On the role of dislocations in fatigue crack initiation

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Chapter 1

Introduction

1.1 Motivation

On June 3, 1998 a high speed train ran through a false switch with a speed of 200km/h close to the city of Eschede in northern Germany. Normally, this is nothing special nor worrying, but on that date it caused all cars after the second to de-rail. Unfortunately, a bridge was located closely behind the switch against which the cars hit. This accident took 101 lives. What had happened? Before departing from the 600km distant Munich, the wheels of the train had been checked by X-ray. However, the very small crack in one of the wheels had not been found. On the way to Eschede the wheel fatigued more and it broke a few kilometers before Eschede. Then, the wheel was dragged along with the train. It got pinned in the false switch and caused the third car to de-rail, which pulled all cars behind it off the track.

This example shows a general characteristic of fatigue life. Considering the initial specimen to be defect free, in the first thousand or even million load cycles very small cracks develop, which are not visible with the naked eye nor with X-ray. This phase is called fatigue initiation. The small cracks then propagate leading to the fatal crack. The engineering approach to this kind of failure is to calculate the time necessary for the crack to propagate from a size which is visible to the critical length which leads to failure of the part. This time is then chosen to be the inspection period to search for cracks, as it was done in Munich that morning.

It may be interesting to note that the first systematical research on fatigue life was conducted by Wöhler [1] in 1870 on the fatigue life of the chassis of train cars. Wöhler investigated the material behavior under a constant loading amplitude. The behavior under specific loading spectra and for different materials have been investigated afterwards by experiments and simulations. Fatigue crack growth and environmental effects have been studied and are understood to some level. However, initiation is not well understood.

We go back and use the simplest configuration of fatigue crack initiation, neglecting all influences that are not necessary for failure. Salty or chemical environments as well as elevated temperatures are such. They decrease the fatigue life but are not essential, since failure occurs also when those influences are not present. It is essential to note that irreversibility is a necessary ingredient in any fatigue model. If the material behavior would be reversible and if a structure does not fail in the first load cycle it would never fail. However, structures fail after a number of cycles, as the tragic example above shows. Therefore, a small and locally-confined irreversibility is necessary. We model a plastically deforming, i.e. irreversible, grain at the free surface surrounded by an elastic, i.e. reversible, continuum. Moreover, we model a metal which has little impurities and which is initially almost dislocation-free. The surface of the material is initially perfectly smooth, i.e. the material has no surface roughness from fabrication. Furthermore, we will focus on face-centered-cubic (fcc) structured metals like aluminum, which is used in aerospace.

The propagation of fatigue cracks in fcc metals with a constant loading amplitude had been successfully modeled with the concept of dislocation dynamics by Cleveringa et al. [2] and by Deshpande et al. [3]. For that reason, this concept will also be used here to study the first step, i.e. fatigue crack initiation.

1.2 Mechanics background

Since continuum mechanics will be used through out the thesis a short summary is given for linear elasticity. Continuum mechanics describes the material behavior, where two neighboring material points stay in each others neighborhood during the deformation. Moreover, continuum mechanics can be subdivided in three parts: the equilibrium equation, the kinematic equation and the constitutive rule.

In the **equilibrium equations**, neglecting inertia effects, the sum of all forces on a body is zero. Therefore, the stress σ_{ij} at an infinitesimal element has to satisfy

$$\sigma_{ij,j} = \mathbf{0}$$

where $_{,j}$ denotes the differentiation with respect to j. The equilibrium equation above is equivalent to the principle of virtual work:

$$\int_V \sigma_{ij}\delta\varepsilon_{ij}\; dV = \int_S t_i \delta u_i\; dA$$

where V denotes the body and S the surface of the domain. $\delta\varepsilon$ is the virtual strain and t and δu are the tractions and virtual displacements on the surface, respectively.

