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Modeling transgranular crack growth in random 3D grain structures under cyclic loading

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ABSTRACT

A probabilistic method to predict the crack formation in polycrystalline materials with a random microstructure under cyclic loading is developed. In particular, transgranular crack growth in 3D grain structures generated randomly by the Voronoï process is considered. The potential crack extension planes in the individual grains are dependent on the different grain orientations and the crystal structure of the considered material. Under cyclic loading fatigue cracks initiate and propagate along the slip planes of the crystal structure. For this reason, an energy-based criterion is used in order to describe the successive material damage under cyclic loading which is completely projected into the crack extension planes and finally causes the crack propagation. Subsequently, the computation of the crack path in a number of randomly generated grain structure models provides a raw data base in order to determine probability distributions of the number of cycles up to a pre-defined crack depth. As an input for many fracture mechanics evaluation concepts which are based on an assumed incipient crack depth, the number of cycles and the corresponding scatter band width up to a postulated incipient crack depth is of great interest.

1. Introduction

Many materials in structural components in operating state are subject to cyclic loading. Since even deformations in the elastic range cause material fatigue, there is a great interest for development of methods for accurate lifetime prediction starting from crack initiation to final fracture. Due to their different damage behaviors, it is necessary to distinguish between short and long crack growth. The linear elastic fracture mechanics evaluation concepts can only be applied to long cracks because the microstructural influence which is very important for short crack initiation and propagation cannot be taken into account. For description of the incipient cracking, methods are required reproducing the microstructural mechanisms, as the movement of dislocations along slip planes in consideration of the crystal structure (Lankford [1], McEvily [2], Hussain [3]).

In Christ et al. [4] three different groups of models to predict short crack growth are identified. Beside models based on an empirical approach to consider grain boundary effects (Hobson [5], Brown [6]) resp. based on discrete dislocations (Doquet [7], Wilkinson [8]), particularly mechanism-based models considering plastic deformation at the crack tip are important for the present study. Based on models of Bilby et al. [9] and Navarro and de los Rios [10], Schick et al. [11] developed a slip band crack model in order to predict short crack propagation and its scatter in a random grain structure. Further 2D probabilistic methods for short crack propagation in polycrystalline materials are described by Bolotin and Belousov [12], Kraft and Molinari [13] and Meyer et al. [14].

With the increase of computing power the generation and using of much more complex 3D models to predict the degradation and failure in polycrystalline materials is possible. A two-scale approach of Benedetti and Aliabadi [15] shows how the implementation of microstructural submodels improve the component assessment on the macroscopic level. The special feature in the method of Rimoli and Ortiz [16] is the explicitly resolved crack propagation path by the computational mesh. Simonovski and Cizelj [17] show that using a cohesive-type contact instead of cohesive elements for modeling the grain boundaries in a polycrystalline structure yield to a significant higher numerical stability. With a 3D phase-field model Abdollahi and Arias [18] represent a different approach with the advantage that the interaction of several microstructural mechanisms can be considered.

Complex crystal plasticity approaches are implemented in the 3D models of Lin et al. [19], Proudhon et al. [20] and Wan et al. [21], but the extremely high computation times prohibit an efficient lifetime

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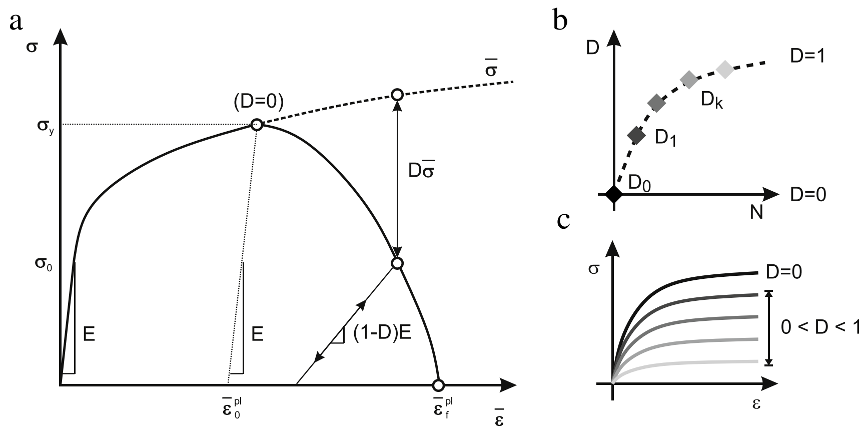

Fig. 1. Damage degradation (a), damage parameter (b) and yield curve (c).

