Simulation of irreversible damage accumulation in the very high cycle fatigue (VHCF) regime using the boundary element method

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Abstract

Many components have to withstand a very high number of loading cycles due to high frequency or long product life. In this regime, the period of fatigue crack initiation and thus the localization of plastic deformation play an important role. Metastable austenitic stainless steel (AISI304) that is investigated in this study shows localization of plastic deformation in bands of intense slip. In order to provide a physically-based understanding of the relevant damage mechanisms under VHCF condition, simulation of irreversible damage accumulation in slip bands is performed. For this purpose, a microstructural simulation model is proposed which accounts for the damage mechanisms in slip bands documented by experimental results. The model describes the damage accumulation through formation of slip bands, sliding and multiplication of dislocations and the amount of irreversibility of such mechanisms in case of VHCF relevant loading conditions. The implementation of the simulation model into a numerical method allows the investigation of the damage accumulation in a real microstructure simulated on the basis of metallographic analysis. The numerical method used in this study is the two-dimensional (2-D) boundary element method which is based on two integral equations: the displacement and the stress boundary integral equation. Fundamental solutions within these integral equations represent anisotropic elastic behavior. By using this method, a 2-D microstructure can be reproduced that considers orientations as well as individual anisotropic elastic properties in each grain. Contours of shear stresses along most critical slip systems are compared with images of slip band formation at the surface of fatigued specimens provided by scanning electron microscopy (SEM). Results show that simulation of slip bands is in good agreement with experimental observations and that plastic deformation in slip bands has a high impact on shear stresses at grain boundaries acting as possible crack origin in the fully austenitic material condition. In contrast to most other publications in the field of fatigue simulation the present paper tackles the problem of modeling cyclic slip irreversibility and gives an insight into its effect on the microstructural damage evolution.
Keywords

simulation; damage accumulation; slip band; cyclic slip irreversibility; boundary element method; very high cycle fatigue

1. Introduction

Design and dimensioning of cyclically loaded components is usually based on the classical fatigue limit below which the component should not fail for any number of cycles. Mostly the classical fatigue limit is based on fatigue tests up to 10 million cycles. But observations in the regime of VHCF beyond 10 million cycles reveal that failure arises even at stress amplitudes below the conventional high cycle fatigue limit (as discussed in the series of VHCF conferences since 1998, e.g. Ref. [1]). For that reason the exploration of fatigue mechanisms in that regime and the characterization of fatigue life become more and more important. In the VHCF regime the period of fatigue crack initiation consumes the majority of the total fatigue life and cyclic plastic deformation is heterogeneously distributed due to low stress amplitudes. In this context, sites of stress concentration get a dominant life controlling meaning. The localization of cyclic plastic deformation in the metastable austenitic stainless steel considered in this study is conducted by motion of dislocations arranged in slip bands. Slip bands are accepted as very important feature of cyclic straining in crystalline materials and represent the first sign of fatigue damage [2]. As the cyclic strain becomes localized in slip bands, a rough surface relief with extrusions and intrusions develops at the traces of emerging slip bands, which are believed to be critical precursors to the nucleation of fatigue cracks. These slip bands are affected by cyclic slip irreversibility, which even in VHCF regime leads to a sizeable irreversible accumulated plastic slip deformation and finally leads to significant microstructural changes up to crack initiation [3].

The prediction of fatigue life under VHCF condition requires the knowledge and understanding of the basic microstructural fatigue damage processes. For this purpose the present study focuses on the investigation of slip bands, which - as mentioned before - primarily sustain the localization of cyclic plastic deformation. In Ref. [4] several slip band modeling approaches are summarized, which describe the formation of surface roughening due to slip bands, e.g. the well-known model by Essmann, Gösele and Mughrabi [5] or the model by Tanaka and Mura [6]. The slip band model adopted in this study combines some ideas of the models proposed in Ref. [4]. The model is applied on a mesoscopic scale and accounts for the mechanisms of slip band formation, motion and multiplication of dislocations, its cyclic irreversibility and - as an effect of the mechanisms mentioned before - cyclic hardening. In the following the motion and multiplication of dislocations is expressed with the term sliding and the mechanisms of sliding, irreversibility and hardening are related to the slip band as a whole.