The **kinematic equations** give the relationship between displacement u_i and strain ε_{ij}. For small-strain, this expression is defined as

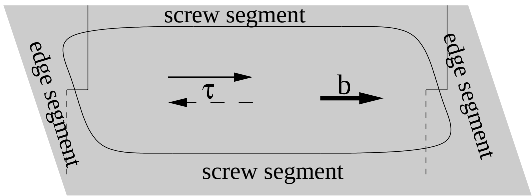


Figure 1.2: Edge and screw segments in a dislocation

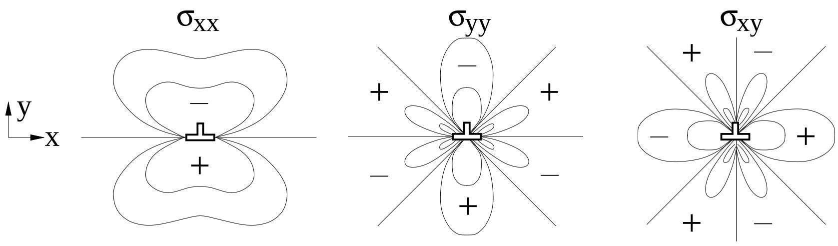


Figure 1.3: Contours of the stress distribution around an edge dislocation.

Channel-vein structure
During fatigue the dislocation density rises and dislocations form so-called channel-vein structures, as shown in figure 1.4 (a). Almost all dislocations in the figure are edge dislocations [4], [5]. Mughrabi [4] found also that the edge segments extend very long into the third dimension, as shown in figure 1.4 (b). Moreover, the dislocations in the channel-vein structure travel back and forth across the channels during the cycles. The veins have a dislocation density of $3 \times 10^{15}/\mathrm{m}^2$ [6] and a volume fraction of 50% [7]. The dislocation density in the channels is $10^{11}/\mathrm{m}^2$ [7].

PSB
During fatigue, the channel-vein structure transforms into to ladder-like structure found inside Persistent Slip Bands (PSB), which is also shown in figure 1.4. The PSBs follow the primary slip direction, i.e. the direction of the Burgers vector of those dislocations which experience the maximum resolved shear stress. These PSBs give rise to more plasticity than the channel-vein structure that surrounds the PSBs. Their development is not some sudden event but they grow in length [8] and in width [5] until they span the entire crystal. As in the channel-vein structure, dislocations travel from the very dislocation dense walls through the channel to the next wall. The dislocations loops, of which one edge segment travels across the channel, are initially almost circular [9] and afterwards extend normal to the plane shown in figure 1.4 once the edge segment reaches the other wall. The walls of a PSB are regularly spaced and have a dislocation density of around $6 \times 10^{15}/\mathrm{m}^2$ [6].

