thesis for the degree of licentiate of engineering in solid and structural mechanics

Computational modeling of oxygen-assisted fracture in nickel-based superalloys

Kim Louisa Auth

CHALMERS
UNIVERSITY OF TECHNOLOGY

Department of Industrial and Materials Science
Chalmers University of Technology
Gothenburg, Sweden, 2022

Computational modeling of oxygen-assisted fracture in nickel-based superalloys

Kim Louisa Auth

Technical Report No. IMS-2022-7
This thesis has been prepared using LaTeX.

Department of Industrial and Materials Science
Chalmers University of Technology
SE-412 96 Gothenburg, Sweden
www.chalmers.se

COVER IMAGE: Von Mises stress distribution in a polycrystal during oxygen-assisted intergranular fracture.

Printed by Chalmers Reproservice
Gothenburg, Sweden, September 2022

Für Anita & Wolfgang

Abstract

Nickel-based superalloys are a commonly used material in applications where high strength is required at high temperatures. A typical such example is jet engines and, in the case of polycrystalline nickel-based superalloys, components like turbine disks. Under severe loading conditions, such as cyclic loading combined with sustained dwell times at high temperatures, polycrystalline nickel-based superalloys are known to experience accelerated fatigue crack growth in oxygen-rich environments compared to vacuum. Environmentally assisted crack initiation could for example be identified as cause for turbine disk fracture in some cases of mechanical turbine failure of passenger airplanes. It has been shown by experimental work in the past that oxygen is the main deteriorating species in the case of intergranular fracture in nickel-based superalloys.

In this work we develop a fully coupled chemo-mechanical cohesive zone model accounting for the interaction between oxygen transport into the grain boundaries and their stress state. The model is presented in a thermodynamic framework. Additionally, a chemo-mechanical cohesive finite element carrying both the displacement and the concentration field is suggested. The finite element formulation is complemented by a moving boundary condition for the concentration field, accounting for the increase in environment-exposed surface as edge cracks grow into the structure. Aside from handling edge cracks, the moving boundary condition yields physically meaningful results even in the case of crack initiation at interior grain boundaries.

Numerical experiments are conducted on bi- and polycrystals. It is shown that the modeling framework can qualitatively reproduce experimentally observed phenomena, like the reduction of tensile strength in oxygen rich environments, the acceleration of crack growth rates upon increasing environmental oxygen concentration and saturation thereof for high environmental oxygen levels. It is also demonstrated that edge cracks can be propagated past preexisting cracks inside the polycrystal while maintaining realistic oxygen boundary conditions.

Keywords: Intergranular fracture, Grain boundaries, Crystal plasticity, Stress-assisted diffusion, Polycrystal, Crack propagation, Crack growth rate, Moving boundary condition.

List of Publications

This thesis is based on the following publications:

[A] **Kim Louisa Auth**, Jim Brouzoulis, Magnus Ekh, "A fully coupled chemo-mechanical cohesive zone model for oxygen embrittlement of nickel-based superalloys". *Journal of the Mechanics and Physics of Solids*, vol. 164, 140880, Jul. 2022. DOI: 10.1016/j.jmps.2022.104880.

[B] **Kim Louisa Auth**, Jim Brouzoulis, Magnus Ekh, "Modeling of environmentally assisted intergranular crack propagation in polycrystals". *To be submitted for publication.*

Preface

This thesis is a result of my work at the Division of Material and Computational Mechanics, Department of Industrial and Materials Science, Chalmers University of Technology between January 2020 and September 2022. The project has been funded by the Swedish Research Council (Vetenskapsrådet) under the grant numbers 2018-04318 and 2018-06482. The majority of the simulations were performed on resources at the Chalmers Centre for Computational Science and Engineering (C3SE) provided by the Swedish National Infrastructure for Computing (SNIC).

Acknowledgments

First and foremost, I would like to thank my supervisors Magnus Ekh and Jim Brouzoulis for their guidance, encouragement and support. I am grateful for being able to come to your open office doors, for all of our discussions and for the time you take whenever I have a question, but most of all for taking me serious from the very first day.

I want to thank the other `Ferrite.jl` devs, in particular Kristoffer, Fredrik, Elias and Maximilian, collaborating with you has been so much fun! A special thank you goes to Fredrik Ekre, who introduced me to `Julia` and guided me through my first steps in open-source software development. I much appreciate our discussions and am grateful for all of the computing knowledge you have shared with me.

My colleagues make coming to the office a joy. The warm, welcoming, and friendly environment here has made me want to stay from the beginning. Particularly, thanks to my fellow PhD student colleagues, who have made a great effort to become a group of friends! I also want to thank Alexander Hildebrandt, who has been an important part of my decision to become a PhD student. Your mentoring guided me to see how much there is I want to learn.

Finally, I want to thank my family. I am grateful to Anita and Wolfgang for showing me how to always look at the positive side of things and never give up. You are my role models. I thank my parents for raising me in the belief that I can be whomever I want. And I thank my partner Markus for his infinite support and for believing in me every step of the way.

