Simulation of stage I short crack propagation in an austenitic-ferritic duplex steel

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Abstract

The propagation of short fatigue cracks is simulated in the microstructure of an austenitic-ferritic duplex steel by means of a mechanism-based model. Due to strong interactions with microstructural features, such as grain and phase boundaries the growth rate of these short cracks is substantially non-uniform. The strength of these barriers has been quantified by a Hall-Petch analysis and the findings have been implemented into a two-dimensional model for stage I crack propagation, which considers the orientation of available slip systems and can predict the crack growth in a real microstructure. The model allows the activation of secondary slip systems at the crack tip resulting in a crack propagation on multiple slip bands. To study the effect of a misorientation between two slip planes on crack propagation the stress field at the tip of a surface crack is calculated using a three dimensional extended crack model. Crack growth simulations carried out with the model show good agreement with experimental data.

1 Introduction

Many components in industrial applications are subject to a cyclic loading in the high cycle fatigue regime at stress amplitudes, which are close to the fatigue limit. Under these conditions, the phase of crack initiation and short crack growth can last up to 90% of the total lifetime. These cracks exhibit strong interactions with microstructural features such as grain boundaries and the growth mechanism (stage I) is significantly different from that of long cracks. Thus, the propagation rate cannot be described by the methods of linear elastic fracture mechanics.

In polished test specimens fatigue cracks often initiate at locations in the microstructure, which are subject to elevated stresses. This stress increase can be caused by inclusions or the anisotropic elastic properties of the grains. Once initiated, a stage I-crack can grow on individual favourably orientated slip bands characterized by a high Schmid factor and the propagation rate is controlled by the crack tip slide displacement *CTSD* (Fig. 1a). The grain boundaries act as obstacles to crack propagation, as they prevent a transmission of slip into the neighbouring grain. This yields a dislocation pile up in front of the barrier resulting in a decreased crack growth rate. If the boundary is broken, the stress intensity will be relieved by slip in the next grain and the crack propagation rate will increase again, resulting in an oscillating crack growth.

With increasing crack length additional slip systems are activated at the crack tip and the crack grows on alternating slip systems. The crack path is deflected from a plane with maximum shear stress into a direction perpendicular to the applied load. As long as the length of the active slip bands at the crack tip is still determined by the microstructure, the crack can still be regarded as microstructurally short. Even a return to crack propagation on a single slip system is possible if there are not enough favourably orientated slip systems available.

A stage I short crack model has to predict the abnormal propagation behaviour described above. Approaches that fulfil this requirement are the analytical models of Taira [1] and Navarro and de los Rios [2]. There, the extension of the plastic zone is blocked by the next grain boundary until a critical stress in a dislocation source behind the barrier is reached to activate a new slip band. Based on this idea a two dimensional model has been developed, which is able to predict crack growth in a real microstructure and considers the orientation of available slip systems in the crystals. The boundary value problem is solved numerically by means of a discretisation with dislocation dipole boundary elements.

According to Navarro and de los Rios, the fatigue limit of a material can be interpreted as the stress amplitude below which crack propagation stops at grain boundaries. Because of that it is essential for a model to predict the stress state in a dislocation source behind a grain boundary correctly. The two dimensional model already considers the tilt angle between two slip systems of two neighbouring grains. Nevertheless, more accurate results could be obtained by a three dimensional model that considers the real orientation of slip planes including the twist angle between them. Thus, the two dimensional model is extended to a three dimensional one for surface cracks in a semi-infinite body so that the shear stress in a dislocation source can be calculated correctly. The three dimensional surface crack can be modelled by a continuous distribution of dislocation loops [3]. The effect of the twist angle has been analysed and the findings are considered in the two dimensional model.

The model is applied to the microstructure of an austenitic/ferritic duplex steel (X2CrNiMoN 22 5 3), thus both grain and phase boundaries have to be considered.

2 Two-dimensional short crack model

In order to model the propagation of microstructurally short cracks a two dimensional yield strip model has been developed. The model allows an opening and a tangential displacement of the crack flanks. If the shear stress τ reaches the critical value for dislocation motion τ^b a plastic deformation due to slip on the active slip band in front of the crack tip occurs.

An extension of the plastic zone is blocked by the next grain boundary until a critical stress intensity is reached on a dislocation source beyond the barrier in the neighbouring grain. If this critical stress intensity is reached, the respective slip band is activated and the plastic zone grows into the new grain. The crack propagation rate, which decreased significantly in front of the grain boundary, increases again. This results in an oscillating crack growth rate that is characteristic for microstructurally short cracks. The critical stress intensities for grain and phase boundaries were quantified experimentally by a Hall-Petch analysis [4].