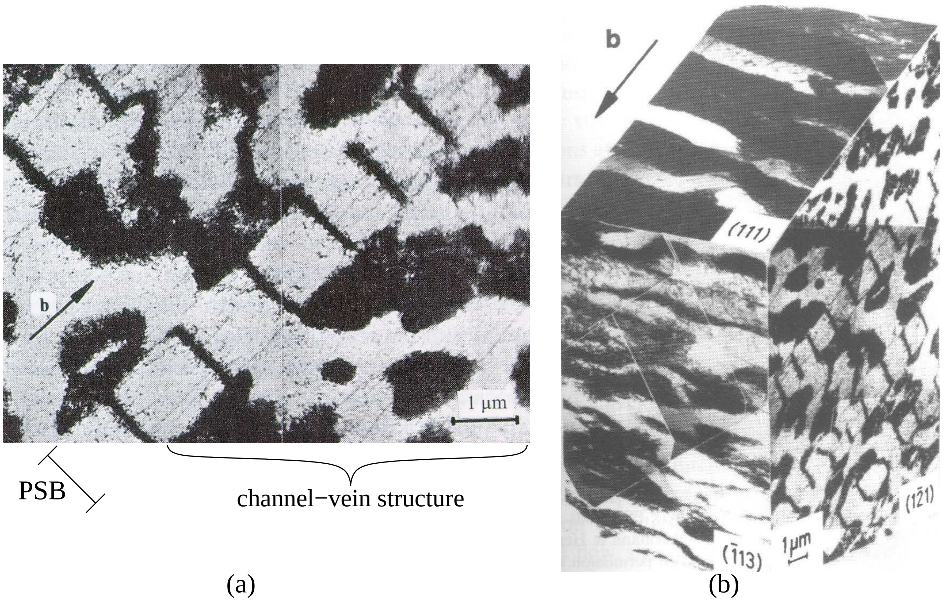


Figure 1.4: Channel-vein structure and persistent slip band (PSB) (From [4]).

Although the dislocation density in the walls is much higher than in the veins, the overall dislocation density in the PSB is roughly half of the density in the channel-vein structure, because the volume fraction of the walls in the PSB, roughly 10%, is smaller than the volume fraction of the veins in the channel-vein structure.

Ex- and intrusions

A dislocation leaving the crystal produces a surface step. If two dislocations of opposite sign move out of the crystal on different but parallel slip planes they produce an ex- or intrusion, depending on whether the dislocations form an interstitial or a vacancy dipole, respectively. A schematic drawing of ex- and intrusions and other terms is shown in figure 1.5. Moreover, in copper, intrusions and extrusions have a similar shape and size, as shown by Basinski and Basinski [10].

An area where massive material is extruded is called protrusion, see e.g. figure 1.6. These protrusions extend over the PSBs and are an evidence of the strong localization of plasticity inside the PSB. However, not all PSBs lead to a protrusion at the free surface [10]. Often, there are many smaller ex- and intrusions in a protrusion, as shown in figure 1.5 and 1.6.

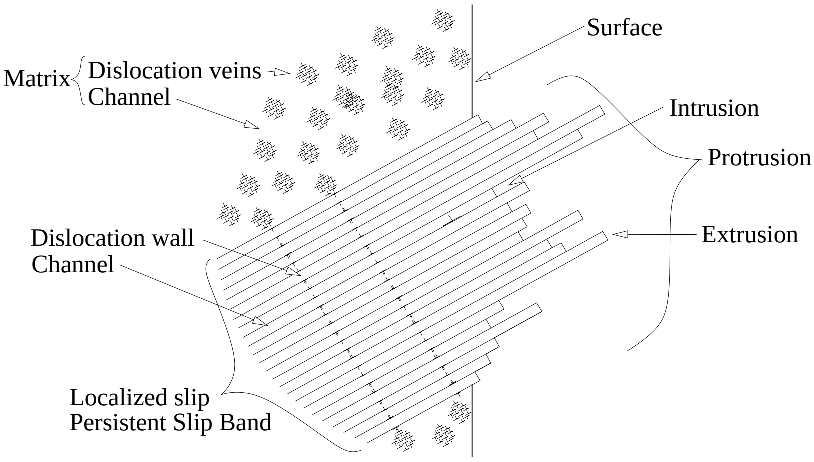
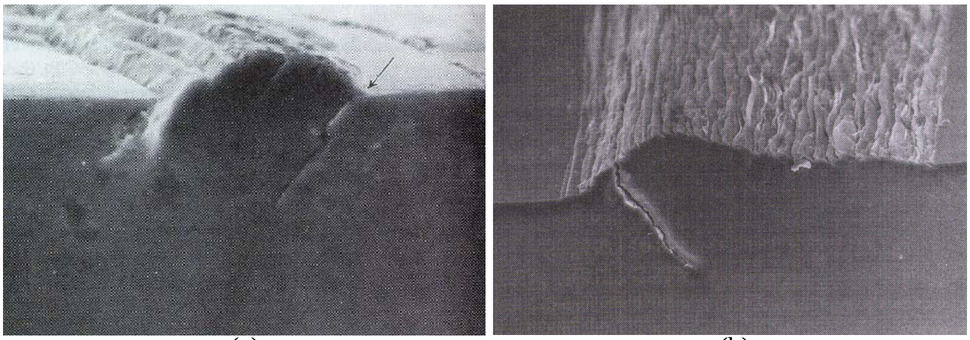


Figure 1.5: Definition of terms.