To investigate the effect of the suggested slip band model on damage relevant parameters such as shear stresses or sliding deformation it is adapted to real simulated microstructures. Because of the high geometrical complexity of real microstructures and a variety of possibly occurring slip bands, the computation of damage relevant parameters can hardly be done analytically. It is advisable to use a numerical method. Several studies in the field of microstructural modeling and simulation of fatigue damage use the finite-element method (FEM) in conjunction with crystal plasticity models. Zhang et al. [7] explicitly model multiple slip bands within individual grains of a polycrystalline material by using a shear-enhanced crystal plasticity model implemented in the FEM. Simulated slip bands are in qualitative agreement with SEM observations. Although the FE-method combined with crystal plasticity models has been devoted to a wide range of applications the implementation of the newly proposed slip band model of this study would present some difficulties: formation of new slip bands would require a remeshing algorithm and computation of sliding displacement in slip bands would necessitate special finite elements like cohesive-zone elements. Furthermore, various models (e.g. Ref. [7]) adopted by the FE-method presently do not reflect the mechanism of irreversibility nor do they employ any predictive means to account for it, particularly models based on crystal plasticity [8].

In this study a two dimensional boundary element method (BEM) is applied, in which the proposed slip band model can be implemented very effectively. The most outstanding feature of this method is that it uses displacement differences or sliding displacements directly as unknowns on slip band
layers. The proposed BEM can simulate slip bands in a two dimensional microstructure consisting of grains with individual anisotropic elastic properties. In the following paragraphs at first the simulation model with its slip band mechanisms is presented and then the numerical method is specified. The irreversible damage accumulation in slip bands is investigated in a model representing the morphology of a real microstructure characterized by means of SEM in combination with the electron backscattered diffraction (EBSD)-technique and the orientation imaging microscopy (OIM) analysis.

2. Simulation Model

In the previous section, it was introduced that by means of a BEM a 2D microstructure consisting of grains with individual anisotropic elastic properties can be simulated. Plastic material behavior by localization of cyclic plastic deformation in slip bands will be considered by mechanisms which define the properties of formation, sliding, irreversibility and hardening of a slip band as follows. Although the metastable austenitic stainless steel implies further microstructural inhomogeneities such as deformation induced martensite or inclusions, in this study the focus is on slip band evolution as it is the predominant process in the fully austenitic condition.

Formation of a slip band is assumed to occur at sites of shear stress concentration \([9,10]\). Once a critical resolved shear stress in the most critical slip system is exceeded, a slip band is generated at the critical position and propagates along the intersection line of the corresponding slip system and the surface plane of the two dimensional microstructure. The critical resolved shear stress is defined as \(\tau_{\text{crit}} = 80\text{MPa}\), which corresponds to the threshold for slip band formation observed in Ref. [11].

Fig. 1 shows a transmission electron microscopy (TEM) micrograph of the dislocation arrangement in metastable austenitic stainless steel in the fully austenitic condition fatigued under VHCF condition. The micrograph indicates that dislocations are arranged in pile-ups at grain boundaries. Therefore, the model used in this study is based on the theory of dislocation pile-ups at grain boundaries [12], in order to determine the sliding distribution along the slip band. Due to the equilibrium of forces produced by external loading and repulsive forces between dislocations a characteristic dislocation distribution occurs. Taking into account the distortion of a dislocation, which is defined by the magnitude of the Burgers vector, a sliding distribution \(\Delta u(\xi)\) can be determined:

\[
\Delta u(\xi) = \frac{2 \cdot (1 - \nu)}{G} \sqrt{(l/2)^2 - \xi^2} \cdot (\tau - \tau_{\text{crit}}), \tag{1}
\]

where \(\nu\) and \(G\) are Poisson's ratio and shear modulus in the slip plane, respectively (Table 1). \(l\) is the length of slip band and \(\xi\) is the coordinate along the slip band starting at the dislocation source. \(\tau\) and \(\tau_{\text{crit}}\) represent the shear stress existing in the dislocation source and the critical resolved shear stress. In order to account for mutual influences between slip bands, the sliding distribution in equation (1) is converted into a qualitative shape function. In this way, the quantitative sliding values of the slip bands result from the simulation by predefining the critical resolved shear stresses in the dislocation sources. The sliding distribution model assumes that dislocations perform planar slip. This assumption appears reasonable for the material considered presumably because of the existence of short range order [13].
Fig. 1. TEM micrograph of dislocation pile-ups at a grain boundary in metastable austenitic stainless steel fatigued under VHCF condition (loading amplitude: 240MPa, number of cycles: $10^7$).