Contents

Part I

Overview

CHAPTER 1

Introduction

1.1 Motivation

Nickel-based superalloys are a class of high-strength, heat resistant materials. For polycrystalline nickel-based superalloys, a shift from transgranular to intergranular fracture is observed if they are subjected to a combination of an oxygen-rich environment, high temperatures and tensile loading sustained over a significant dwell time. In applications that require this class of materials, e.g. gas turbines, parts often experience such a severe combination of loading conditions.

Several cases of intergranular oxygen-assisted fracture have occurred in jet engines in the past. In September 2000, the stage 1 turbine disk of a Boeing 767-2B7(ER) broke during a maintenance ground run; part of the disk broke through a fuel tank and the left wing [2]. In December 2002 on a passenger flight, a Boeing 767-219ER had to return to its origin six minutes into the flight because the left engine failed after a loud noise was heard. The engine failure was caused by fracture of the first-stage high pressure turbine (HPT) disk, which is shown in Figure 1.1 [1]. In June 2006, the stage 1 HPT disk of a Boeing 767-223(ER) failed during a maintenance ground run. The disk

Figure 1.1: Rear face of the broken stage-1 HPT disk from a Boeing 767-219ER (General Electric CF6-80A high-bypass turbofan engine). The fracture originated on the left side of the disk, the initial part of the crack broke intergranuarly. [1]

completely split the engine [3]. In September 2015, the takeoff of a Boeing 777-236ER had to be aborted because the left engine failed and took fire during the takeoff ground roll. Failure was caused by fracture of the stage 8 high pressure compressor disk [4].

These four examples have in common that the fracture through the turbine disks was initiated by intergranular cracking, followed by a transition to transgranular fracture until rupture. All disks were made from polycrystalline nickel-based superalloys. Note that while turbine blades are often manufactured from single-crystalline nickel-based superalloys, disks are commonly made from polycrystalline material. The technical failure investigations indicate that the fractures were initiated by environmentally assisted fatigue crack growth, resulting in stress concentrations at the crack tips that in turn led to failure by other fracture mechanisms. Further detailed information on the metallurgical investigations performed for the 2006 and 2016 engine failures can be found in the metallurgical investigations report by GE [5] and the Materials Laboratory factual report by NTSB [6], respectively.

The measures for avoiding such type of failure of turbines focus on non-destructive crack detection during maintenance. However, in order to be able to design parts which are less likely to experience environmentally assisted cracking, it is crucial to understand the chemo-mechanical fracture phenomenon and to be able to make predictions under which conditions it is likely to occur.

1.2 Research objectives

It would be beneficial for future component design and material choices to improve the understanding of environmentally assisted intergranular fracture of nickel-based superalloys by using modeling and simulations. However, only few modeling efforts have been focused on capturing the interaction between environmental and mechanical effects. The objectives of the first part of this research project have focused on the environmentally assisted and thus intergranular fracture behavior:

- Understand which factors influence environmentally assisted intergranular fracture in polycrystalline nickel-based superalloys.
- Build a numerical framework for predicting the interaction between environmental effects and the mechanical behavior of the polycrystals.
- Capture the dependence of intergranular crack propagation rates on different environmental and loading conditions, including varying dwell times and cyclic loading.

Continuing, for the second part of the project there are several possible research objectives such as:

- Extend the model by a fracture model for transgranular cracks. Investigate the transition regime from transgranular to intergranular fracture and try to predict under which conditions trans- or intergranular fracture occurs. A focus could be on the influence of microstructural mechanical effects on the crack path.
- Extend the model for intergranular fracture to a 3D setting and investigate the influence of out-of-plane effects. A focus could be on the suitability of 2D modeling as a computationally cheaper approximation.

Both possible future research objectives lead to a significant increase in the computational cost and therefore open up for research on strategies for handling expensive models. Such strategies include for example nonlinear preconditioning, GPU assisted linear solvers and adaptive mesh refinement.

CHAPTER 2

Experimental observations

Over the past decades, a significant amount of experimental work has been performed in order to understand the impact of oxygen on intergranular fracture of nickel-based superalloys at high temperatures. This chapter gives a brief overview of experimental work that constitutes the basis for the chemo-mechanical modeling of oxygen-assisted intergranular fracture in this work. The experimental findings are summarized in the list below and translate into different aspects of the model, which will be described in Chapter 3.