Crack nucleation

Cracks often nucleate at or close to protrusions, as shown in figure 1.6. Basinski and Basinski [5] found that cracks nucleate most likely at thin PSBs that were generated just prior to fracture initiation. Furthermore, removal of the surface roughness leads to an increase in fatigue life, as observed by Hahn and Duquette [11]. Moreover, it has been observed that deep intrusions sometimes develop into cracks (e.g. [10]).



(a) (b)

Figure 1.6: Experimental observation of an early crack by Ma and Laird [12] (a) and by Vehoff [13] (b).

In many cases more than one crack nucleates. In the first stage all cracks grow and follow the PSB, but at some point one crack finally wins and grows into the final crack. This period is called stage I fatigue. Since this crack follows the primary slip direction, and this direction has the maximum resolved shear stress, stage I fatigue is commonly associated with mode II fracture (cf. figure 1.1). In a subsequent, second stage the crack deviates from the PSB direction and continues normal to the free surface due to the macroscopic stress field. This stage II is associated with mode I fracture, because the maximum tensile stress is normal to the crack.

1.4 Existing dislocation models of fatigue initiation

There are several models in the literature that attempt to explain fatigue crack initiation or combine dislocation structuring and crack initiation. These models can be divided into two groups. On the one hand there are continuum based models, which treat the dislocations not individually but as an average over a region, e.g. [14]. On the other hand there are models which are based on discrete dislocation or discrete slip plane events, e.g. [15]. The latter try to explain experimental observations by a sequence of physical mechanisms. Only a few of these are mentioned here due to space reasons.

One of the first models was proposed by Mott [16] in 1958. He suggested that vacancies are generated below the surface as a result of the production of extrusions; since Mott found more extrusions than intrusions on the surface, he concluded that vacancies accumulate inside. These clusters of vacancies then grow and form cracks underneath the surface, as illustrated in figure 1.7.

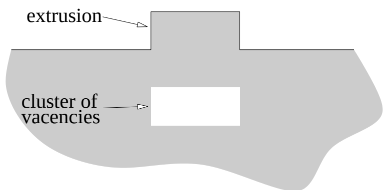


Figure 1.7: Schematic of a cluster of vacancies below the surface that may give rise to crack initiation according to Mott [16].

Antonopoulos et al. [17] extended Mott's idea and proposed a model based on vacancy dipoles, which are more likely to form than interstitial dipoles because their formation energy is lower than that of interstitials. Due to the difference in formation energy, interstitials are more likely to escape before examining the material by transmission electron microscopy than vacancies according to Antonopoulos. Furthermore, they argue that there would be twice as many vacancies as interstitials in the PSB during fatigue. To that end, adding up the dislocation dipoles in a PSB wall, the resulting dislocation dipole is a 'super' vacancy dipole and is then placed at either end of the wall, as illustrated in figure 1.8. These form a row of 'super dislocations' along the PSB–matrix interface. Antonopoulos et al. proposed that in the PSB this configuration leads to tension normal to the PSB–matrix interface. Moreover, they also computed the volume increase due to the growth of protrusions from the density of vacancy dipoles, which agrees with the values measured in experiments.