The crack problem is solved numerically by means of a discretization with dislocation dipole boundary elements, which represent a constant relative displacement over the element. The elements in the plastic zone consist of a negative and a positive dislocation tangential to the crack so that a slip displacement can be modelled (Fig. 1b). In addition to that a crack element also allows an opening displacement that is achieved by a dislocation dipole normal to the crack. The stress state in the material around the growing crack can be calculated by so called sensor elements.

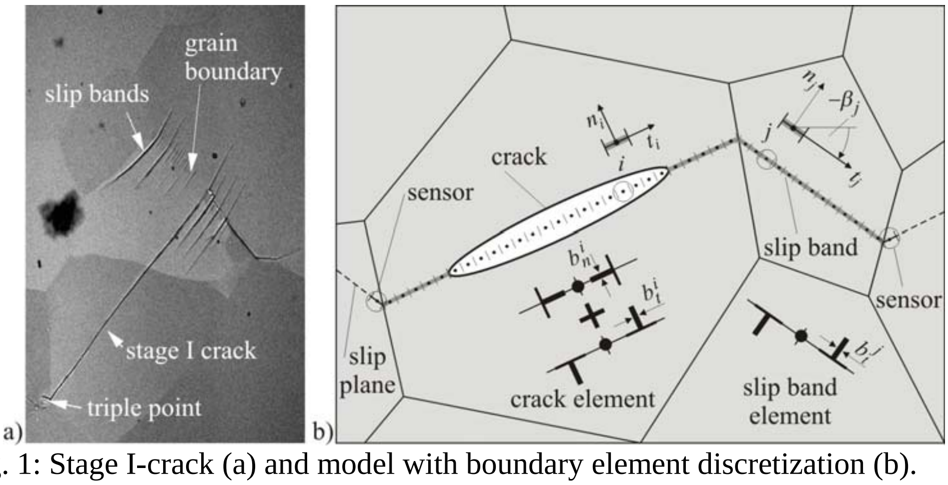

Fig. 1: Stage I-crack (a) and model with boundary element discretization (b).

The elements are connected to each other by the influence function G^{ij}, which describes the stress in an element i due to a displacement in an element j. The total stress σ^i_{nn} and τ^i_{tn} is obtained by summation over all elements plus the external normal and shear stress $\sigma_{nn}^{i\infty}$ and $\tau_{tn}^{i\infty}$. The consideration of the boundary conditions yields the following system of inequalities:

$$\sigma_{nn}^{i} = \sum_{j=1}^{p} G_{nn,n}^{ij} b_n^j + \sum_{j=1}^{p+q} G_{nn,t}^{ij} b_t^j + \sigma_{nn}^{i\infty} \leq 0 \qquad i = 1 \ldots p \tag{1}$$

$$\left|\tau_{tn}^{i}\right| = \left|\sum_{j=1}^{p} G_{tn,n}^{ij} b_n^j + \sum_{j=1}^{p+q} G_{tn,t}^{ij} b_t^j + \tau_{tn}^{i\infty}\right| \begin{cases} = 0 & i = 1 \ldots p \\ \leq \tau^b & i = p+1 \ldots p+q \end{cases} \tag{2}$$

$$b_n \geq 0 \qquad i = 1 \ldots p \tag{3}$$

Here, p is the number of crack elements and q the number of elements in the plastic zone. To consider roughness induced crack closure a penetration of the crack flanks is prevented (Eq. 3). The crack propagation is calculated from the range of the crack tip slide displacement $\Delta CTSD$ by a power law function (Eq. 4), which is analog to the model of Navarro and de los Rios.

$$\frac{da}{dN} = C \cdot \Delta CTSD^m \tag{4}$$

In Eq. 4, C is a material specific constant and m is an exponent that is usually very close to one. A more detailed description of the short crack model can be found in [5].

With growing crack length the stress intensity on additional slip planes in front of the crack increases [6,7]. This can yield an activation of an inactive slip plane at the crack tip, which is the beginning of crack propagation in double slip mechanism. To identify the activation of a second slip band, additional sensor elements representing other slip planes of the grain are positioned at the crack tip to determine the shear stress on those slip planes (Fig. 2a). Once a critical value is reached on one of these sensors the respective slip band is activated and plastic deformation occurs on this plane. In the model the activation of a second slip band is considered by meshing it with plastic zone elements (Fig. 2b). Then, crack growth results from the crack tip slide displacement on two slip bands, which results in a deflection of the crack growth into a plane perpendicular to the applied load (Fig. 2c).