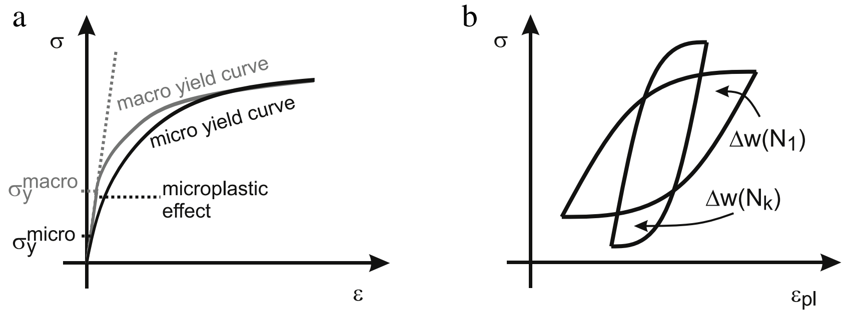

Fig. 2. Microplastic yield (a) and dissipated hysteresis energy per cycle (b).

prediction in the application of component assessments. For this reason, Gulizzi et al. [22] represent a method to reduce extensively the computational cost of polycrystalline micro simulations. The same objective pursue Benedetti et al. [23] by a reduction of the degree of freedoms in their polycrystalline models using a 3D grain-boundary formulation for small strains crystal plasticity.

In the present study, as an extension of Schick et al. [11], a stochastic finite element method based on microstructural characteristics, as grain size distributions and crack growth along slip planes, is developed in order to predict not only the number of cycles up to an incipient crack depth but also to identify the corresponding scatter band width with a numerically efficient approach. This model is a benefit as an input for fracture mechanics concepts for fatigue assessment, using a postulated incipient crack, because the initial crack depth to be used as a starting point for these concepts as well as the lifetime up to this starting point can be integrated much more accurately.

2. Fatigue and damage definition

Material damage due to fatigue caused by cyclic mechanical loading is a typical damage mechanism for metallic materials. In particular, for components in operating state it is crucial that material fatigue may arise out of cyclic loading far below the macroscopic material yield strength. On the microstructural level, the clash of grains with different orientations and the presence of inhomogeneities, such as inclusions, lead to stress concentrations. Consequently, material fatigue due to microplastic yield caused by movement of dislocations along activated slip planes under cyclic loading occurs. In this relation, the grain boundaries constitute a barrier so that crack nucleation arises due to an irreversible accumulation of dislocations. By further cyclic loading the crack growth is induced at the most severe pile-up to the completely material failure.

Based on this damage mechanism Tanaka and Mura [24] developed a model of damage accumulation considering that in particular slip band cracks are expected for high shear stress values. In the case of uniaxial stress the maximum shear stress occurs if the normal of the slip plane and the slip direction are inclined at 45° to the stress axis.

In the present study the failure on material level is described by the continuum damage equation

$$\boldsymbol{\sigma} = (1 - D)\bar{\boldsymbol{\sigma}} \tag{1}$$

with the scalar damage parameter D, the stress tensor $\boldsymbol{\sigma}$ and the effective undamaged stress tensor $\bar{\boldsymbol{\sigma}}$. A schematic representation of the damage degradation referred to Eq. (1) is pictured in Fig. 1(a) with the elasticity modulus E, the yield stress $\boldsymbol{\sigma}$ and the equivalent plastic strain $\bar{\varepsilon}_0^{pl}$ at the onset of damage and at failure $\bar{\varepsilon}_f^{pl}$ resp. As plotted in Fig. 1(b), the value of the damage parameter is $D = 0$ for the undamaged state and achieves its maximum $D = 1$ for complete material failure. The influence of an increasing damage parameter on the material yield curve is sketched in Fig. 1(c).

For the additional field variable D, an additional field equation is required. This equation is provided in terms of the damage evolution equation. Using a load-cycle based approach, the damage degradation per cycle

$$\frac{\partial D}{\partial N} = \frac{k_1}{L} \Delta w^{k_2} \tag{2}$$

is defined by an energy-based criterion (Abaqus [25]) with the dissipated microplastic energy Δw per load cycle N, the model-dependent characteristic length L and the material constants k_1 and k_2. In this context, the term microplasticity refers to a plastic deformation occurring below the static yield limit due to cyclic dislocation movements with plastic strains far below their elastic counterparts.