1. Reduction of ultimate tensile strength
A reduction of ultimate tensile strength and of ductility is observed in oxygen-rich environments compared to those observed in vacuum. In particular, this effect occurs if the exposure to oxygen is combined with mechanical loading. Oxygen exposure without mechanical loading does not cause material degradation to the same degree. [7]

2. Acceleration of crack growth rate
Crack propagation is accelerated in oxygen-rich environments compared to a vacuum. This effect is particularly pronounced when the specimens are exposed to a dwell time in the oxygen-rich environment during tensile or

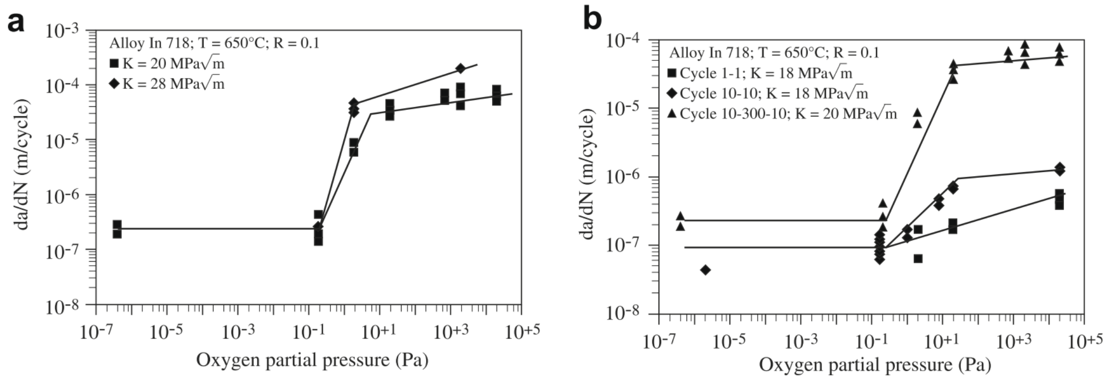

Figure 2.1: Crack propagation rates da/dN increase for increasing oxygen partial pressure in the environment. For higher oxygen partial pressures, a higher stress intensity factor leads to faster crack growth. The crack propagation is also accelerated for lower cyclic loading frequencies (compare the 1s-1s cycle to the 10s-10s cycle in b)). Figure reprinted with permission from [10], original results from [11].

cyclic loading [8], [9], [10].

3. Saturation of crack growth rate upon reaching a critical amount of oxygen
The acceleration of the crack growth rate in oxygen rich environments has been quantified in several experimental studies. The crack growth rates are found to depend on the environmental oxygen content [11], [9] and on the imposed dwell time [12], [8], [13], [14]. Exemplary results for these dependencies are shown in Figures 2.1 and 2.2, respectively.

The dependence of the crack growth rate on the environmental oxygen content is described in Figure 2.1 in terms of the oxygen partial pressure in the environment. Crack propagation per cycle is displayed for increasing oxygen partial pressure for different load levels (compare Figure 2.1a) and for varying dwell time (compare Figure 2.1b). It can be observed that the crack propagation rates are not dependent on the environmental oxygen concentration if it is low. For increasing concentration, there is a region with quickly increasing crack growth rate around 1 Pa of oxygen partial pressure followed by a saturation of the crack propagation rates for high environmental oxygen concentration. It is additionally important to notice that the cracks propagate intergranularly for high oxygen concentrations, but transgranularly for low oxygen concentrations. There is a transitioning region with mixed inter- and transgranular fracture that coincides with the beginning of the region with

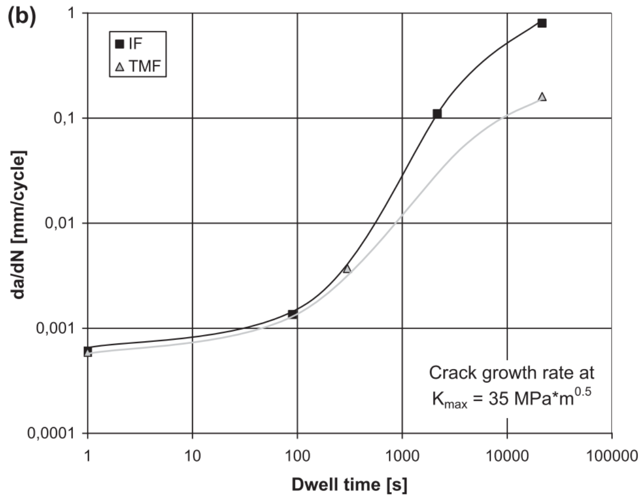

Figure 2.2: Crack propagation rates da/dN increase for longer dwell times at maximum load, both in isothermal fatigue (IF) and in thermo-mechanical fatigue (TMF). For very short and very long dwell times, saturation of the crack growth rate is approached. Figure reprinted with permission from [13]

quickly increasing crack growth rates.

Furthermore, cracks propagate faster for higher loads and for longer dwell times. The latter is quantified in Figure 2.2 by showing crack propagation per cycle for cyclic loading with varying dwell time at the maximum load level. Similarly to the dependence on oxygen pressure, short dwell times have a small impact on the crack growth rate, but with increasing dwell times the cracks grows increasingly fast and for very long dwell times saturation of the crack propagation rates is approached. Like for increasing oxygen concentration, a transition from transgranular crack growth for short dwell time to intergranular crack growth for long dwell times has been observed.