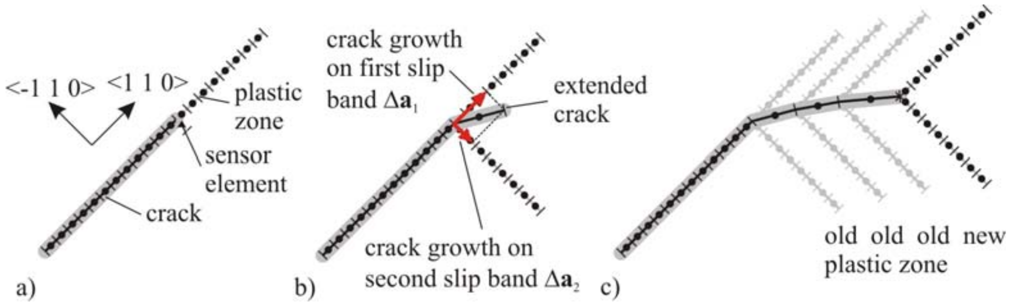

Fig. 2: Transition from crack growth in the single slip mechanism to the double slip mechanism.

3 Three-dimensional extension of the short crack model

3.1 Modelling of three-dimensional cracks

In order to consider the real orientation of slip systems the presented short crack model is extended to three dimensions. Thus, an arbitrary planar surface crack S in a semi-infinite solid under remote loading σ_{jk}^{∞} is considered. The relative displacement between the crack faces can be represented by a continuous distribution of infinitesimal dislocation loops dS [3]. As the stress field at a position $\mathbf{x}$ due to an infinitesimal dislocation loop of strength $b_m dS$ in $\mathbf{x}'$ is known, the stress induced by the crack can be calculated by integration over the crack surface S. By enforcing that the surface of an open crack is traction free the following integral equation is obtained:

$$\sigma_{jk}(\mathbf{x}) = \int_S K_{jkm}(\mathbf{x},\mathbf{x}')b_m(\mathbf{x}')dS + \sigma_{jk}^{\infty}(\mathbf{x}) = 0 \tag{5}$$

The kernel K_{jkm} can be split into a singular part K_{jkm}^{s}, which results from the crack in an infinite space, and a regular part K_{jkm}^{r} that considers the free boundary of the half space. For the planar crack it is sufficient to calculate the stress components σ_{xz}, σ_{yz} and σ_{zz} in the local crack coordinate system where the z-axis is normal to the crack surface. However, the calculation of the shear stress on slip bands in neighbouring grains requires the calculation of the complete stress tensor. In general K_{jkm}^{s} is given by [8]:

$$\begin{aligned} K_{jkm}^{s}(\mathbf{x},\mathbf{x}') = \frac{C_{ilm3}}{8\pi(1-\upsilon)r^3}\Bigg\{&(1-2\nu)\left[\delta_{ij}\delta_{kl}+\delta_{ki}\delta_{jl}-\delta_{jk}\delta_{il}-\frac{3r_l}{r^2}\left(\delta_{ij}r_k+\delta_{ki}r_j-\delta_{jk}r_i\right)\right] \\ &+\frac{3}{r^2}\left(\delta_{jl}r_k r_i+\delta_{kl}r_j r_i+\delta_{il}r_j r_k\right)-\frac{15 r_j r_k r_i r_l}{r^4}\Bigg\} \end{aligned} \tag{6}$$

C_{ilmn} is the tensor of the elastic constants, $r_i = x_i - x'_i$ and $r = \sqrt{r_i r_i}$. The regular part, which accounts for free boundary is also given in [8].

Since the Kernel K^s_{jkm} is hypersingular with a singularity of r^{-3} when r approaches zero the integral exists only in a finite part sense. To calculate the integral the semi-analytical method proposed by [3] is applied.

To solve Eq. 5 numerically, the crack surface is meshed with finite dislocation loop elements. The relative displacement in each element is approximated by a linear interpolation function. These elements have been proposed by [3] and show a better convergence compared to elements with constant displacements.

3.2 Stress field at the tip of a three dimensional crack

The three-dimensional model is used to analyse the shear stress field on a dislocation source behind a grain boundary. Thus, a semi-circular surface crack is considered, which is perpendicular to the free surface and inclined about 45° to the loading axis (Fig. 3). To consider the critical situation with a maximum shear stress acting on possible slip planes beyond the grain boundary it is assumed that the crack front is located directly in front of this barrier. According to Navarro and de los Rios, short crack growth stops at this point at stress amplitudes below the fatigue limit.