In Fig. 2(a) the microplastic effect is sketched in an exaggerated manner in order to show that for modeling a micro yield curve is

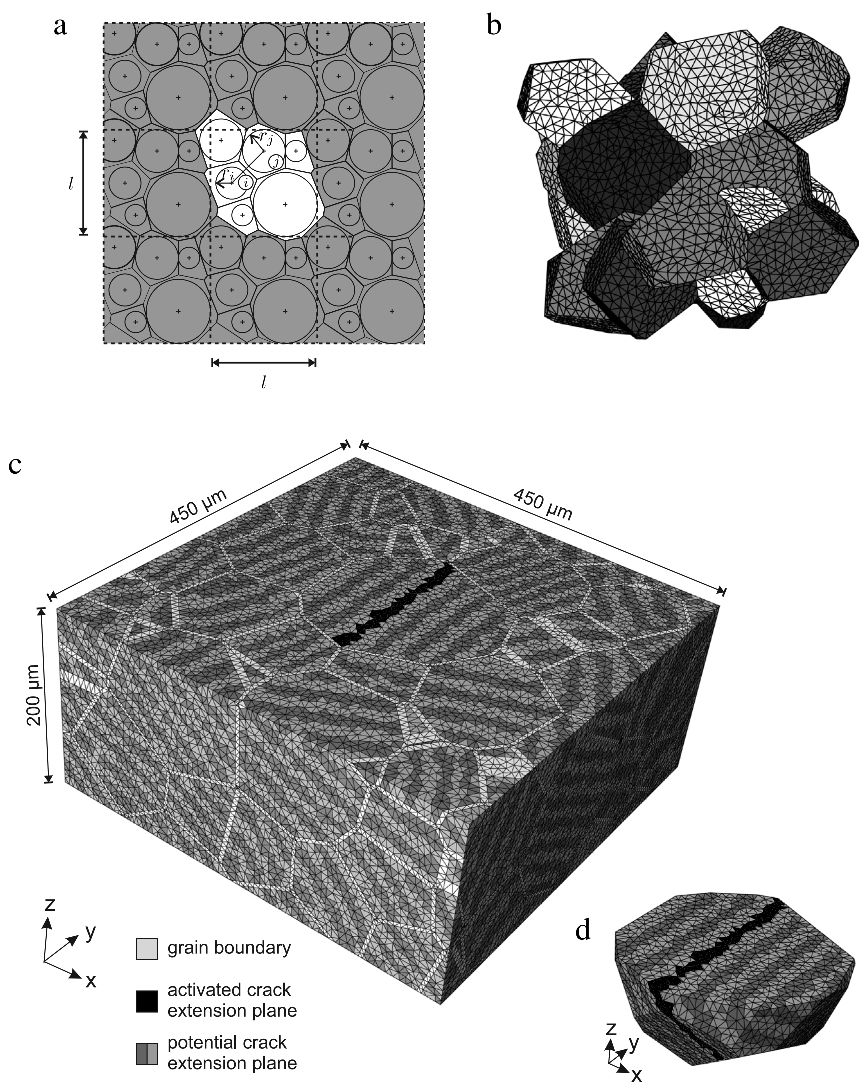

Fig. 3. Voronoï process (a), periodic grain structure (b), crack extension model (c) and grain with crack extension plane (d).

necessary because fatigue is a material failure process taking normally place in the macroscopically elastic range. The damage degradation is reproduced in the model by accumulation of the dissipated energy per cycle. As sketched in Fig. 2(b), the energy amounts in each of the cycles differ in their values because not only the local loading is varied over the time but also the material yield curve continuously changes in dependence on the damage parameter. However, it can be assumed that the dissipated energy amounts in a sequence of cycles is approximately equivalent.

3. Crack extension model

For computation of the load-cycle-dependent crack growth and its scatter finite element models are generated randomly. The scatter in the size of the grains is reproduced by using the Voronoï process in Laguerre geometry [26] which is a randomized space division algorithm. A 2D sketch in Fig. 3(a) illustrates this approach. The first step is the random generation of nucleation points inside a square with the edge length l. In order to obtain structures which correlate to given grain size distributions an environment defined by a radius r_i in which no other nucleation point is allowed to exist is assigned to each nucleation point $s(i)$. In order to obtain a periodic computational model for the microstructure these nucleation points are copied into the surrounding neighborhood. Subsequently, the grain belonging to nucleation point $s(i)$ is defined by

$$\mathbf{\Omega}^{g(p)} = \left\{ x_i \mid x_i \in \mathbb{R}^3,\ r_L(x_i,\ x_i^{s(p)}) \leq r_L(x_i,\ x_i^{s(q)}),\ q \neq p \right\} \ ,$$
$$p,\ q = 1,\ 2,\ \dots\ ,\ n \tag{3}$$

with the distance $r_L(x_i,\ x_i^{s(p)}) = \left[\left(r_E(x_i,\ x_i^{s(p)}) \right)^2 - (r(p))^2 \right]^{\frac{1}{2}}$ in Laguerre geometry and the Euclidean distance $r_E(x_i,\ x_i^{s(p)})$ as the set of spatial points, for which the Laguerre distance r_L to the respective nucleus $s(p)$ is smaller than for all other nuclei. A 3D grain structure after meshing with tetrahedral finite elements is shown in Fig. 3(b).

