6 Conclusion and Outlook

Fatigue crack initiation and short fatigue crack growth are strongly influenced by the underlying microstructure, which is documented by Tokaji et al. [119] and Suresh [14]. An improved understanding of the deformation features on microstructural scale helps to understand the complex interactions between cracks and microstructure and helps to introduce new methods in designing materials with improved fatigue properties.

With the implemented numerical framework it is possible to link microstructural features directly to fatigue properties. With the implemented tool it is possible to identify and quantify influencing parameters based on a microstructural basis. Currently applied models describe the fatigue behaviour of materials as function of the global stress state, neglecting the microstructural influence on local deformations, which are however important for fatigue crack initiation. In most experiments the local stress state and deformation cannot be measured directly, which stresses the importance of numerical tools on microscale. In this thesis the focus is set on accumulation of irreversible deformation, fatigue crack initiation and short fatigue crack growth on microstructural scale. With the help of the dynamical microstructure generator statistically similar RVEs with prescribed grain size distribution can be reproduced. Material deformations are described by a crystal plasticity model with three distinct hardening formulations and the occurring deformations can be analysed with respect to fatigue susceptibility. Additionally, fatigue crack growth can be modelled. The results of the studies performed in chapter 5 and the drawn conclusions are summarized in the following. The derived understanding of microstructural influence on fatigue ranging from accumulation of irreversible deformation to final coalescence of crack networks is pointed out.

Derived micromechanical fatigue understanding

The understanding is derived from the simulations performed in this study. It is valid for polycrystalline materials fatigued under cyclic loading conditions with \( R = -1 \), where failure is known to be affected by the accumulation of plastic deformation. Fatigue modelling up to the stage of final coalescence of the crack network on RVE level can be subdivided into four different parts. The parts are visualized in figure 6.1 summarising the main results of the different simulations performed. The mechanisms taking place during localisation of deformation are derived from the results presented in detail in section 5.1.
Figure 6.1: Overview of derived micromechanical fatigue understanding subdivided into four regimes which take place sequentially. Accumulation and localisation of irreversible deformations is followed by fatigue crack nucleation. Initiated cracks grow in the short fatigue crack growth regime and fatigue crack coalescence takes place in the final stage of crack propagation.
Mechanisms taking place during crack initiation are extracted from [section 5.2]. Impacts of microstructure on fatigue crack growth and final fatigue crack coalescence are derived from [section 5.3]. In the following, the main conclusions are summarized, while a more detailed description can be found in the description of the individual regimes.

**Regime 1: Localisation of deformation**

Before fatigue crack nucleation takes place, irreversible deformations accumulate during cyclic loading. During this accumulation, significant irreversible deformations accumulate, which will finally lead to fatigue crack initiation if reaching a critical point. Complex processes of dislocation accumulation, nucleation and structure evolution take place that are influencing material hardening and, thus, the further evolution of plastic deformation. These effects can be described on phenomenological basis by the crystal plasticity model implemented. The anisotropic nature of elastic and plastic deformation is captured by the crystal plasticity model as well as the hardening evolution during cyclic loading. To capture cyclic hardening correctly, it has to be differentiated between isotropic hardening, kinematic hardening and dislocation structure evolution. While isotropic hardening determines the initial work hardening of materials, kinematic hardening captures the Bauschinger effect appearing during load reversal. Especially dislocation structure evolution turns out to lead to localized plastic deformation and gives insight in slip band formation. The consideration of dislocation structure evolutions leads to regions developing a smaller resistance against plastic deformation and thus a localisation of plastic deformation. The evolution of these regions and their spreading in the material depends on the applied strain range. Depending on the actual material considered, the different hardening mechanisms might be more or less pronounced.

**Regime 2: Fatigue crack nucleation**

The regime of localised plastic deformation is followed by the fatigue crack initiation regime. Fatigue crack initiation can be based on fatigue indicator parameters that are able to describe the detrimental effect of irreversible deformation within the polycrystalline material considered. Depending on the material, the loading condition and the failure mode, different indicator parameters can be used. Fatigue crack initiation takes place in regions of localized plastic deformation. During the simulations it turned out that possible localisation regimes are regions of grains prone to plastic deformation, grain boundary regions between grains showing a strong difference in plastic deformation or regions located in the vicinity of defects. Depending on the defect size, the defect type and the defect position and also on the applied loading range, defects are more detrimental or less. This thesis has shown that often multiple regions in the microstructure nucleate cracks, which are evolving independently in the beginning of the fatigue simulation.
in cases of very localized deformation, a crack from a single nucleation point develops. The actual locations of crack nucleation depend on various microstructural features, which lead to localized plastic deformation and, thus, a prediction of exact crack nucleation regimes previous to the calculation is not possible. Nonetheless, grains with favourable orientation for plastic slip indicated by the maximum Schmid factor, grain boundaries between grains having a strong difference in maximum Schmid factor and especially regions next to defects have shown to be favoured regions for crack nucleation, while the interplay of all influencing effects is complex.

