# Discrete dislocation modelling of near threshold fatigue crack propagation

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## ABSTRACT

At low crack propagation rate in metals and alloys the discrete nature of plasticity is essential to understand the fatigue phenomena. A short overview of the different types of performed discrete dislocation simulations of cyclically loaded cracks and their essential results are presented. The discrete dislocation mechanics deliver the changes of the stresses and displacement during cyclic loading. However, it does not give directly the crack propagation rate. In the simulations one has to assume a propagation mechanism. A comparison implies two things: the different simulations, the experimentally observed crack growth behaviour and crystallographic features will be used to show, which crack propagation mechanism is more appropriate in which case.

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## 1. Introduction

The description and as a consequence the prediction of the fatigue crack propagation requires different types of modelling tools. This becomes clearly evident if one takes into account the different phenomena. For modelling it is very helpful to separate these phenomena into three groups: the material separation processes, i.e. the generation of new fracture surface, the monotonic and cyclic deformation in the vicinity of the crack tip and the bridging and closure of the crack flanks. The latter two phenomena are usually called extrinsic mechanisms. The separation phenomena are called intrinsic mechanisms [1] and they are controlled by deformation processes in the vicinity of the crack tip. The difference in the length scales in all these phenomena and the variation of the loading parameter, where fatigue crack propagation occurs, shows even more clearly why different modelling tools are necessary. The crack propagation rate varies between one atomic spacing per cycle and a few hundred thousand atomic spacings per cycle. The size of the zones where monotonic plastic deformation and cyclic plastic deformation occur can be a few 10 nm, in very high strength materials near the threshold, up to the size of the sample or component in low strength metals at large crack propagation rates, or at very short crack lengths.

In this paper we will restrict our considerations to low crack propagation rates, where atomistic techniques and discrete dislocation mechanics are the appropriate methods to describe fatigue crack propagation. The atomistic modelling tools, ab initio techniques and molecular dynamics can be used to answer the questions: What does the dislocation core looks like and as a consequence how easy it is to generate and to move the dislocation? The discrete dislocation mechanics is an appropriate tool when very local plastic deformation takes place and when the description of stresses in the nm regime is important. Fatigue crack propagation in metals is a consequence of the plastic deformation at the crack tip, especially cyclic plastic deformation. In order to understand better, what happens near the threshold, a detailed understanding of the cyclic plastic deformation as well as a detailed understanding of the stresses near the crack tip in the nm regime is necessary.

Several discrete dislocation simulations [2–20] devoted to the fatigue crack propagation have been performed in the last 20 years. The aim of this paper is to summarize the most important consequences of these simulations for the understanding of the fatigue crack propagation behaviour near the threshold. In order to introduce the reader to the special phenomena caused by the discrete nature of plasticity, the plastic deformation and the changes of the local stress field during moderate cyclic loading of a mode I crack will first be considered in detail (Section 2). In Section 3 the different consequences of discrete nature on the near threshold behaviour of idealized long mode I cracks will be summarized. Some important features of the discrete dislocation simulation of cyclic loaded short cracks of the group of Melin [15–18] will be shortly introduced in Section 4. Discrete dislocation simulations deliver the plastic response, although they do not directly provide the crack propagation mechanism. In Section 5 the simulations of van der Giessen and Needleman are used to discuss the effect of propagation mechanisms, because a different type of mechanics was used in their simulation.

## 2. Moderately loaded fatigue cracks

Discrete dislocation modelling is a linear elastic description of stress and strain fields or displacements, where the nonlinearity is taken into account by the movement of dislocations on pre-defined slip planes.

In the following the computer algorithm, which we have used to simulate the plastic deformation is shortly described. It contains the following steps:

- an incremental increase of the applied load or, in the case of unloading an incremental decrease,
- inspection of dislocation generation,
- inspection of fracture surface contact and determination of the contact stresses,
- seeking of equilibrium positions. We usually determined a stable equilibrium configuration, i.e. the dislocations move away from the crack tip if the stress is larger than the friction stress and it moves to the crack tip if it is smaller than the negative friction stress.

A two-dimensional mode I crack is used, and the generate dislocations are parallel to the crack front. At the beginning of the loading of the infinite cracked body, the body is free from dislocations. The crack tip is assumed to be the dislocation source. Dislocations are formed, when the local stress intensity is larger than a critical value $k_e$. That is very similar to dislocation generation at a source very near the crack tip (few nm). Where the source stress has to overcome a certain critical value, this type of dislocation generation criterion is used, for example, by [6,15,16]. A symmetric emission of dislocation is assumed, which makes the calculation somewhat easier. In our simulations a "surface forming" crack propagation mechanism is assumed. In Fig. 1 the mechanism is schematically depicted. The generated dislocations form a V-shaped notch. The next dislocations are generated at the tip of this notch, hence, the spacing between slip planes of the successive emitted individual dislocations is equal to the Burger's vector. During unloading, the emitted dislocations return to the tip and resharpen the crack, but in the simulation the crack does not reweld. In real fatigue crack propagation experiments the oxidation of the new generated surface at the crack tip prevents a reversible blunting.