Due to the fact that a periodic structure is given (Fig. 3(a)), it is possible to shift volume fractions of grains in such a way that in contrast of the meshed model in Fig. 3(b) a rectangular-shaped model, as shown in Fig. 3(c), can be obtained. Furthermore, the meshing is adapted in such a way that the region near the grain boundaries is represented by layers of finite elements. Moreover, for computation of transgranular crack growth, crack extension planes inside individual grains are necessary (Fig. 3(d)). For this reason, a finite element mesh reproducing a number of parallel potential crack extension planes is implemented in each grain. The orientation of these planes is chosen in such a way that for each grain in the model the most critical orientation for the randomly determined crystalline orientation and the prescribed external loading direction is obtained.

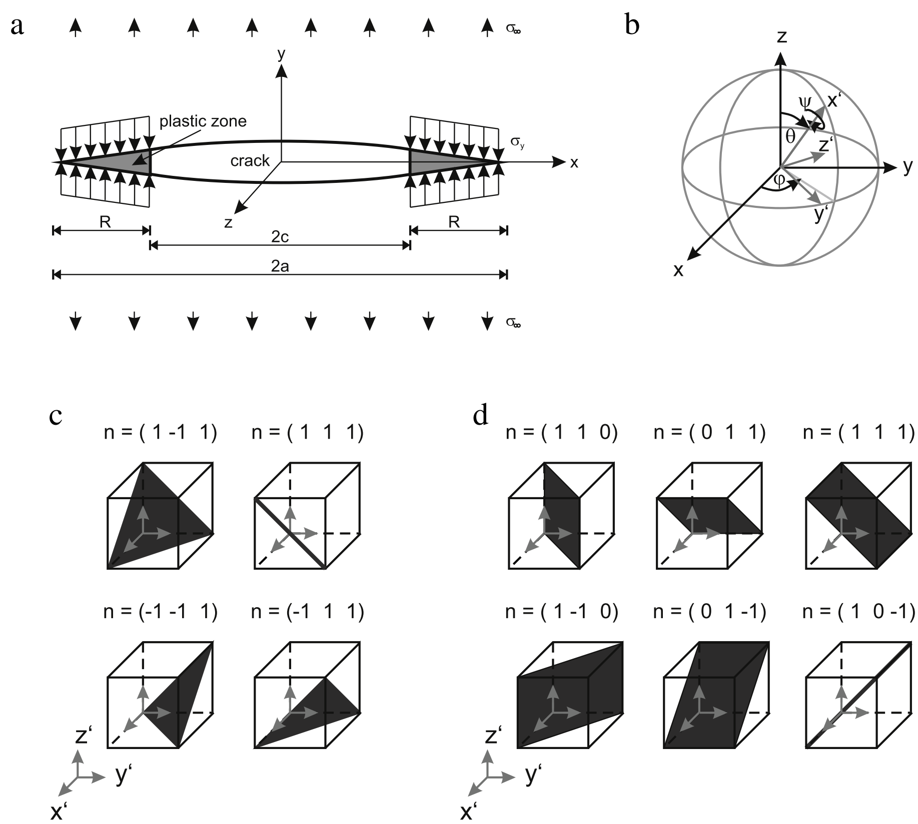

Fig. 4. Dugdale–Barenblatt plastic zone model (a), orientation of the cubic system in space (b), primary slip systems in a body-centered cubic system (c) and primary slip systems in a face-centered cubic system (d).

To simplify the model, the fatigue damage under cyclic loading is modeled using a Dugdale [27] and Barenblatt [28] type model (Fig. 4(a)) with successively projected crack extensions planes. For this reason, initially all finite elements in the model obtain elastic material properties with the exception of the finite elements in the crack extension plane in the largest grain close to the surface. To reproduce the fatigue damage, these elements have from the start of the computation elastic–plastic material properties in terms of a micro yield curve (Fig. 2(a)) and can be damaged successively (Section 2). As soon as the crack front gets close to the grain boundaries, elastic–plastic material properties are allocated to the most critical crack extension plane in the neighbored grain in order to make a further crack propagation possible.