Concluding these observations, the right halves of Figures 2.1 and 2.2 are related to intergranular fracture. It is further concluded that a critical amount of oxygen is needed for causing the acceleration of crack growth. This critical amount of oxygen must be available from the environment in the first place. If it is available, there must be sufficient time for the critical amount of oxygen to enter into the structure. After the material has been damaged by a sufficiently high oxygen concentration, further increase of the oxygen concentration in the material does not affect the intergranular fracture process.

4. Presence of oxygen only along grain boundaries
Oxygen is found exclusively along grain boundaries and does not significantly diffuse into the grains [15], [16]. Notice that this is a major difference from hydrogen embrittlement where hydrogen diffusion into the bulk material is a relevant process.

All four above described effects are based on the presence of oxygen in the environment and in the material ahead of the crack tip. This work takes the fundamental assumption that oxygen diffusion into the grain boundaries ahead of the crack tip happens and that oxygen causes degradation of the grain boundaries. However, no assumption is made on what the chemo-mechanical phenomenon causing the material degradation is.

CHAPTER 3

Modeling

3.1 Chemo-mechanically coupled cohesive zone model

As the possible crack paths are a priori known to be intergranular, cohesive zone modeling is used for representing the cracks. Hence, cohesive elements are introduced along all grain boundaries. An adaption of the well known Xu-Needleman cohesive law ([17]) by Kolluri *et al.* [18] that adds irreversible damage is used as a base model for the mechanical behavior of the grain boundaries. In this section, an overview of the additions made to the base cohesive law in order to account for the chemo-mechanical phenomena discussed in Chapter 2 is given. For a complete model formulation, the reader is referred to Paper A.

A concentration field c is introduced on the grain boundaries, i.e. in the cohesive elements. As it is known that oxygen is present only along grain boundaries, there is no need for a concentration field in the bulk material. Firstly, the effect of the concentration field on the cohesive law will be described. Secondly, the oxygen transport into the structure is discussed.

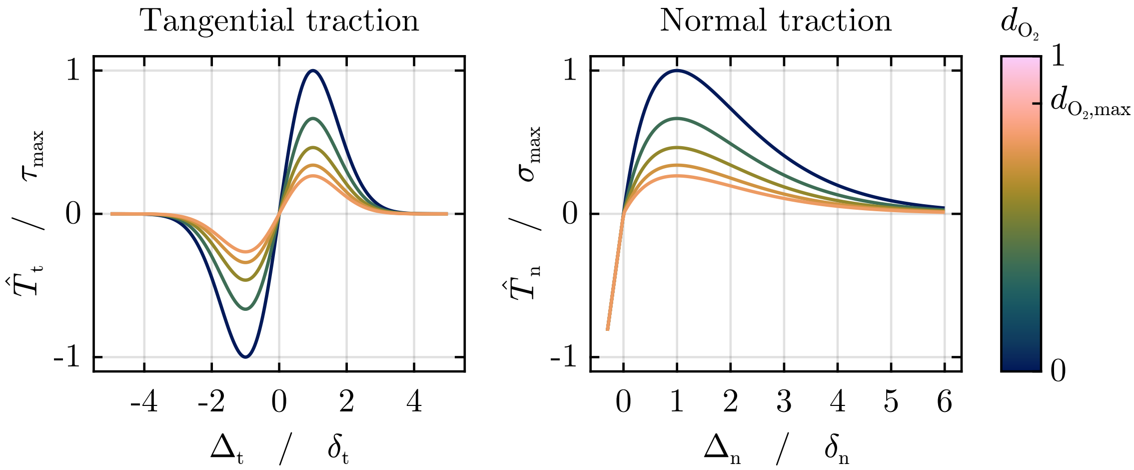

Figure 3.1: Environmental degradation of cohesive law. Initially, the strength of the cohesive law is $\tau_{\max}$ in tangential and $\sigma_{\max}$ in normal direction. The maximum traction in each direction is reached when the respective jump Δ_t / Δ_n reaches its characteristic value δ_t / δ_n. For increasing environmental damage d_{O_2}, the tractions in normal and tangential direction decrease.

Environmental damage

To account for the reduction of ultimate tensile strength and thereby give rise to the accelerated crack growth, the tractions resulting from the base cohesive law $\boldsymbol{T}^{\text{base}}$ are reduced by an environmental damage variable d_{O_2} such that

$$\hat{\boldsymbol{T}} = \left(1 - d_{O_2}\, \mathcal{H}\left(\Delta_n\right)\right) \boldsymbol{T}^{\text{base}}\,, \tag{3.1}$$

where Δ_n is the normal jump along the interface and $\mathcal{H}$ is the Heaviside function. The resulting tractions $\hat{\boldsymbol{T}}$ are represented in Figure 3.1. The strength of the cohesive law, and thus the fracture energy, is reduced upon increasing the environmental damage d_{O_2}. The reduction only happens for positive normal separation jumps $\Delta_n > 0$. Notice that the initial stiffness of the cohesive law is also reduced.