The crack growth increment per cycle, $\Delta a$, is therefore

$$\Delta a = \Delta N \cdot b \cdot \cos \theta$$

where $\Delta N$ is the number of generated dislocation pairs per cycle and $\theta$ is the angle between the slip plane and the crack plane. Such propagation mechanisms have been experimentally observed in [21,22] and were proposed very similarly [23–25]. For the details to determine the stresses on the dislocations – which are the sum of stresses caused by the applied $K$ – stresses from all other dislocations, the image stress and the stresses caused from possible fracture surface contacts and the detail of the calculation procedure, see [11,14].

In order to illustrate what happens during such discrete dislocation simulation at the crack tip during cyclic loading at a stress intensity range $\Delta K$ somewhat smaller than the effective threshold, $\Delta K_{eff\ th}$, and at a $\Delta K$ larger than $\Delta K_{eff\ th}$, the movement of the dislocations and the local stress in the vicinity of the crack tip are considered in the following. The material parameters used are the shear modulus $\mu = 80{,}000$ MPa, Poisson's ratio $\nu = 0.3$, a lattice friction stress of $\mu/1000$, a critical stress intensity to generate a dislocation at the crack tip $k_e = 0.4\mu\sqrt{b}$ and an angle between the crack plane and the slip plane of 70.3°. The stress ratio $R = K_{min}/K_{max} = 0.1$. For all simulations in Figs. 2–7 the same material
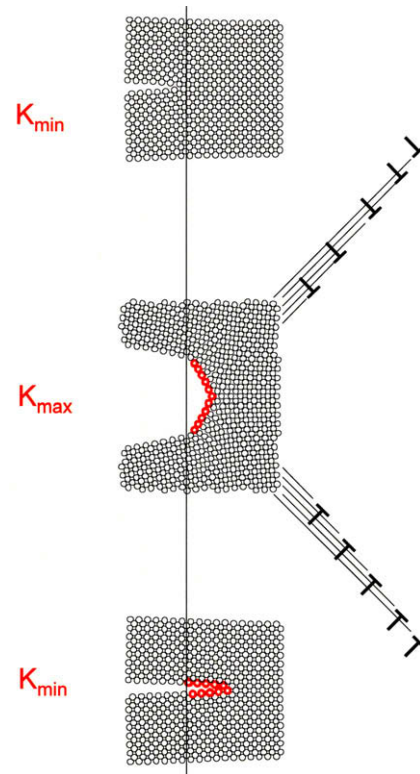


**Fig. 1.** Schematic representation of the assumed fatigue crack propagation mechanism: the blunting and resharpening of the crack tip on the atomistic scale is shown. Only the cyclically activated dislocations are sketched.

parameters and $R$ are used. The simulation starts with a crack in a "mathematical"[1] crystal without dislocations. If $K_{max}$ is smaller than $k_e$, no dislocations will be generated. During cyclic loading at such small load amplitudes a pure elastic loading and unloading and therefore no crack extension will take place. Since no dislocations are generated, the local stress field at the crack tip in the vicinity of the crack tip is determined by the applied stress intensity factor $K$ solely. For $K_{max}$ somewhat larger than the critical stress intensity factor $k_e$, the deformation, i.e. the movement of the dislocations and the variation of the local stress field at the crack tip, are depicted in Fig. 2. During the first loading a pair of edge dislocations is generated at the crack tip, when $K$ is equal to $k_e$. They will move away from the crack tip till they reach their equilibrium positions, where the local stress acting on the dislocation is equal to the friction stress. These dislocations reduce the stress field at the crack tip, i.e. they shield the crack tip [26,12]. The stress field in the immediate vicinity of the crack tip – in a region of about 1/5 of the distance to the nearest dislocation – can be described by the standard linear elastic stress field of a crack, characterized by means of a local stress intensity, $k$. During further loading the dislocations move away and the local $k$ increases similarly to the applied $K$ till again $k = k_e$, then the next pair of dislocations is emitted. Due to the repulsive force the first emitted dislocation is pushed away from the crack tip till it again reaches its equilibrium position. This process of the dislocation movement away from the crack tip, increasing of the local stress intensity till $k = k_e$, emission of a new pair of dislocation and pushing away from the crack tip of the pre-existing dislocations continuous till the applied $K$ reaches $K_{max}$. During unloading the stresses acting on the dislocations decrease. The reduction in the local $k$ is, in this case of the quasi-static consideration, exactly equal to the reduction of the applied $K$.

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[1] No crystallographic orientations are assumed.