As described in Section 2, a fraction of energy is dissipated in each cycle and causes the material damage. Due to the fact that the amount of dissipated energy is nearly the same for several cycles, one cycle in the computation may represent a number of cycles in a real fatigue test in order to perform the computations in a numerical efficient way.

4. Probabilistic approach

For computation of the load-cycle-dependent crack growth and its scatter it is assumed that the heterogeneous microstructure significantly affects the rate of crack growth. For this reason, a probabilistic approach is applied which is based on the determination of the probabilities of occurrence for the spatial orientation of the crack extension planes. As an example the primary slip systems of a body-centered cubic system (bcc) and a face-centered cubic system (fcc) are shown in Fig. 4(c) resp. Fig. 4(d). By rotation of the cubes in space (Fig. 4(b)) all possible orientations of the crystal structure are sampled and the critical slip plane direction of the considered crystal structure referring to crack growth under the present loading direction is determined. With this procedure the probabilities of occurrence for arbitrarily oriented crack extensions planes in space, as sketched in Fig. 5(a), can be determined.

Considering that the results obtained in the numerical analysis of one of the microstructural modes (i. e. the crack dimensions for a prescribed cycle number under a specific external load case) have the same probability as the probability of occurrence of the underlying microstructure, the probability distributions for the respective output properties are obtained. For this purpose, the results (e. g. the number N of cycles required to reach a prescribed crack depth a) are rearranged into ascending order (Fig. 5(b)). Each datum is provided with its individual probability of occurrence p (coinciding with the probability of occurrence of the underlying microstructure). Subsequently, the cumulative probability for the respective datum is obtained as the sum

$$F(N_i) = \sum_j p_j \quad \text{with} \quad N_j \leq N_i \tag{4}$$

of the individual probabilities p_i of all results which are smaller than the considered datum N_i. In a similar manner, the probability distributions for the crack depth at a prescribed number N of cycles can be computed.

The benefit of this method is that the results of the models with differently oriented crack extension planes can be weighted with their real probability of occurrence (Fig. 5(b)). This is an advantage to an equally weighted assessment because it can be assumed that crack extension planes which have a strongly deviating orientation referring to the most critical direction for crack growth supply results which may underestimate the considered material properties on the macroscopic level in a very large number of cases.

5. Example

For illustration of the developed stochastic finite element method the scatter in the crack growth in a polycrystalline grain structure under cyclic load is considered. In order to keep the numerical effort within acceptable bounds, the number of models to be computed is limited to eight models representing the entire range of possible grain or crack

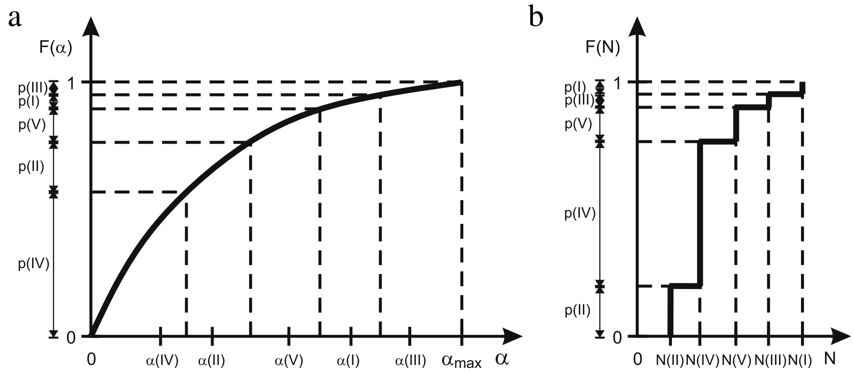

Fig. 5. Probabilities of occurrence for the potential orientations of the crack extension planes (a) and probability distribution of the number of cycles up to a pre-defined crack depth (b).