The spatial domain of standard mechanical cohesive elements is their mid-plane, thus the dimension of the domain is reduced by one compared to the overall spatial dimension. In order to differentiate between quantities defined in the spatial dimension and on the mid-plane, the oxygen concentration on the mid-plane of the cohesive elements is introduced as grain boundary con-

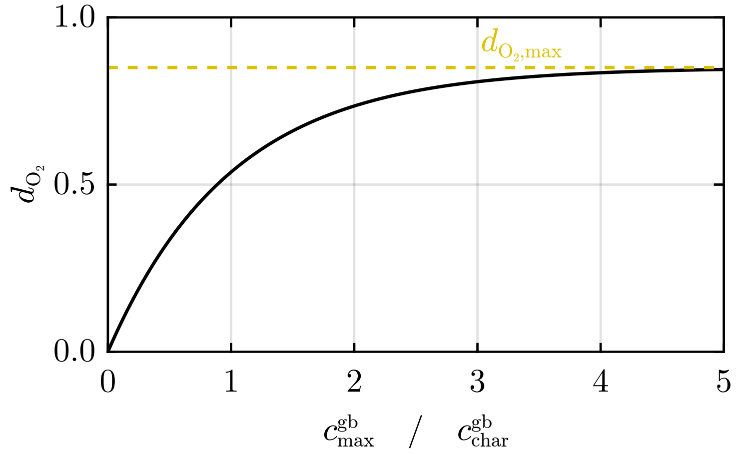

Figure 3.2: Relation between the environmental damage variable d_{O_2} and the maximum grain boundary concentration c^{gb}_{max}. The damage variable increases quickly around a characteristic oxygen concentration c^{gb}_{char}, which can be related to the regions of high crack rate acceleration in Figure 2.1.

centration c^{gb} and all quantities denoted with superscript gb subsequently refer to the domain of the cohesive elements.

The environmental damage is the main model feature for causing the accelerated crack growth rate. Therefore, the experimentally observed saturation effects in crack rate acceleration come into the model at this point. As explained in Chapter 2, it is assumed that the saturation effects can be related to reaching a critical amount of oxygen in the grain boundaries. The crack growth rate increases quickly around a characteristic oxygen concentration c^{gb}_{char} and approaches saturation for much larger concentrations. This is reflected in the model by using an exponential relation between the oxygen concentration and the environmental damage

$$d_{O_2} = d_{O_2,max} \left(1 - \exp\left(-c^{gb}_{max} \,/\, c^{gb}_{char}\right)\right) , \tag{3.2}$$

where the history variable c^{gb}_{max} has been introduced as maximum experienced oxygen concentration in a material point in order to ensure irreversibility. Additionally, an upper limit of the environmental damage $d_{O_2,max}$ is introduced as a model parameter. The relation between oxygen concentration and environmental damage is shown in Figure 3.2.

Stress-assisted oxygen diffusion

The base assumption for oxygen transport into the structure is that oxygen diffuses along the grain boundaries. This is accounted for by a diffusive oxygen flux $\boldsymbol{j}^{\mathrm{gb}}_{\mathrm{chem}}$ according to Fick's law. Additionally, it is known that accelerated crack growth is associated with oxygen exposure under mechanical loading. In order to account for this, the assumption of stress-assisted diffusion towards high hydro-static stresses (originally suggested by Sofronis and McMeeking [19] in the context of hydrogen embrittlement) is adopted. As the hydrostatic stress is not readily available in cohesive elements, the mechanically assisted flux $\boldsymbol{j}^{\mathrm{gb}}_{\mathrm{mech}}$ is instead assumed to be proportional to the gradient of normal traction $\boldsymbol{\nabla}^{\mathrm{gb}}\hat{T}_{\mathrm{n}}$. The oxygen flow in the grain boundaries $\boldsymbol{j}^{\mathrm{gb}}$ can then be expressed as

$$\boldsymbol{j}^{\mathrm{gb}} = \underbrace{-\,D\,\boldsymbol{\nabla}^{\mathrm{gb}} c^{\mathrm{gb}}}_{\boldsymbol{j}^{\mathrm{gb}}_{\mathrm{chem}}} + \underbrace{D\,c^{\mathrm{gb}}\,\frac{V_{\mathrm{O_2}}}{\mathrm{R}\,T}\,\boldsymbol{\nabla}^{\mathrm{gb}}\hat{T}_{\mathrm{n}}}_{\boldsymbol{j}^{\mathrm{gb}}_{\mathrm{mech}}}\,. \tag{3.3}$$