It is concluded that the evolution of slip bands is related to cyclic slip irreversibility [3]. To be able to consider this mechanism in the simulation model, the slip band is approximated by two closely located layers, on which dislocation motion occurs separated in tensile and compressive loading (Fig. 2), as Tanaka and Mura suggested in their model [6]. By doing so, irreversible slip can be regarded separated in both loading half cycles.

Fig. 2. Approximation of slip band by two closely located layers.

A special procedure was adopted to accumulate the irreversible fraction of cyclic slip. Fig. 3 shows exemplarily the variation of shear stress $\tau$ as a function of time in a slip band (in both layers) caused by external loading and illustrates the development of the resulting maximum sliding $\Delta u'^I$ in layer I and $\Delta u'^{II}$ in layer II, which are affected by irreversibility.

Fig. 3. Exemplary variation of fatigue shear stress $\tau$ as a function of time in a slip band and resulting maximum sliding $\Delta u'^I$ in layer I and $\Delta u'^{II}$ in layer II.

Once the critical resolved shear stress $\tau_{\text{cr}}$ in the first tensile loading is exceeded, layer I starts to slide by conducting the pile-up sliding model. As the shear stress decreases, sliding is fixed at its maximum value $\Delta u'^I$. During compressive loading layer II is activated as soon as the shear stress exceeds the critical resolved shear stress in the opposite direction and concurrently in layer I, the fixed sliding $\Delta u'^I$
is reduced to an irreversible fraction \( p \cdot \Delta u_1^i \). The cyclic slip irreversibility \( p \) defines the fraction of plastic shear deformation that is irreversible in a microstructural sense [3]. One full cycle later the maximum sliding \( \Delta u_1^i \) is reduced again, but this time to an accumulated irreversible fraction expressed as \( p \cdot (\Delta u_1^i + \Delta u_2^i) \) taking the irreversibility of the previous sliding into account. The maximum irreversible fraction of sliding in cycle \( i \) can generally be written as:

\[
\Delta u_{irr}^i = p \cdot \sum_{n=1}^{i} \Delta u_{n/H}^i .
\]  

(2)

Summarizing, compatible sliding displacements of slip bands are completely defined by the condition that sliding increases once a critical resolved shear stress is exceeded, sliding is fixed as shear stress decreases and sliding is reduced to an irreversible fraction once critical resolved shear stress is exceeded in the opposite direction. This procedure in combination with approximation of the slip band by two closely located layers is capable to account for the irreversible fraction of sliding.

Hardening is assumed to result from an increasing dislocation density within the slip band. This work-hardening is considered to follow the well-known Taylor relationship, which affects the critical resolved shear stress as follows [14]:

\[
\tau_{crit} = \alpha G b \sqrt{\rho} + \tau_{0}^{crit} ,
\]  

(3)

where \( \alpha \) and \( b \) are a material-specific parameter and the magnitude of the Burgers vector, respectively (Table 1). \( \rho \) is the dislocation density and \( \tau_{0}^{crit} \) the initial resolved shear stress. The dislocation density in the model is linearly raised according to the plastic slip deformation in the slip band. After the slip band mechanisms are well defined in the simulation model in the following the numerical method is presented.