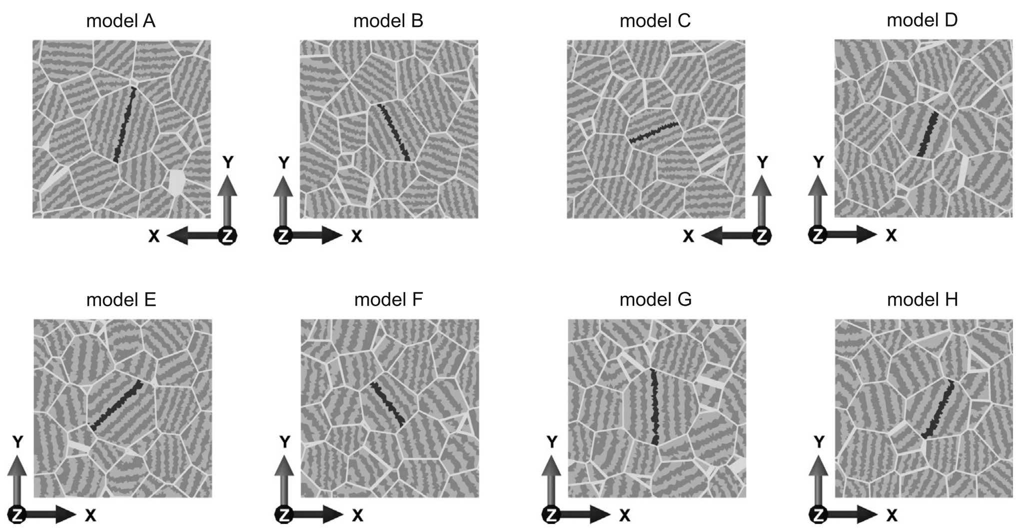

Fig. 6. Surfaces of the finite element models with crack extension planes.

orientations. The size of the models is 450 µm × 450 µm × 200 µm and a random grain structure consisting of 45 grains in each model are generated with the Voronoï process in Laguerre geometry. The average equivalent sphere diameter of the grains is 60 µm and the scatter band is 35 µm to 100 µm.

The periodic grain structure is cut in such a way that the largest grain is located in the center of the model because large crack extension planes are particularly critical for crack initiation. For this reason, it is defined that the crack always starts from the upper resp. lower surface depending on which side the considered grain has the larger extension in direction of depth. The surfaces of the eight models with the most critical crack extension plane in each case are plotted in Fig. 6. Elastic material properties with a Young's modulus of $E = 210$ GPa and a Poisson ratio of $\nu = 0.3$ are allocated to all finite elements. For simplicity isotropic elastic behavior is used, assuming that the orientation of the crack planes is the dominant anisotropy effect in fatigue crack formation and initial propagation. Compared to the anisotropy induced by the crack orientation, the elastic anisotropy usually is of minor importance. The finite elements in the crack extension plane are assigned with plastic material properties in terms of a microplastic fitted yield curve for structural steel. The cyclic loading is applied uniaxially in x-direction with a stress ratio of $R = 0.1$. Moreover, one loading cycle in all the models is consistent to $1 \cdot 10^4$ cycles in a real experimental fatigue test and the model is fixed in one point so a constraint in y- and z-direction is non-existent. Noted at this point that periodic boundary conditions are little useful since in this case the model would be a model for a periodic multi-crack array. The grain orientations are arbitrarily and a body-centered crystal structure is assumed. The corresponding probabilities

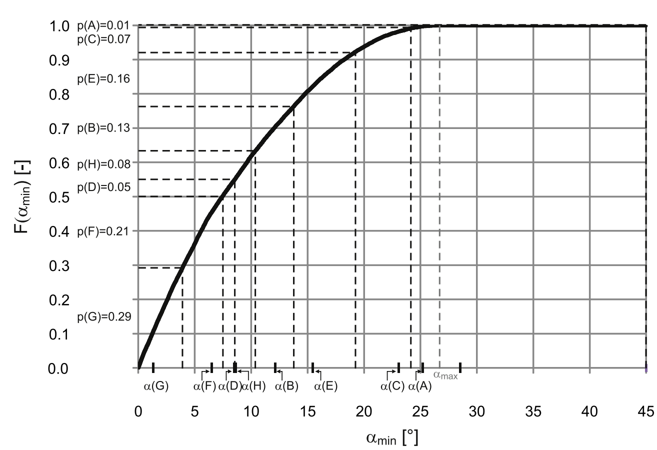

Fig. 7. Probabilities of occurrence for the models A to H based on a body-centered cubic system.

of occurrence for the models A to H are shown in Fig. 7. It is pointed out that the models are distributed over the whole range of possible orientations. This legitimate to do the computations on the base of the low number of eight generated models.