**Regime 3: Short fatigue crack growth**

The microstructural short crack growth regime is the regime where cracks are strongly influenced by the underlying microstructure. After first crack initiation, which takes place at the aforementioned regions, a crack network starts to develop. The actual crack growth kinetics and the subsequent crack network evolution is governed by the landscape of accumulated plastic deformation evolving in the microstructure during cyclic loading. The more influenced this landscape is by a single strong defect, the more likely it is that a single crack nucleates and grows within the microstructure, while a very homogeneous plastic deformation landscape leads to multiple crack initiation points. Simulations without defects have shown that mostly multiple cracks nucleate at grain boundary regions. Within these simulations, multiple fatigue cracks initiate as several regions in the microstructure have accumulated similar amounts of plastic deformation and reach the critical accumulated shear strain nearly contemporaneously. Initial fatigue crack growth mostly takes place at interface regions, where different cracks develop in the microstructure. If defects within the microstructure are considered from the beginning of the simulation, the plastic deformation landscape is very heterogeneous and defect near regions have accumulated considerably more plastic deformations compared to the defect free case. Crack initiation sites, which are in case of defect free RVEs located at certain grain boundaries, shift from these grain boundary regions to defect-near regions. This leads mostly to a more localized crack initiation point and a defect dominated crack initiation and growth within the microstructure.

Additionally to the microstructural features discussed, also the applied loading range plays a role during fatigue crack initiation. Simulations have shown that the smaller the loading amplitude, the more localized plastic deformation takes place. Projecting this on the crack growth behaviour, the smaller the loading amplitude the more likely it is that only a single crack evolves within the RVE.
Regime 4: Fatigue crack coalescence

Fatigue crack coalescence takes place after the regime of short fatigue crack growth and is mainly determined by the type of applied loading. If cracks have developed to sizes in a considerable length compared to the RVE dimensions, cracks start to interact within the microstructure and, due to periodicity, also over the periodic boundaries of the RVE. While the driving force for strain controlled loading shows a retarding trend on fatigue crack growth rate during cyclic loading conditions especially for smaller strain amplitudes, for stress controlled loading crack growth rates accelerate with increasing crack length rather independent on the actual applied stress range. During fatigue crack coalescence the evolved subcracks within the microstructure collapse and form a connected crack network. Due to the pronounced localisation between adjacent subcracks, subcracks connect rather independently from microstructural features. The connection is mostly oriented in a $45^\circ$ inclination towards the loading direction.

Outlook

The implemented framework is built on a modular basis consisting of three main modules. First the generation of representative volume elements, second the material model and third the fatigue evaluation. In the following, suggestions for future improvements are given.

- The irreversibility factor is an important parameter if quantitative predictions of the model are in the centre of interest. An experimental method to characterise the irreversibility factor can be found in [127], but identification of exact values is difficult and the understanding is still not complete. Nowadays, molecular dynamics simulations are capable of accessing systems and cycle numbers that are large enough to determine influencing parameters of the cyclic slip irreversibility and will give a more fundamental understanding of relevant processes. Complementary, very sensitive eigenfrequency fatigue experiments [132] can be performed which are capable to track the development of slip bands and small fatigue cracks and will give a more detailed insight.

- The implemented crystal plasticity model does not capture strain gradient effects, but describes dislocation interaction mechanisms via phenomenological models. On the one hand, the phenomenological models, which have a high number of material parameters, need to be fitted to experiments if one specific material is investigated. On the other hand, higher order crystal plasticity models, that are described by more physically based models, capture the effects implemented by the phenomenological models inherently. They might make the complex fitting process of phenomenological parameters easier, as their parameters are easier accessible.
from lower scale models, which leads to an improved understanding of the influence of individual parameters. Additionally, with the usage of higher order plasticity models size effects, that are currently not included into the model, are inherently considered.