Table 1 Material parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau_{crit}^{0} )</td>
<td>80 MPa</td>
</tr>
<tr>
<td>( \nu )</td>
<td>0.3</td>
</tr>
<tr>
<td>( G )</td>
<td>80 GPa</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>0.4</td>
</tr>
<tr>
<td>( b )</td>
<td>0.0002 ( \mu )m</td>
</tr>
</tbody>
</table>

3. Numerical Method

The boundary element method is well suited to investigate the effect of the proposed slip band model. The formulation used in this study combines the traditional displacement BEM as well as the displacement discontinuity BEM [15]. By doing so, sliding displacements can directly be evaluated in slip bands and element discretization is confined to outer boundaries such as grain boundaries and to slip bands. Thus, a sophisticated remeshing algorithm is not necessary. Furthermore, because of its semi-analytical character, the BEM shows a high accuracy concerning singularities.

The BEM used in this study is described by means of a problem statement, which consists of a two-dimensional homogeneous, anisotropic and linear elastic solid containing a finite slip line as shown in Fig. 4.
Fig. 4. An anisotropic solid including a slip line.

On the external boundary \(\Gamma_b\) displacements and tractions with components \(u_i\) and \(p_i\) are predefined, while relative displacements \(\Delta u_i\) and stresses \(\sigma_{ij}\) are considered on one face \(\Gamma_s\) of the slip line. Here, relative displacements consist only of tangential relative displacements, because slip lines in contrast to cracks cannot perform opening but sliding. Throughout the analysis the conventional summation rule over double indices is applied, Roman and Greek indices can only have the values 1 and 2. The procedure is based on two boundary integral equations: the displacement boundary integral equation, which is applied on the external boundary, and the stress boundary integral equation, which is used on the slip line face. The displacement boundary integral equation for a solid containing a slip line can be written as [15,16]:

\[
\int_{\Gamma_b}^{* u_{ij}}(x,y) \cdot p_i(y) - p_{ij}^*(x,y) \cdot u_i(y) \, d\Gamma_y + \int_{\Gamma_s}^{* p_{ij}}(x,y) \cdot \Delta u_i(y) \, d\Gamma_y, \quad x \in \Gamma_b, \quad (4)
\]

where \(c_{ij}\) equals 0.5 when \(\Gamma_b\) is smooth and \(u_{ij}^*(x,y)\) and \(p_{ij}^*(x,y)\) are the displacement and the traction fundamental solutions. Vector \(x\) denotes the positions, where displacements are determined, and \(y\) denotes the integration points on the boundaries \(\Gamma_b\) and \(\Gamma_s\). The stress boundary integral equation is obtained by substituting equation (4) into Hooke’s law:

\[
\int_{\Gamma_s}^{* \sigma_{ij}}(x,y) = \int_{\Gamma_s}^{* d_{ij}}(x,y) \cdot u_i(y) - s_{ij}^*(x,y) \cdot \Delta u_i(y) \, d\Gamma_y, \quad x \in \Gamma_s, \quad (5)
\]

where \(d_{ij}^*(x,y)\) and \(s_{ij}^*(x,y)\) are the stress and the higher-order stress fundamental solutions. The displacement fundamental solution in equation (4) is given in Ref. [17] by Wang. He derived two-dimensional elastostatic fundamental solutions for general anisotropic solids by the use of Stroh’s formalism [18]. The displacement fundamental solution in equation (4) can be written as an explicit expression:

\[
u_{ij}^*(x,y) = \frac{1}{\pi} \text{Im} \sum_{m=1}^{M} \frac{A_{ij}(\eta_m)}{\partial^n D(\eta_m)} \log[\mathbf{d}_m \cdot (y-x)] \quad (6)
\]

with

\[
A_{ij}(\eta_m) = \text{adj} \left[ \Gamma_{ij}(1,\eta_m) \right], \quad (7)
\]

\[
D(\eta_m) = \det \left[ \Gamma_{ij}(1,\eta_m) \right], \quad (8)
\]

\[
d_m = (1,\eta_m). \quad (9)
\]

In equations (6)-(9) \(\Gamma_{ij}(1,\eta_m)\) is defined by

\[
\Gamma_{ij}(1,\eta_m) = C_{2ij} \cdot \eta_m + (C_{2i1} + C_{2j1}) \cdot \eta_m + C_{1ij}, \quad (10)
\]

where \(C_{\alpha\beta}\) is the elasticity tensor. \(D(\eta_m)\) in (6) and (8) is a polynomial function of order four and has \(M=2\) complex roots \(\eta_m\) and two complex conjugates of \(\eta_m\), which satisfy the following characteristic equation:
\[ D(\eta_m) = 0. \] (11)