In Fig. 8 the computation of the crack extension in model E is shown as an example. As in all other models the finite elements close to the surface in the crack extension plane are deleted in order to obtain a more

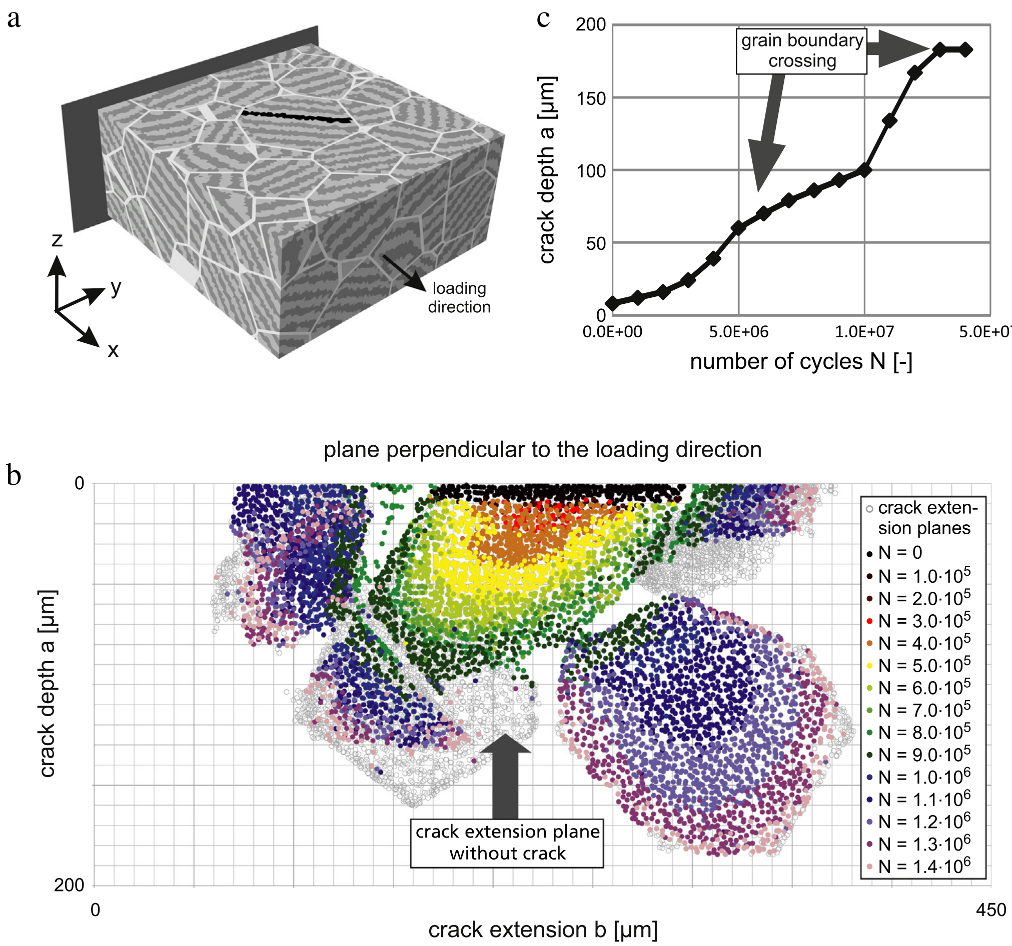

Fig. 8. Model E (a), cycle-dependent crack extension (b) and crack growth (c).

realistic surface with a roughness of around 10 μm. The crack extension under a loading with a stress amplitude of 300 MPa is plotted in Fig. 8(b), as a projection into a plane perpendicular to the loading direction. In addition to the typical semi-elliptical crack growth, it can be observed in Fig. 8(b) that after reaching the grain boundaries of the first grain, the crack does not extend into all neighboring grains, but the further crack growth takes place in particularly favorable crack extension planes, which are characterized by their large size and preferred orientation.

The typical crack propagation in the direction of depth is shown in Fig. 8(c). First, there is a slow rate of crack growth near the surface, then it increases rapidly inside the grain and slows down when approaching the grain boundary. After crossing this barrier anew a fast crack extension can be observed. Close to the next grain boundary the crack growth decelerates again.

For analysis of the scatter in the crack growth behavior, the crack growth across the first grain is computed for all models loaded with three different stress amplitudes of 100 MPa, 200 MPa and 300 MPa. The resulting cycle-dependent crack growth in depth direction for the different models and loading amplitudes is plotted in Fig. 9.

It can be observed that the number of cycles to achieve an equivalent crack depth increases towards lower stress amplitudes. Furthermore, there is a significant scatter in the results for the identical external loading conditions. In particular, the higher cycle numbers for model E are conspicuous. An explanation is given in Fig. 7 in combination with Fig. 6. The angle between the normal vector of the crack extension plane and the loading direction is unfavorable in consideration of crack growth. Only in model A the angle is even worse, but Fig. 6 shows that close to the surface the crack extension plane in model E is much more disadvantageous than in model A and all other models.