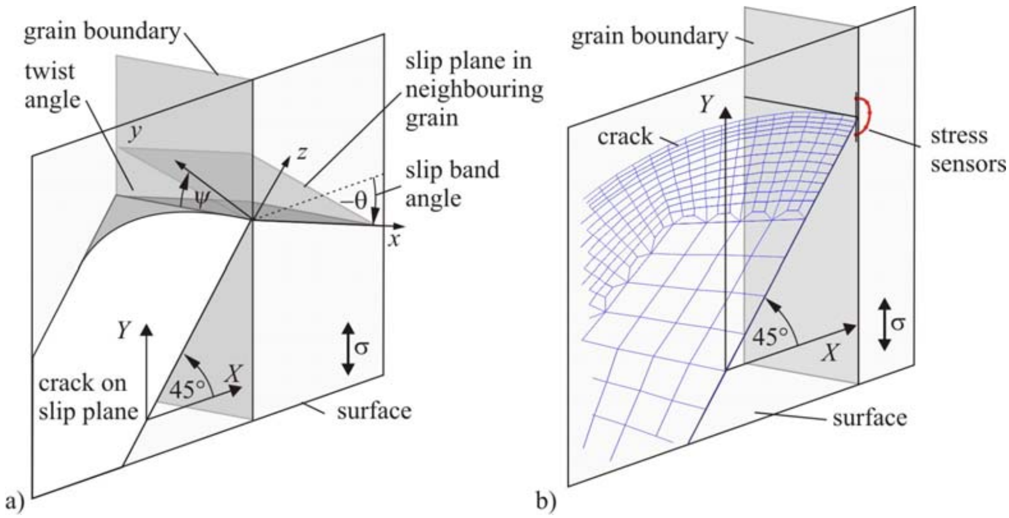

Fig. 3: Misorientation between slip planes in different grains (a) and meshed semi-circular surface crack with stress sensors beyond the grain boundary (b).

Using this model the shear stress distribution is calculated in a constant radius around the crack tip for an external loading of 400MPa. In Fig. 4 the shear stress τ_{xz} in the local *xyz*-coordinate system is plotted for slip band angles between –90° and 90°. In order to study the effect of a twist angle between the crack plane and a slip plane in the neighbouring grain, results are also given for slip planes, which are rotated around the local *x*-axis about the respective twist angle ψ.

The simulations show that an additional twist angle reduces the shear stress on a dislocation source behind the grain boundary significantly. Thus, an activation of the respective slip system gets more and more unlikely with an increasing twist angle.

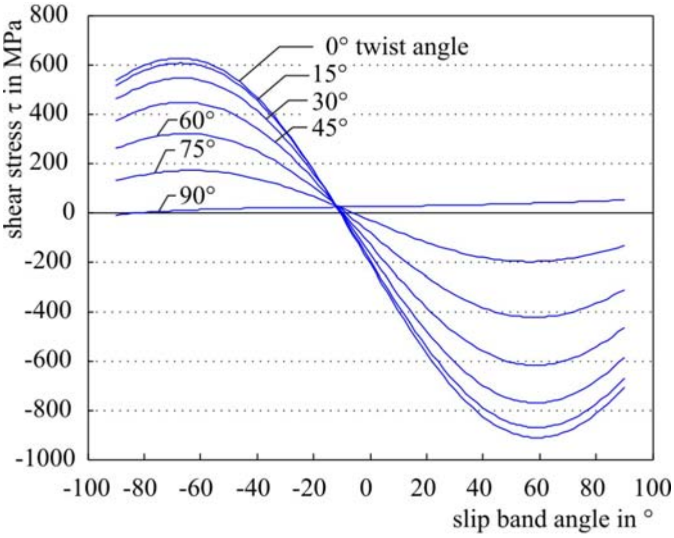

Fig. 4: Shear stress on dislocation source at different slip band angles and twist angles.

The slip bands in the two-dimensional model are the intersection lines of the slip planes in the crystal with the surface. Because of that the three-dimensional orientation of the slip planes and the misorientation between two planes in neighbouring grains is known, but only the tilt angle between two slip planes is considered by the orientation of the sensor elements.

Therefore, the results from the three dimensional model are used to consider the effect of a twist angle also in the 2D-model. As can be seen in Fig. 4 the maximum shear stress occurs on slip planes with a twist angle of 0° at slip band angles of –68° and 59°. The reduction of the shear stress τ_{xz} at these angles with increasing twist angle is shown in Fig. 5. It can be seen that the decrease of shear stress is approximately proportional to $\cos\psi$. Thus, the shear stress on a sensor element in the 2D-modell is multiplied by $\cos\psi$ to account for a twist angle with sufficient accuracy.