The traction fundamental solution in equation (4) is defined by the following closed expression [16]:

\[ p^*_y(x, y) = \frac{1}{\pi} \text{Im} \sum_{m=1}^{M} \frac{B_y(\eta_m)}{\partial_y D(\eta_m)} \frac{d_m \cdot n(y)}{d_m \cdot (y - x)} \] (12)

with

\[ B_y(\eta_m) = \left( C_{2y2} \cdot \eta_m + C_{2y1} \right) \cdot A_y(\eta_m) \] (13)

and the outward unit normal vector \( n \). The stress and higher-order stress fundamental solutions in equation (5) are provided by:

\[ d^*_y(x, y) = -\frac{1}{\pi} \text{Im} \sum_{m=1}^{M} \frac{B_y(\eta_m)}{\partial_y D(\eta_m)} \frac{d_m}{d_m \cdot (y - x)} \] (14)

\[ s^*_y(x, y) = -\frac{1}{\pi} \text{Im} \sum_{m=1}^{M} \frac{C_y(\eta_m)}{\partial_y D(\eta_m)} \left[ \frac{d_m \cdot d_m \cdot n(y)}{d_m \cdot (y - x)} \right]^2 \] (15)

with

\[ B_y(\eta_m) = \left( C_{y2y2} \cdot \eta_m + C_{y2y1} \right) \cdot A_y(\eta_m) \] (16)

\[ C_y(\eta_m) = \left( C_{y2y2} \cdot \eta_m + C_{y2y1} \right) \cdot A_y(\eta_m) \cdot \left( C_{y2y2} \cdot \eta_m + C_{y2y1} \right). \] (17)

The integration of the fundamental solutions (6), (12), (14) and (15) are performed fully analytically. It should be noted that the solutions have a weak logarithmic singularity \( \log|y-x| \) (6), a strong singularity \( 1/|y-x| \) (12,14), and a hypersingularity \( 1/|y-x|^2 \) in the higher-order stress fundamental solution (15). Particularly for the case of hypersingularity, special analytical techniques are used to solve the boundary integrals. For spatial discretization of equation (4) and (5) a collocation method is utilized. It implies that the boundary integral equations are fulfilled in discrete points, the so called collocation points.

Previously, the BEM was derived for a single homogeneous solid. But in case of microstructural modeling the notion of homogeneous material behavior is insufficient. Therefore in Ref. [15] and [19] a substructure technique is presented, which enables coupling of individual homogeneous substructures by use of continuity condition. The implementation of this technique in the present method allows for reproducing heterogeneous material behavior and finally each grain is represented by a homogeneous, elastic anisotropic substructure which is combined with other grains to a continuous microstructure.

In the following, the irreversible damage accumulation in slip bands is investigated.

### 4. Simulation of the microstructural damage evolution

In the previous sections, a simulation model defining the mechanisms acting in slip bands was presented and a numerical method based on a hypersingular boundary element method was derived. The implementation of the simulation model into the BEM allows to simulate damage accumulation in slip bands in a 2-D microstructure. The investigation was carried out on the basis of the real microstructure of a metastable austenitic stainless steel characterized by means of SEM in combination with the EBSD-technique and OIM. To represent the microstructure of the experimentally observed area, a 2-D mesh was created based on the EBSD map. Simulations were carried out by adopting the simulation model combined with the BEM and results were compared with experimental observations. The SEM image and the EBSD map of the considered area are shown in Figs. 5a and 5b. In addition to grain boundaries, the SEM image also highlights markings of emerging slip bands at the surface after cyclic loading. The EBSD map in Fig. 5b with related stereographic triangle indicates the crystallographic orientation of each grain.
Fig. 5. (a) SEM image and (b) EBSD map of the examined area of surface grains (loading amplitude: 240MPa, number of cycles: \(10^7\)).