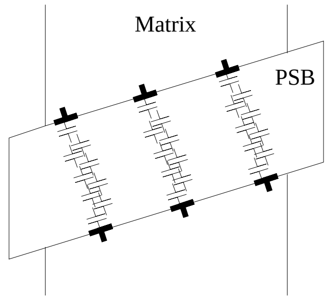
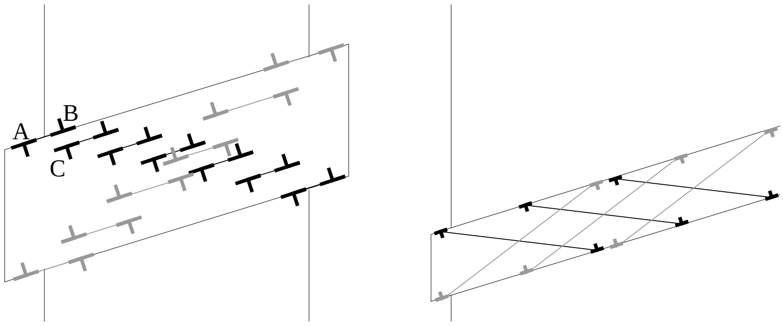


Figure 1.8: Construction of 'super dislocations' as it was used for the explanation of fatigue crack initiation by Antonopoulos et al. [17].

Essmann et al. [7] started from the same observation, i.e. pre-dominance of vacancy over interstitial dipoles, but proposed the sequence of events shown in figure 1.9 (a). A dislocation pair $A-B$ nucleates, dislocation A glides to the surface of the grain and produces a surface step while dislocation B stays inside the bulk. Another dislocation pair is generated on an adjacent glide plane. Dislocation C of the newly generated dislocation pair is forming a vacancy dipole with dislocation B. Similar events continue to occur, i.e. gliding and formation of vacancy dipoles, thus, a band of dislocation dipoles forms, as shown in the figure by the dark dislocations. The endpoints of this band are dislocations with the half-plane inside the PSB. A similar band develops from the lower left-hand to the upper right-hand edge, as depicted by the grey dislocation dipoles in figure 1.9 (a). The slope of the bands is a material property. For large crystals similar events occur except the dislocations at the ends of the band do not form surface steps. They stay on the PSB–matrix interface. Several of those bands develop, as shown in figure 1.9 (b) where each band is denoted by a line, for simplicity. At the endpoints of these bands the extra half-plane of the dislocations are inside the PSB.

It is interesting to note that the dislocations on the PSB–matrix interface in the Essmann model (figure 1.9 (b)) are changed in sign compared to the Antonopoulos model, figure 1.8. However, in both models extrusions develop on both sides of the crystal. These extrusions are due to the vacancy dipoles which develop in the PSB.

Moreover, Essmann et al. [7] proposed that vacancies are diffusing along the dislocation loops through pipe diffusion to the matrix which surrounds the PSB. They argued that this effect leads to the growth of protrusions at elevated temperatures. At lower temperatures diffusion is impossible and, therefore, the growth of protrusions is restricted. Repetto and Ortiz [18] gave constitutive rules for vacancy generation and corresponding volumetric



(a) (b)

Figure 1.9: Vacancy dipole model by Essmann et al. [7]. Two bands of dislocation dipoles form in a thin specimen by a sequence of nucleation–glide–formation of dipoles events(a). In a wide specimen several bands form, which are denoted by lines, for simplicity (b).

expansion inside the PSB at elevated temperatures. Moreover, they included the diffusion of vacancies into the matrix. They found that the protrusion would grow and found similarities in the shape of the protrusion between the simulation and experiments. On one side of the protrusion, Repetto and Ortiz found that the free surface forms an acute angle with the protrusion, which is not supported by the experiments shown in figure 1.6 but by the models of Antonopoulos et al. (figure 1.8) and Essmann et al. (figure 1.9). They proposed that fatigue crack initiation is due to the stress singularity arising from this acute angle. Differt et al. [19] extended Essmann's model to capture also the small ex- and intrusions within a protrusion, see figure 1.6, based on the statistical irreversibility of slip.