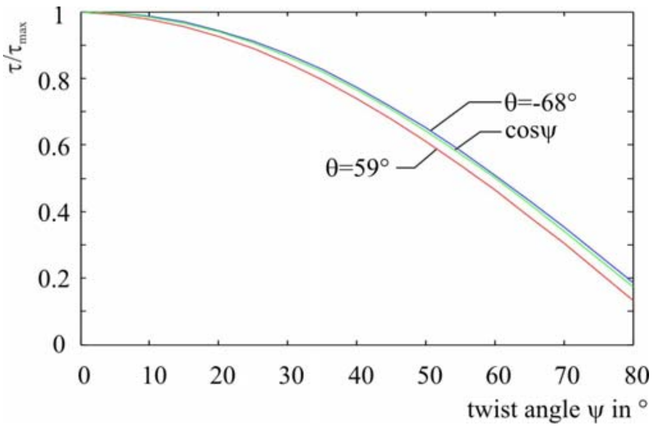

Fig. 5: Decrease of shear stress on a dislocation source with increasing twist angle.

4 Results

The modified two-dimensional model is used to simulate short crack propagation in an austenitic/ferritic duplex steel. Thus, a virtual microstructure of the material has been generated using the Voronoi technique [5], which has the same average grain size and phase distribution as the real microstructure. The crack growth simulation starts with an initial crack on a slip band in one grain (Fig. 6). Then the crack growth through several grains in the single slip mechanism until the stress intensity on an inactive slip system at the crack tip reaches a critical value to activate the slip band, which is the beginning of crack growth in the double slip mechanism. Due to the lower strength of the austenitic phase, the activation of a second slip band occurs usually in an austenitic grain. At the other crack tip crack propagation continues in the single slip mechanism. It is even possible, that the growth mechanism returns from double to single slip after the transition of a grain boundary. This has been observed in fatigue experiments [4] when the crack grows from an austenitic grain into a ferritic one.

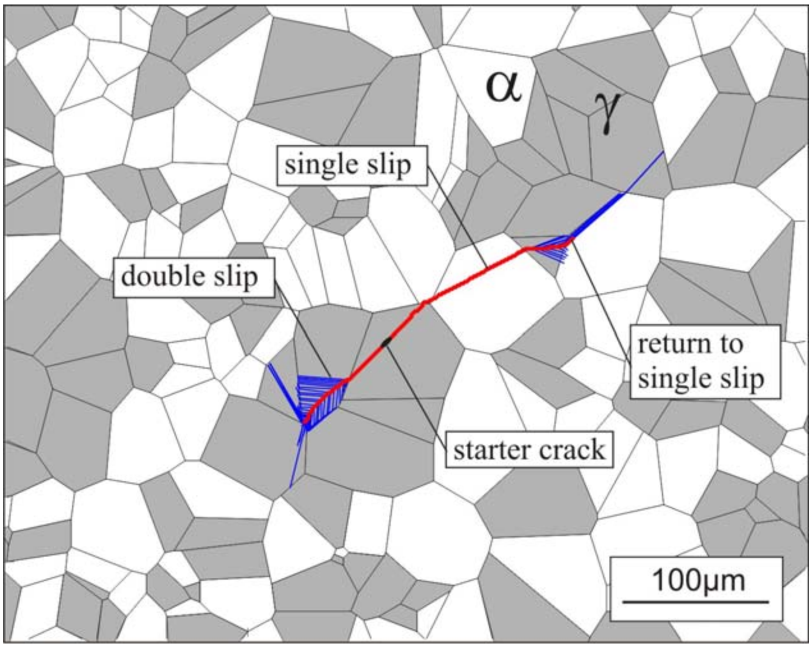

Fig. 6: Crack path in virtual microstructure of an austenitic/ferritic duplex steel.

5 Conclusions

A two dimensional model for stage I crack propagation is presented, which is able to reproduce the barrier effect of grain and phase boundaries and considers crack closure. The model allows the activation of additional slip systems at the crack tip, which yields a crack propagation on multiple slip planes in the double slip mechanism. The twist angle between two slip planes in neighbouring grains influences the barrier effect of the respective grain boundary. To quantify this influence the stress field around a semi-circular surface crack has been calculated. For this purpose, an extended three dimensional model has been developed where the crack is represented by a distribution of dislocation loops. It was found that the shear stress reduces significantly with increasing twist angle so that an activation of the respective slip plane becomes more and more unlikely. The findings were implemented into the two dimensional model, which has been used to simulate crack propagation in a virtual microstructure of a duplex steel.

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