The surface area investigated consists of 47 grains. For certain grains labeled 1-6 in Fig. 5a the orientation angles in Bunge convention and the highest and second highest Schmid factors (SF) are given in Table 2. To identify the corresponding slip systems of surface slip markings in the SEM image (Fig. 5a), the azimuth angles between the surface slip markings and the \(x\)-direction of the first two critical slip systems (depending on SF) are also listed in Table 2. Analyzing the SF and azimuth angles, it becomes apparent that in grains 1 to 3 (Fig. 5a) the surface slip markings belong to the first critical slip system. However, in grain 6 slip markings are apparently resulting from the second critical slip system. In accordance to Ref. [11], obviously slip markings formed in metastable austenitic stainless steel are not limited to grains with highest SF.

Table 2. Orientation angles in Bunge convention, Schmid factors (SF) and azimuth angles of surface slip markings in \(x-y\)-plane for grains 1-6 in Fig. 5a.

<table>
<thead>
<tr>
<th>Grain</th>
<th>Orientation angles [°]</th>
<th>Schmid factors (SF)</th>
<th>Azimuth angles of surface slip markings</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(\phi_1)</td>
<td>(\phi)</td>
<td>(\phi_2)</td>
</tr>
<tr>
<td>1</td>
<td>68</td>
<td>163</td>
<td>272</td>
</tr>
<tr>
<td>2</td>
<td>167</td>
<td>138</td>
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</tr>
<tr>
<td>3</td>
<td>67</td>
<td>42</td>
<td>349</td>
</tr>
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<td>4</td>
<td>17</td>
<td>69</td>
<td>73</td>
</tr>
<tr>
<td>5</td>
<td>164</td>
<td>42</td>
<td>174</td>
</tr>
<tr>
<td>6</td>
<td>202</td>
<td>104</td>
<td>340</td>
</tr>
</tbody>
</table>

Fig. 6 shows the corresponding BEM model of the microstructure. The size of the zone is 55 x 44 \(\mu m^2\). Grain boundaries are meshed by displacement boundary elements. In additional to boundary elements, collocation points are necessary inside grains, where displacements and stresses are computed in a fast post-processing routine. The distribution of these collocation points is refined towards grain boundaries and is indicated in Fig. 6 inside the dashed rectangle. The microstructure is embedded into a much larger surrounding area, which has average isotropic elastic behavior. Thereby incorrect border constraints are relaxed and by using the BEM no elements are necessary inside the surrounding area. External loading is acting at the upper and lower border of the surrounding area by imposing normal stress in the \(y\) direction. A cyclic loading is applied by sampling a harmonic stress curve and running an elastostatic calculation for every sample.
In this study, primarily the contours of shear stresses in the most critical slip systems are observed. For this purpose, in all boundary elements and inner collocation points shear stresses were computed in all of the 12 slip systems of each austenite grain and only the highest corresponding shear stresses were presented in the contours, regardless of highest SF. The elasticity tensor of the austenite phase is defined by the figures of the elastic constants of the cubic material that are $C_{11}=205$ GPa, $C_{12}=135$ GPa and $C_{44}=125$ GPa in the present case. Fig. 7a shows the computed contours of highest shear stresses in the relevant microstructure without modeling of slip bands. The loading amplitude was 240 MPa representing VHCF loading conditions for the material studied. The information, which slip system carries the maximum shear stress, is not included in Fig. 7a. Therefore, Fig. 7b gives an overview, which slip system undergoes maximum shear stresses in the contours of Fig. 7a. For this purpose the slip systems are numbered in the sequence of decreasing SF. As mentioned before, in grain 6 slip markings are occurring in the second critical slip system. Actually, in the upper section of grain 6 in Fig. 7b there appears a limited area where the slip system with the second highest SF undergoes maximum shear stresses. Hence, it is evident that the anisotropic shear stresses in slip systems are an important factor in the selection of the slip system which is activated.

