Summary

Dislocations have been found experimentally to play a fundamental role for fatigue crack initiation. Even prior to macro-scale plasticity, dislocations get generated during cyclic loading, which cluster and form channel-vein structures and later on ladder-like structures. Ladder-like structures are found inside persistent slip bands which carry most of the plastic deformation and lead to surface roughness, in the form of so-called ex-, in- and protrusions.

This thesis presents a study of these phenomena by way of a two-dimensional discrete dislocation model of a grain near a stress-free surface. The neighboring material is assumed to remain elastic, while the grain can deform plastically by edge dislocations moving on multiple slip systems. Their movement is controlled by the Peach-Koehler force, incorporating the singular long-range effects of the other dislocations, the image stress from the free surface as well as the applied load. Dislocation pairs can be generated from Frank-Read sources. Annihilation is taken into account, as well as disappearance of dislocations at the free surface, leading to surface roughening. Finally, dislocations can become pinned at point obstacles, which represent, for instance, forest dislocations and small precipitates. The model predicts high tensile stresses at the grain boundaries, along the primary slip planes and at the free surface. For the chosen material parameters and stress levels, the dislocation density is initially increasing very rapidly and after around 100 cycles the rate of growth decreases. The dislocation density is high along the primary slip planes and along the grain boundaries. The area close to the free surface is almost dislocation-free due to the image force pulling dislocations out of the grain. However, with this model it is not possible to capture the clustering of dislocations.

In a subsequent extended version, three-dimensional effects are included. Here, dislocations can form junctions that act as obstacles or nucleation sites. These junctions are nucleated and broken depending on three-dimensional mechanisms. Additionally, line tension is incorporated. With these extensions, dislocations form stable clusters and dislocation-free regions. Furthermore, the dislocation density is higher due to junctions hindering the dislocation motion. This dislocation distribution is similar to the cell structure found in experiments for multiple slip. However, still no channel-vein structures are found in the

simulations.

The experimental finding that dislocations arrange in structures during cyclic loading has been used by various authors in the past to estimate dislocation-structure induced stresses near a free surface, which may lead to fatigue crack initiation. These structures were highly idealized ones. Here, dislocation statics and dynamics is used for a more realistic calculation of the stresses near the surface as the dislocation configuration evolves during cyclic loading.

A single dislocation moving out of the grain at the free surface leaves a surface step. Multiple of these events produce intrusions and extrusions, which continue to grow with continuing load cycles. These surface steps produce stress singularities, which may assist in triggering fatigue crack initiation. The stress field due to the surface steps is approximated analytically using the wedge solution from the theory of elasticity. This approximation is compared to approximations proposed by other authors and to numerical calculations. It is found to be fair close to the surface step, but to overestimate the stresses in the bulk.

Stress-strain curves are considered to investigate the influence of grain shape and size as well as the loading condition. Dislocation dynamics predicts a size effect, i.e. small grains are harder. Furthermore, under stress-controlled conditions the maximum strain is decreasing over time due to hardening. For the same reason, the maximal stress increases in strain-controlled simulations.

Cohesive surfaces, which account for both mode I and mode II opening, are added to model crack initiation. The stress leading to crack opening includes contributions from the dislocation distribution as well as from the surface roughness. Initially the cohesive opening at the free surface behaves elastically and the dislocation density builds up as without cohesive surfaces. Afterwards, the dislocation density increases significantly and this leads to an increase in the cohesive opening up to the formation of a crack. The model prefers the crack to initiate normal to the free surface. Moreover, the contribution to fatigue crack initiation from the dislocation distribution is stronger than the contribution from the surface roughness.

The simulation predicts, without any assumptions about dislocation structures, that dislocations can cause fatigue crack initiation with the help of the surface roughness they produce. Fatigue cracks initiate without any environmental influence, i.e. damage to the atomic structure due to the oxidation of the crack surface, or thermal effects, like climbing of dislocations to form clusters of vacancies. Furthermore, fatigue initiation is associated to mode I crack opening and not to mode II, as commonly believed.

The main obstacle to continue the simulations, to use more physical material properties and to use the three-dimensional extension together with the cohesive surface model is the computational expense. The long-range dislocation interaction forces are computationally

very expensive thereby limiting the number of cycles that can be simulated. Different algorithms to accelerate the simulations are suggested but they fail due to the chaotic nature of dislocation interactions. More work in this direction is needed in the future in order to be able to perform more physically realistic simulations.

Quo vadis 2D dislocation dynamics? Except for the numerical issues mentioned before, one path is to model the grain boundary behavior and the interaction between two neighboring grains. Nucleation of dislocations at grain boundaries is a first step. An additional step is the material behavior of the grain boundary, which has to allow grain boundary sliding and an evolution of the grain boundary structure depending on the elastic fields. The last step would be to model penetration of grain boundaries by dislocations and the continuation of the dislocation motion of a different slip system. This is definitely the most difficult task and needs detailed input from either atomistic simulations or experiments.

An additional path is coupling dislocation dynamics with atomistic simulations and crystal plasticity. This compilation could be used to model fracture propagation. The atomistic part would model areas close to the crack tip to incorporate dislocation nucleation from the crack tip and the interaction of dislocations with the tip. The grain which surrounds this area would then be modeled by dislocation dynamics to incorporate the long-range interaction of the crack tip with dislocations. The other grains surrounding the grain of interest would be modeled by crystal plasticity to allow for plastic anisotropic deformation in the polycrystalline material.

2D dislocation dynamics is a matured material model, which cannot only model fatigue crack initiation but also propagation of fatigue cracks, two-stage hardening under uniaxial tension, hardening caused by large inclusions, the stress build-up in thin films and much more. 3D dislocation dynamics is still bound to smaller dimensions, lower dislocation densities and shorter time-scales. Therefore, there are large areas of material problems which can be modeled by 2D dislocation dynamics. Quo vadis?