Therein, the introduced model parameters are the base diffusivity along grain boundaries D and for the partial molar volume of oxygen in metal $V_{\mathrm{O_2}}$. Further, R is the universal gas constant and T is the absolute temperature. In the damage zone, the mechanical flux $\boldsymbol{j}^{\mathrm{gb}}_{\mathrm{mech}}$ is the dominant phenomenon transporting oxygen into the grain boundaries, thus ensuring that significantly less oxygen can enter the structure without mechanical loading ($\boldsymbol{\nabla}^{\mathrm{gb}}\hat{T}_{\mathrm{n}} = \boldsymbol{0}$). However, the chemical flux $\boldsymbol{j}^{\mathrm{gb}}_{\mathrm{chem}}$ plays an important role in the initiation of the degradation process, as it is the first phenomenon bringing small amounts of oxygen into the structure. The oxygen starts to degrade the cohesive law according to Equation (3.1), resulting in increasing traction gradients between regions with and without oxygen. This in turn gives rise to the traction assisted oxygen flux.

3.2 Moving boundary condition

In order to compute crack propagation rates in polycrystals, it is crucial to be able to propagate cracks through polycrystals and to track their crack tips. This requires a criterion to determine if a material point is broken and a way to compute the crack length. Further, specific treatment of the chemical

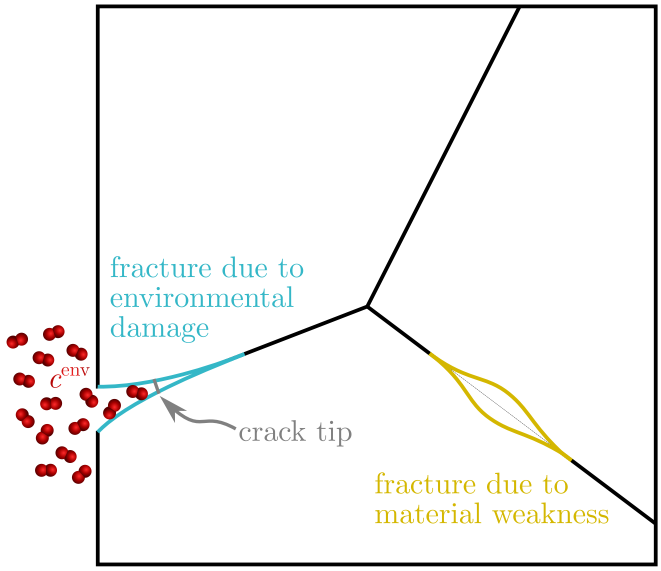

Figure 3.3: Different fracture scenarios: Edge cracks (blue / left) should fill up with oxygen, while interior cracks (yellow / right) should not.

boundary conditions is needed, as the outer boundary of the structure changes when cracks open up.

A local fracture criterion based on the remaining strength of the grain boundaries in the normal direction σ_r is used here. For a given fracture limit value T_f, broken regions Γ_f are a subset of the grain boundaries Γ_s and are defined as

$$\Gamma_f = \{\boldsymbol{X} \in \Gamma_s : \sigma_r \leq T_f\}. \tag{3.4}$$

For details, the reader is referred to Paper B.

As cracks grow from the domain boundary into the structure and open up, the crack flanks are also exposed to the environmental oxygen concentration c_{env}. Consider the fracture due to environmental damage in Figure 3.3 (blue). Originally, only the domain boundary was exposed to c^{env}. In the state depicted in the Figure, the crack has propagated, leaving the crack flanks (left from the crack tip) exposed to the environment. As the crack propagates further, the fractured domain Γ_f changes.

The coupled chemo-mechanical cohesive zone model presented in Paper A describes the material behavior ahead (i.e. right in Figure 3.3) of the crack tip. It is therein assumed that the oxygen concentration behind the crack tip (in the broken regions) is the environmental oxygen concentration c^{env}.

Therefore, an oxygen boundary condition that moves along with the crack tip is needed. Additionally, cracks can in general originate anywhere, not only at the outer boundary of the structure. A crack that initiates inside the structure (e.g. due to a material weakness, compare with the yellow / right crack in Figure 3.3) should not fill up with oxygen as long as it is not connected to the oxygen supply.

To fulfill these requirements, a penalty approach that penalizes the concentration gradient $\boldsymbol{\nabla}^{\mathrm{gb}} c^{\mathrm{gb}}$ in the broken regions Γ_{f} is proposed. Combined with Dirichlet boundary conditions on the concentration field at the outer boundary of the structure, this approach enforces the environmental oxygen concentration in edge cracks, as spatial changes of the concentration are not allowed wherever the grain boundaries are broken. On the other hand, for a crack unconnected to the boundary, the only effect is a constant concentration throughout the crack. This corresponds to an instantaneous oxygen flow through it.