The simulation model is implemented into the BEM model of the microstructure in the following way. Once the condition of slip band formation is fulfilled (see the description about the simulation model given above), the slip band is formed if the corresponding slip system is the most critical one along the possible slip band trace in the $x$-$y$-plane. The minimum distances between slip bands are limited by a given value. The 2-D BEM presupposes that exclusively in-plane sliding displacements in the $x$-$y$-plane are observed in the simulation. Therefore, the sliding distribution model based on the theory of dislocation pile-ups was adopted into the 2-D BEM by predefining shear stresses in the dislocation...
sources within the $x$-$y$-plane of the microstructure and not directly in the slip direction. To evaluate the equivalent shear stress within the $x$-$y$-plane, at first the critical resolved shear stress is predefined in the real 3-D slip direction in the correspondingly rotated stress tensor. Then the stress tensor is rotated back into the $x$-$y$-system in order to get the appropriate in-plane shear stress as constraint in the model. Out-of-plane sliding displacements and thus the emerging of slip bands out of the surface are not considered. So, the focus here is not the development of surface roughening, rather the dislocation pile-ups at grain boundaries are represented such as they are expected to occur in the bulk. Due to the fact, that surface roughening is strongly affected by out-of-plane sliding displacements, simulations in this study are not able to directly represent the surface roughening shown in Fig. 5a. However, in order to validate the mechanism of slip band formation that depends on the shear stresses in real 3-D slip systems, the orientations of surface slip markings in Fig. 5a are useful.

Fig. 8 shows the development of the contours of the simulated shear stresses in the microstructure when the simulation model is enabled. Due to high computational effort, slip band modeling was confined to 6 grains labeled 1-6. Contours were chosen from the first, third, fifth and seventh simulated loading cycle and in each case at the maximum external loading of 240MPa. It should be noticed that one cycle in the simulation represents the microstructural damage evolution resulting from many cycles in the experiment. This was achieved by adapting the parameter of cyclic slip irreversibility $p$ and by increasing the effect of cyclic hardening. In the simulation the cyclic slip irreversibility $p$ is 0.2 that is much higher than usually observed for VHCF. For example in Ref. [3] a value of $p=0.000034$ for copper polycrystals fatigued at low amplitudes was assessed. The effect of cyclic hardening was similarly increased in the simulation.

It turned out in the simulation that directly at the beginning of fatigue loading, initial slip bands spread out over entire grains. The comparison between surface slip markings found in the SEM image (Fig. 5a) and simulated slip band layers (Fig. 8) illustrates that slip bands are formed in the correct slip systems. The maximum shear stresses in the slip systems that are relevant for determining the corresponding slip systems are therefore suitable for the prediction of the active slip systems. Grain 6 in Fig. 8 includes slip bands in two different slip systems. In the lower region of grain 6 slip bands occur in the first slip system (highest SF) and in the upper region slip bands occur in the second slip system because of the highest shear stresses occurring there, as shown in Fig. 7b. A closer investigation showed that after slip bands have developed in the first slip system in the lower region of grain 6, the area of maximum shear stress in the second slip system increases so that finally half of the grain is filled by slip bands of the second system. This is in good agreement to SEM observations (Fig. 5a in combination with Table 2).

Sliding displacements in slip band layers lead to a decrease of the shear stresses within the grains, while at the end of the slip bands significant stress peaks arise. This is particularly demonstrated in grain 4 (Fig. 8). Stress peaks at the end of slip bands arise due to the notch effect at the tips resulting from the sliding distribution model based on dislocation pile-ups. Similarly, Yang et al. [9] simulated stress fields of persistent slip bands and found that stresses at the tips of persistent slip lines are much higher than in other regions. In the present study, stress peaks at grain boundaries are additionally intensified, because grain boundaries possess a barrier effect resulting from the change in crystal orientation.

The SEM image in Fig. 5a shows that grains 4 and 5 exhibit no visible surface roughening. However, the simulation results presented in Fig. 8 indicate that these grains possess many slip bands. It was found that the most critical slip systems in these grains have a small angle between slip direction and the surface plane. So, the component of out-of-plane sliding and the corresponding surface roughening are low and can therefore hardly be identified in the SEM image. However, it is a plausible assumption that in-plane sliding displacement exists, as it was simulated in this study.
Fig. 8. Contours of simulated maximum shear stresses in the most critical slip systems in the (a) 1st, (b) 3rd, (c) 5th and (d) 7th loading cycle (loading amplitude: 240MPa, hypothetical cyclic slip irreversibility of $p=0.2$ (in order to represent many experimental cycles in one simulated cycle)).