Brown and Ogin [20] arrived at the same 'super dislocation' distribution at the PSB–matrix interface as Antonopoulos. However, they arrived at this distribution in a different way, which is discussed in detail in chapter 3. Based on that dislocation distribution, they calculated the stress at the free surface and in the material.

Neumann [15] developed a model based on the activation of two slip systems, as illustrated in figure 1.10. In the first tensile stroke slip planes 1 and 2 get activated after each other and the material opens up. In the compression phase the dislocations glide back. However, they cannot totally heal the material because both side of the evolving crack touch macroscopically like ordinary pieces of metal. Therefore, a crack has initiated along slip plane 1 to the intersection with slip plane 2. Consequently, the crack propagates in a zig-zag fashion, as shown by the dashed line in figure 1.10.

All these models, with the exception of the one by Neumann, depend on the assumption that there are more vacancy dipoles than interstitial dipoles in a PSB. Several researchers looked into the change in electrical resistivity of metals during fatigue to investigate the dipole formation. Johnson and Johnson [21], Helgeland [22], Eikum and Holwech [23],

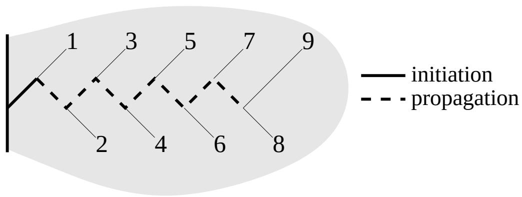


Figure 1.10: Fatigue crack initiation and propagation model by Neumann [15].

Polák [24] and Kromp and Weiss [25, 26] found an increase in the number of point defects during fatigue. But none of them were able to quantify the number of vacancies with respect to interstitials. However, if two-thirds of the defects are assumed to be vacancies, the number of vacancies in those experiments is in agreement with the values predicted by Antonopoulos et al. [17] and Essmann et al. [7], which are based on the size of the protrusion.

1.5 Outline of thesis

All the models mentioned above either assume a specific sequence of slip events (i.e. Neumann) or assume that a PSB has already formed, which will then nucleate a crack. Additionally, none of the models explains the channel-vein or the ladder-like structure in PSBs. The general objective of this thesis is to shed more light on fatigue crack initiation by numerical simulations with discrete dislocation plasticity. Rather than making ad-hoc presumptions about a dislocation structure, I start from the initial elastic field and, with a set of constitutive rules for the dislocations, the simulations will lead to the development of a dislocation structure with its residual stress field.

In chapter 2 I describe dislocation dynamics and the model of a grain at the free surface, which is subjected to a uniform remote cyclic stress. For this – so called – 2DD model a set of simple constitutive rules is used to mimic the nucleation of dislocations and the short-range interaction between dislocations. This chapter concentrates on events inside a grain that is close to the free surface. This model serves as a basis for further extensions, summarized in figure 1.11. First, in chapter 2 the 2DD model is extended by the constitutive rules given by Benzerga et al. [27] to incorporate three-dimensional effects, such as line tension and the formation of junctions and segments that can act as dislocation sources. We call this extended model the 2.5DD model.

Brown and Ogin [20] proposed a model for the elastic fields caused by a PSB, which yields a logarithmic stress singularity at both ends of the PSB on the free surface. This model is described in chapter 3 and compared to static dislocation calculations. The dislocation arrangement proposed by Brown and Ogin is then used to investigate the stresses inside a PSB analytically. Finally, these results are compared to the results obtained from