The penalty condition is imposed by adding an additional term to the weak form of the mass conservation of oxygen

$$p_{\mathrm{bc}} \int_{\Gamma_{\mathrm{s}}} \mathcal{H}\left(T_{\mathrm{f}} - \sigma_{\mathrm{r}}\right) \, \boldsymbol{\nabla}^{\mathrm{gb}} c^{\mathrm{gb}} \cdot \boldsymbol{\nabla}^{\mathrm{gb}} \delta c^{\mathrm{gb}} \, \mathrm{d}A \,, \tag{3.5}$$

where p_{bc} is a penalty coefficient and δc^{gb} is the variation of c^{gb}. The Heaviside function cancels the term in non-broken material points. Notice that this term can also be interpreted as an additional oxygen flux due to the moving boundary condition $\boldsymbol{j}_{\mathrm{bc}}^{\mathrm{gb}}$. This oxygen flux should however be a strictly trailing phenomenon to the fracture process and only interact with the coupled cohesive zone model in terms of supplying realistic conditions behind the crack tip.

In practice, the penalty term also needs to be regularized in order to avoid numerical difficulties. Details of the regularization are given in Paper B.

3.3 A perspective: Inter- vs. transgranular fracture

The presented model is a cohesive zone model that predicts fracture in the grain boundaries. However, as discussed in Chapter 2, fracture only occurs intergranularly under certain conditions and a transitioning region with both trans- and intergranular fracture has been experimentally observed. Such a mixed fracture region has also been observed in the turbine disks discussed in section 1.1. While transgranular fracture is (not yet) possible with the present model, the model can be used as the tool accounting for intergranular fracture in a mixed trans-/intergranular fracture setting.

The following scenario is suggested for incorporating transgranular fracture and including a transitioning region to intergranular fracture: Undamaged grain boundaries have a higher strength than the bulk material. Thus the base fracture mechanism would be transgranular fracture, as observed e.g. in vacuum or in a lack of time for oxygen to enter the structure. A possible choice for modeling fracture through the grains is to adopt a phase-field model. A similar approach has recently been suggested by Valverde-González *et al.* [20] for hydrogen embrittlement.

Upon oxygen exposure, the grain boundaries are weakened until they become weaker than the bulk material. If sufficiently much oxygen is supplied and it enters the structure sufficiently fast, fracture becomes purely intergranular. The mixed fracture region naturally arises from the transition between these two scenarios. If the strengths of the grains and the grain boundaries are approximately equal, the local chemo-mechanical conditions determine where the crack growths. Possible factors influencing the crack growth in this case could e.g. be the grain size, crystal orientations or local stress concentrations (for example arising from material defects or at grain boundary intersections).

CHAPTER 4

Concluding Remarks and Future Work

Environmentally assisted intergranular fracture is a phenomenon that reduces the life-time of components made of nickel-based superalloys. Examples of such components are turbine disks of jet engines. While the phenomenon has been known and experimentally investigated for many years, there has been less work on numerical modeling of the interaction between the environment and the mechanical behavior of polycrystals.

In this work, we present a numerical framework for predicting the interaction of oxygen, acting as embrittling element, and accelerated intergranular fracture of polycrystals. The framework is based on chemo-mechanical phenomena which were inferred from a literature study of various experimental results on intergranular fracture of nickel-based superalloys. The framework is thermodynamically consistent, and it has been shown in Paper A that it can qualitatively reproduce important experimental results, such as stress relaxation in oxygen-rich environments. In Paper B the framework is extended to allow for crack propagation and computation of crack growth rates. It has therein been demonstrated that reasonable relations between the environmental oxygen content and the crack growth acceleration in the case of intergranular fracture can be predicted.

With these results, the major part of the first set of research objectives has been achieved. However, the results from Paper B are thus far limited to monotonic loading. Most realistic loading conditions, e.g. in the turbine disk examples, include cyclic loading. In the case of the turbine disks the loading / unloading would correspond to starting / stopping the engines, with a significant dwell time under loading while the engine is running. Thus, the work in Paper B should be complemented by applying the presented model to cyclic loading scenarios.

Coming to the second half of this project, there are several possible paths to follow. So far, in all simulations a 2D plane strain assumption has been adopted. An evaluation of the importance of 3D effects and the suitability of the 2D assumption would be relevant for future numerical research on this topic, especially when trying to approach simulations on a structural rather than a micro-structural scale. Another possibility could be an extension of the current model to fully resolve the micro-structural behavior and also allow for transgranular fracture. It would especially allow evaluations of the micro-mechanical effects that influence the transition from trans- to intergranular fracture.

Either of these paths lead to significantly increased computational cost of the current model. The full simulation code for this project has been written in the Julia programming language, making use of open-source software packages. Hence, we have full access to all parts of the program. We intend to use this for investigating strategies for handling and reducing the computational cost, by using e.g. non-linear preconditioning, GPU assisted linear solvers and adaptive mesh refinement.

References

[1] Australian Transport Safety Bureau, "In-flight uncontained engine failure and air turn-back, Boeing 767-219ER, ZK-NBC 8," *Aviation Safety Investigation Report*, no. 200205780, 2002.