- The established numerical framework is checked for functionality without referring to a specific steel grade comparing homogenised properties of the RVE. In detail, numerically determined stress-strain hysteresis are compared to experimentally measured ones in figures 5.14 and 5.18. For an exact calibration and verification of the material model used, local deformations have to be compared. Therefore, digital image correlation techniques can be used that are capable of measuring local deformations, which are predicted by the crystal plasticity model. Digital image correlation (DIC) techniques are already successfully applied for the analysis of fatigue or damage mechanisms on a microstructural scale in [133, 134]. As this thesis proposes a statistical equivalent representation of microstructures, local deformations have to be statistically evaluated using the methods proposed in section 4.3 and compared to results of the DIC on a statistical basis. Additionally, the modelled crack paths need to be compared to experimentally observed ones, which is already exemplary shown in figure 5.34 on a qualitative basis.

- During numerical assessment of fatigue experiments numerical expenses are always a problem. Mostly it is not possible to simulate every single cycle and mechanisms have to be extrapolated. An enhanced ansatz to overcome this problem is the usage of the wavelet transformation which is proposed for crystal plasticity simulations within the finite element method by the research group of Gosh [120, 121]. The implementation of an improved method will help to simulate more cycles and reduce the extrapolation errors.

- Currently the critical accumulated plastic slip is approximated based on values determined by Manonokul and Dunne [109]. For an improved quantitative predictability of the model an experimental determination following the concepts of Manonokul and Dunne is proposed.

- In this thesis the normalized effective crack length of the whole crack network within the RVE is determined. Further evaluations are based on this quantity. For an improved identification of microstructural influences on crack growth different sub-cracks and their crack tip evolution have to be triggered. In this case crack growth kinematics can be more closely investigated, as the effects are not superposed by several growing sub-cracks which are analysed combined.

- Additionally to the proposed enhancements of the code, the current framework can be applied to additional applications. Interesting extensions are the application
to larger RVEs, the generation of more realistic microstructures with improved
defect distributions, the consistent usage of three-dimensional models and detailed
parameter variations of the crystal plasticity model. As a first order approximation
of grain size effects, a Hall-Patch like behaviour can be included into the hardening
mechanisms used and the influence of grain size can be tested.

- The influence of misorientation, which is documented in [135, 136] is not reproduced
  by the model used in this thesis. In this thesis cracks nucleated at the grain boundary
in case of defect free RVEs, but prone sites for these initiation effects are not found
to be regions with high misorientation between grains. Instead grain boundaries
spererating grains with high differences in susceptibility for plastic deformation are
found to initiate cracks. As only limited number of defect free RVEs is studied, a
study investigating a higher number of RVEs will show if the effect of misorientation
on fatigue crack initiation spots is already captured with the local crystal plasticity
model. If this is not the case, the effect of misorientation on the crack growth
behaviour, might be reproduced if higher order crystal plasticity models are taken
into account. These crystal plasticity models might be capable of reproducing the
effect of grain boundaries on fatigue crack growth more accurately. Pile up effects
at grain boundaries having a higher misorientation are the natural outcome of
such models like shown by Boeff, Ma and Hartmaier [105] for monotonic loading
conditions and might influence the crack path evolution.

- The studies enable to analyse the crack growth kinetics as function of properties
  that influence crack growth, which are shown by the crack growth rate

\[
\frac{da}{dN} = f (\text{loading type, loading range, defects, microstructure})
\]  

(6.1)

that depends on the aforementioned influencing factors. In section 5.3 the influence
of these effects on fatigue crack initiation and growth is shown, while the strength of
individual influences can be extracted comparing the crack growth kinetics visible
in figures 5.17, 5.19, 5.26 and 5.27. It is shown that loading range and loading type
strongly influence the crack growth kinetics. Additionally, the distinct influence of
different defects is analysed and the influence of microstructure is analysed. In order
to understand the strength of influencing factors on fatigue crack growth, all these
influencing parameters and their strength need to be determined. By comparison of
the effect of influencing factor on the crack growth kinetics the strength of defect can
be dimensioned. Examples for this are given in figures 5.26 and 5.27 for the influence
of voids and microstructure on crack growth rates. For statistically relevant results
a larger number of simulations with larger RVEs need to be performed and the
strength of influencing factors in equation (6.1) can be determined. Due to the modular structure of the numerical framework developed in this thesis, improving or exchanging modules is simple.