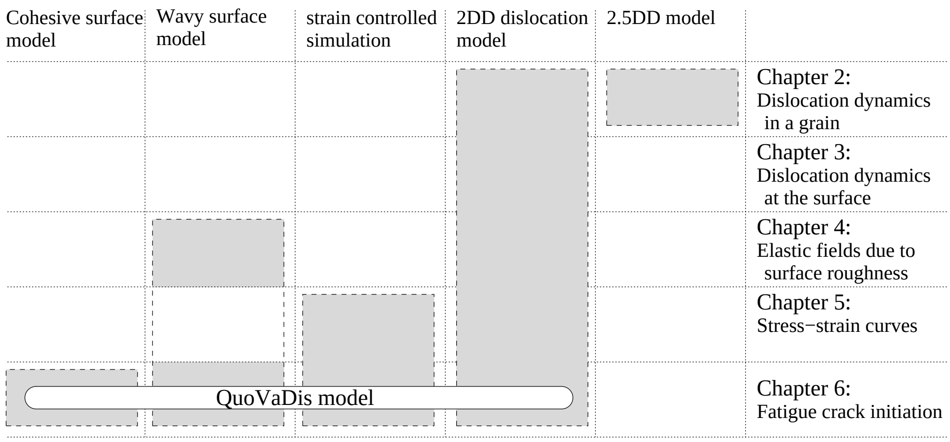


Figure 1.11: Outline of models and chapters

the 2DD model.

Fatigue inevitably involves surface roughness. In chapter 4 the elastic fields due to surface roughness are evaluated in order to include their influence on fatigue. Three approximate models are proposed to mimic the influence of the surface steps on the stress and displacement fields. These models and others given in literature are compared to a numerical calculation. Then we choose the approximation that agrees best with the numerical results.

In chapter 5 we supplement the results of chapter 2 with simulations of the stress-strain behavior using displacement-controlled boundary conditions. This requires a more elaborate analysis , where boundary conditions are incorporated by means of a superposition method [28]. The results are compared to experimental observations. Furthermore, the influence of the grain shape and size is investigated.

In chapter 6 we incorporate three models: the COhesive surface model of Xu and Needleman [29], the model for the WAvy surface and the DISlocation dynamics model, into the COWADIS model, which we will give the phonetic name 'QuoVaDis'. It will be shown that this model is able to predict fatigue crack initiation – with a minimum of ad-hoc assumptions.

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right)$$

Finally, the **constitutive rules** relate the strains to the stresses. In this thesis Hooke's law is used:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$$

Here, C_{ijkl} denotes the stiffness tensor of the material, which incorporates the material properties as shear modulus and Poisson's ratio. However, an elastic material behavior cannot lead to fatigue.

The motion of discrete dislocations produces plasticity. The discrete dislocations are in the center of interest in this thesis. The methodology is introduced in chapter 2. In addition to continuum mechanics, fracture is used in the later chapters of this thesis. To characterize different cracks, standard fracture mechanics uses three different modes which are shown in figure 1.1. The difference between the modes is the direction of loading with respect to the crack.

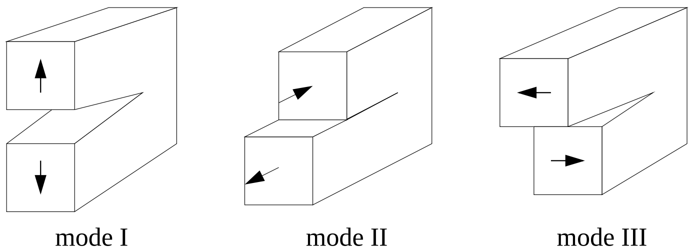


Figure 1.1: Standard fracture modes.

1.3 Experimental observations & Definition of terms

Before applying a load, most crystalline materials are not defect-free, but there are dislocations and precipitates. Dislocations are lattice defects, which nucleate from existing dislocation segments, move and then can act as nucleation points for new dislocations. Moreover, dislocations are shear loops made up of two edge dislocation and two screw dislocation segments, as shown in figure 1.2. If mode II loading is subjected along a slip plane material does not fracture, but edge dislocations move on this plane, as seen by the comparison of figure 1.1 and 1.2. Likewise, if mode III loading is subjected along a slip plane material does not fracture, but screw dislocations move on that slip plane. The stress fields of an edge dislocation are shown in figure 1.3.