[2] J. Hall, "Safety Recommendation, A-00-121 through -124, GE CF6-80C2B2 engine failure," *NTSB Safety Recommendation*, 2000.

[3] M. V. Rosenker, "A-06-60 to -64, Report on General Electric CF6-80A engine failure from June 2, 2006," *NTSB Safety Recommendation*, 2006.

[4] Jean-Pierre Scarfo, "NTSB Powerplant Group Chairman's factual report, General Electric GE90-85BG11 turbofan engine failure," *NTSB Factual Report*, 2016.

[5] B. G. Gieseke, "METALLURGICAL EVALUATION OF CF6-80A HPT STAGE 1 DISK / SHAFT DISK SEPARATION EVENT AT LAX ON JUNE 2 , 2006," *GE Aviation, MPED-Metallurgical Investigations*, 2006.

[6] D. Kramer, "Report No. 15-131, General Electric GE90-85BG11 turbofan engine failure," *NTSB Materials Laboratory factual report*, no. Report No. 15-131, 2016.

[7] C. T. Liu and C. L. White, "Dynamic embrittlement of boron-doped Ni3Al alloys at 600°C," *Acta Metallurgica*, vol. 35, no. 3, pp. 643–649, 1987, ISSN: 00016160.

[8] E. Andrieu, R. Molins, H. Ghonem, and A. Pineau, "Intergranular crack tip oxidation mechanism in a nickel-based superalloy," vol. 154, pp. 21–28, 1992, ISSN: 09215093.

[9] J. A. Pfaendtner and J. J. McMahon, "Oxygen-induced intergranular cracking of a Ni-base alloy at elevated temperatures - An example of dynamic embrittlement," *Acta Materialia*, vol. 49, no. 16, pp. 3369–3377, 2001, ISSN: 13596454.

[10] A. Pineau and S. D. Antolovich, "High temperature fatigue of nickel-base superalloys - A review with special emphasis on deformation modes and oxidation," *Engineering Failure Analysis*, vol. 16, no. 8, pp. 2668–2697, 2009, ISSN: 13506307.

[11] R. Molins, G. Hochstetter, J. C. Chassaigne, and E. Andrieu, "Oxidation effects on the fatigue crack growth behaviour of alloy 718 at high temperature," *Acta Materialia*, vol. 45, no. 2, pp. 663–674, 1997, ISSN: 13596454.

[12] H. Ghonem and D. Zheng, "Depth of intergranular oxygen diffusion during environment-dependent fatigue crack growth in alloy 718," *Materials Science and Engineering A*, vol. 150, no. 2, pp. 151–160, 1992, ISSN: 09215093.

[13] J. J. Moverare and D. Gustafsson, "Hold-time effect on the thermo-mechanical fatigue crack growth behaviour of Inconel 718," *Materials Science and Engineering A*, vol. 528, no. 29-30, pp. 8660–8670, 2011, ISSN: 09215093.

[14] H.-J. Christ, K. Wackermann, and U. Krupp, "Materials at High Temperatures Effect of dynamic embrittlement on high temperature fatigue crack propagation in IN718-experimental characterisation and mechanism-based modelling Effect of dynamic embrittlement on high temperature fatigue crack propagation," 2016, ISSN: 1878-6413.

[15] L. Viskari, M. Hörnqvist, K. L. Moore, Y. Cao, and K. Stiller, "Intergranular crack tip oxidation in a Ni-base superalloy," *Acta Materialia*, vol. 61, no. 10, pp. 3630–3639, 2013, ISSN: 13596454.

[16] M. Hörnqvist, L. Viskari, K. L. Moore, and K. Stiller, "High-temperature crack growth in a Ni-base superalloy during sustained load," *Materials Science and Engineering A*, vol. 609, pp. 131–140, 2014, ISSN: 09215093.

[17] X. P. Xu and A. Needleman, "Void nucleation by inclusion debonding in a crystal matrix," *Modelling and Simulation in Materials Science and Engineering*, vol. 1, no. 2, pp. 111–132, 1993, ISSN: 1361651X.

[18] M. Kolluri, J. P. Hoefnagels, J. A. Van Dommelen, and M. G. Geers, "Irreversible mixed mode interface delamination using a combined damage-plasticity cohesive zone enabling unloading," *International Journal of Fracture*, vol. 185, no. 1-2, pp. 77–95, 2014, ISSN: 03769429.

[19] P. Sofronis and R. M. McMeeking, "Numerical analysis of hydrogen transport near a blunting crack tip," *Journal of the Mechanics and Physics of Solids*, vol. 37, no. 3, pp. 317–350, 1989, ISSN: 00225096.

[20] A. Valverde-González, E. Martínez-Pañeda, A. Quintanas-Corominas, J. Reinoso, and M. Paggi, "Computational modelling of hydrogen assisted fracture in polycrystalline materials," *International Journal of Hydrogen Energy*, no. xxxx, 2022.