It is shown in Fig. 8 that slip bands deform differently depending on the specific polycrystalline boundary value problem. In the first cycle, sliding is very low so that it barely affects the shear stresses (Fig. 8a). In the third cycle, the slip bands are already fully developed (Fig. 8b). In cycles 5 and 7, the irreversible fraction of sliding that is fixed on opposite layers influences the deformation of slip bands in such a way that sliding becomes more pronounced. Finally, the comparison of contour plots in Fig. 8 in the first, third, fifth and seventh loading cycle shows that with increasing number of simulated loading cycles shear stresses at the end of the slip bands and thus at grain boundaries increase. This is a result of the irreversible damage accumulation, which leads to a higher amount of fixed sliding displacement on the opposite layers and in turn raises the sliding displacement on the active layers and hence increases the activation of mobile dislocations. Considering the shear stresses in critical slip systems to be a damage relevant parameter, in simulations it turned out that grain boundaries are most critical sites in the microstructure.

It has been noted before that emerging of slip bands out of the surface is not represented in this study. Therefore, the sites of stress concentration as a consequence of extrusions and intrusions cannot be identified. For this purpose, a full 3-D characterization of the microstructure would be necessary. To reduce this shortage of the 2D-BEM, the generalized plane-strain condition, which assumes columnar grains in $z$-direction, might be beneficial [7]. The well-known phenomenon that slip bands with a high out-of-plane sliding component exhibit higher deformation due to free surface condition of surface grains is not considered. By knowing the effect of free surface condition on the sliding activity, a corresponding parameter might be defined and implemented into the simulation model. In addition, in the simulation model constant slip band thickness is assumed, though it is known that the thickness of slip bands increases with increasing plastic deformation. Moreover, the $x$-$y$ section view of slip bands for different grains are different, because of the various orientation angles of the slip planes. When the angle between the slip plane and the $x$-$y$ section decreases, the thickness and distance of slip bands shown in the $x$-$y$ section increases.

It should also be noted that the size of the simulated area is relatively small and damage evolution was simulated only in 6 grains. Such a small area is inadequate to statistically represent the microstructure. Future work will focus on a reduction of the mentioned inaccuracies. Moreover, the
simulation has to be further adapted to the "real microstructure" with its various inhomogeneities other than the grain morphology.

5. Conclusion

In this study, a simulation model is proposed which describes the damage mechanisms occurring in slip bands under VHCF condition. The formation of a slip band is assumed to occur at sites of shear stress concentration, while sliding distribution arises from the theory of dislocation pile-ups at grain boundaries. The irreversible slip character is represented as the slip band is approximated by two closely located layers and a special procedure was adopted to accumulate the irreversible fraction of cyclic slip. Hardening of the slip band results from an increasing dislocation density. To investigate the effect of the suggested slip band model in a real 2-D microstructure, it was implemented into a BEM. The method is based on two boundary integral equations: the displacement boundary integral equation, which is applied on the external boundary, and the stress boundary integral equation which is used in slip bands. Hypersingular fundamental solutions for general anisotropic elastic solids were implemented and by means of a substructure technique a 2D-microstructure with individual anisotropic elastic behavior in each grain is considered. Simulation of the microstructural damage evolution was conducted in a real 2-D microstructure. The 2-D mesh is based on the characterization of the grain morphology by means of EBSD-technique. Results are shown as contours of maximum shear stress in the microstructure. It turns out that slip planes of the generated slip bands are in good agreement with SEM observation. Sliding displacements in slip bands lead to a decrease of shear stresses within grains, while at the end of slip bands significant stress peaks arise. With increasing number of simulated loading cycles, deformation in slip bands accumulate due to sliding irreversibility. It is shown that accumulation leads to higher shear stresses at the end of slip bands at grain boundaries. Emerging of slip bands out of the surface was not considered, since the simulation of sliding displacements is confined to the surface plane.

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References