided here, for (i) the power-law CP formulation of Section 3.4.2 with 4-noded generalised plane strain elements, (ii) power-law CP with 20-noded, brick elements and (iii) strain-gradient CP for the large deformation implementation of Section 3.4.2, also with 20-noded, brick elements. In each case fully reversed cyclic loading is applied for the strain range ±0.5%.

Figure A.2: Mesh sensitivity study for 2D generalised plane strain power-law CP, including (a) distributions of $W_{\text{cyc}}$, (b) stabilised hysteresis loops and (c) maximum values of $W_{\text{cyc}}$ and $p_{\text{cyc}}$, for each mesh density. The final mesh density used is highlighted in red for each case.
The first study, carried out to ensure sufficient mesh refinement in Chapter 4, is applied to the 2D polycrystal geometry of Fig. 4.3 for generalised plane strain elements, using CP constants identified for 316L in Table 4.3. Five simulations are carried out for meshes containing 4157, 6453, 12454, 19266 and 25430 elements, where the model used in Chapter 4 for calibration of $p_{\text{crit}}$ and $W_{\text{crit}}$ corresponds to the mesh with 12454 elements. Results for the mesh sensitivity study are shown in Fig. A.2, where the final mesh used is highlighted in red. The comparison of $W_{\text{crit}}$ distributions in Fig. A.2 (a) shows little difference across all mesh densities, while macroscopic hysteresis response for each mesh in Fig. A.2 (b) are practically indistinguishable and peak cyclic fatigue indicator parameters (FIPs) for the final mesh appear to be close to convergence from Fig. A.2 (c).

The second mesh sensitivity study is for the power-law CP formulation applied to 3D polycrystal geometries, as used in Chapters 5 and 8. The polycrystal

![Figure A.3: Polycrystal meshes used for 3D mesh sensitivity studies, where the final mesh density is highlighted in red.](image)
morphology of Fig. 5.10 is modelled, using the power-law CP constants identified for the L605 CoCr alloy in Table 5.4, for six mesh densities containing 1000, 2197, 3375, 5832, 8000 and 10648 elements, where the mesh density used in the aforementioned studies corresponds to the mesh with 3375 elements. Unlike simulations for the 2D polycrystal geometry, voxel meshes are used for the 3D models. Therefore, there are minor differences between grain morphology for different mesh densities, as shown in Fig A.3. Results for the mesh sensitivity study are shown in Fig. A.4, where, again, the final mesh used is highlighted in red. As for the previous mesh sensitivity study, minor differences are visible in $W_{crit}$ distributions (Fig. A.4 (a)) and are likely partly accounted for by slightly
different grain morphologies. Again, the macroscopic hysteresis responses in Fig. A.4 are difficult to distinguish and peak cyclic FIPs, shown in Fig. A.4 (c), appear to reach a relatively stabilised level for the mesh containing 3375 elements.

The final study investigates mesh sensitivity for the large deformation strain-gradient CP implementation, used in Chapters 7 and 8. Only the first four meshes of Fig. A.3 are simulated in this study, due to the computational expense associated with 3D strain-gradient CP analyses. The constants identified for the L605 CoCr alloy in Table 7.1 of Chapter 7 are used. Results for the mesh sensitivity study are shown in Fig. A.5. Again, differences in $W_{\text{crit}}$ distributions

![Figure A.5: Mesh sensitivity study for 3D strain-gradient CP, including (a) distributions of $W_{\text{cyc}}$, (b) stabilised hysteresis loops, (c) maximum values of $W_{\text{cyc}}$ and $p_{\text{cyc}}$ and (d) (c) and (d) peak $\rho_{\text{GND}}$ and $\rho_{\text{SSD}}$, for each mesh density. The final mesh density used is highlighted in red for each case.]

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of Fig. A.5 (a) are small. Slight hardening of the macroscopic hysteresis response is seen with increasing mesh density in Fig. A.5 (b). Little variation is seen in peak FIP values in Fig. A.5 (c), while peak GND and SSD densities increase with mesh density, but appear to be converging.

A.3. HCF Testing Protocol

A description of the protocol used for HCF testing of foil specimens in the EnduraTEC® is provided in this appendix. The EnduraTEC measures axial displacement via a linear voltage displacement transducer and applies load via electromagnetic linear actuators, controlled by an input voltage. The tests run in this project are carried out under load-control under a feedback loop with proportional, integral, derivative and offset (PIDO) settings. A number of issues arise during high frequency tests, primarily related to feedback control. Aside from identification of appropriate PIDO settings, the following protocol has been developed based on dummy testing for minimisation of risk of specimen damage and traceability of issues in hindsight:

Initial Set-Up

- Align and tighten grips
- Turn on PC, open previous fatigue test file, save as new file and set up folders
- Input block amplitude and data acquisition settings
- Save screen shot of block settings
- Set up amplitude control and PIDO settings
- Set displacement bandwidth for peak-valley data to 0.1%
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- Set up limits and limit actions for checking PIDO settings
- Ensure stop level set at 0.1 N at frequency of 50 Hz

Specimen Set-Up

- Turn on EndraTEC
- Check that both load and displacement transducers are working
- Auto tare load and displacement channels
- Align specimen and tighten top grip
- Tighten bottom grip and save screen shot of load history
- Cut support struts, turn on local energy and save screenshot of load history
- Close chamber door and put up sign on chamber frame
- Test PIDO settings for up to 10 Hz at 2 – 8 N and save screenshot of output:
  - Ensure input load levels are reached
  - Ensure peak-valley points are captured

Start Test

- Set up fatigue test limits and limit actions (upper load limit = high load level + 10 N)
- Recheck block, amplitude control and PIDO settings
- Start test from zero
- Save screenshot when load range for 50 Hz frequency stabilises
- Put up sign on computer

End Test

- Save screen shot of test end and manually record $N_f$
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- Press abort and transfer to displacement control
- Use position tool to move grips slowly close to home position
- Remove specimen and turn off local energy
- Save files (check that all are present), save project file and close software

While some of the steps in the protocol may seem trivial, the order of appearance of some items are in fact quite important. For example, placement of a sign on the EnduraTEC® frame during a test can cause ‘noise’ which affects feedback control and can potentially trip a limit. A parameter sheet, shown in Fig. A.6, is filled out for each test, including specific load levels applied, data recording details, limits and an area for recording issues which may arise.

![Parameter Sheet](image)

**Figure A.6:** Typical parameter sheet for prompting and recording test proceedings.
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