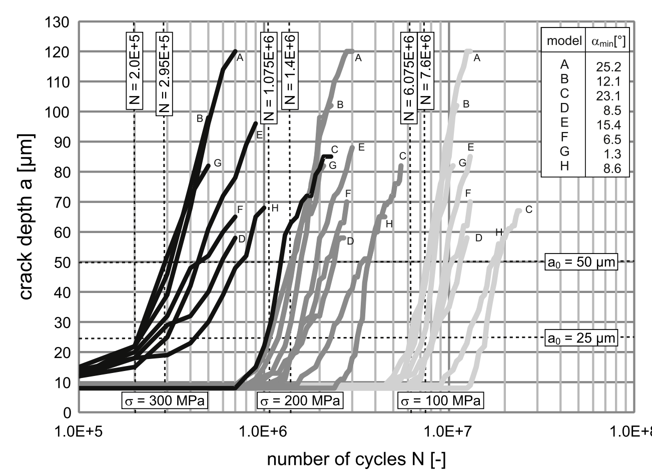

Fig. 9. Initial crack growth.

Nevertheless, such cases may occur and are included in the probability distributions in Fig. 10(a). In this diagram the results of the eight models are weighted according to Fig. 7. The plotted distributions show impressively the scatter in the number of cycles which are necessary to obtain a crack depth of 25 μm resp. 50 μm for the different loading conditions. In particular, the results for the computation with the highest stress amplitude across one grain identify a scatter band width for the number N of cycles by a power of ten. Executing a simulation over a number of grains, it can be expected that the spreading in the

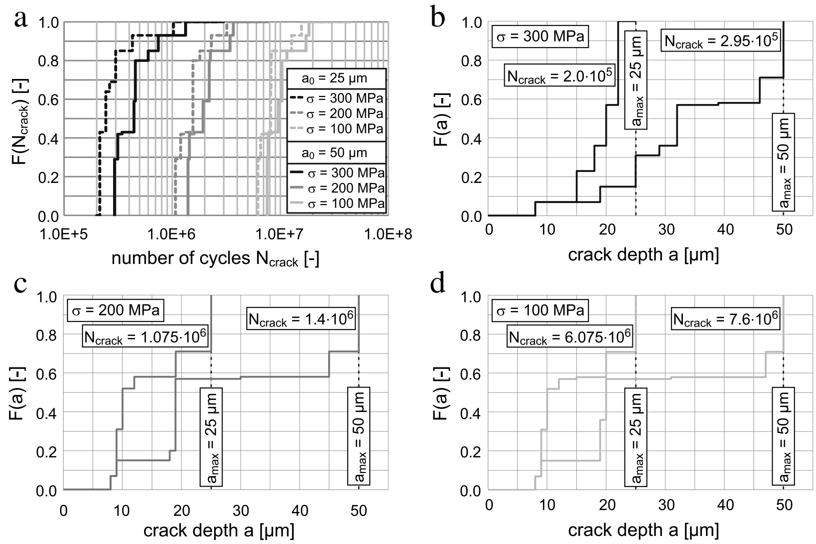

Fig. 10. Number of cycles up to a pre-defined incipient crack depth (a), incipient crack depth distributions (b–d).

results increases because arrangements of grains can occur with different crystallographic orientations which are more or less critical related to crack propagation.

Alternatively, the crack depth in all models is determined for the number of cycles in which the first model achieves a crack depth of 25 µm resp. 50 µm. The corresponding crack depth distributions $F(a)$ for the different stress amplitudes are plotted in Fig. 10(b) to (d). Such assessments are of interest in many fracture mechanics evaluation concepts which determine the further crack growth on the base of a postulated incipient crack. The present stochastic finite element method is able to predict the number of cycles which is necessary to obtain a crack with the postulated crack depth under cyclic loading and the corresponding scatter band width.

6. Conclusions

The present contribution proposes a stochastic finite element method predicting macroscopic fatigue crack propagation properties and the corresponding scatter on the base of a heterogeneous microstructure. As an example, transgranular fatigue crack growth in grain structures generated with the Voronoï process in Laguerre geometry is considered. The orientation of the grains is chosen randomly, but the most critical slip plane direction in each grain is determined considering the crystalline structure of the material. Depending on the probabilities of occurrence for the differently oriented crack extension planes the results for the individual models are weighted in order to obtain probability distributions of the most important fatigue crack formation properties as the number of cycles up to a pre-defined crack depth or in the other way round crack depth distributions for a prescribed cycle number. The considered example shows impressively the influence of the random microstructure with its different grain sizes and orientations on the macroscopic material behavior in term of significant scatter band widths.

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