MESOSCOPIC SIMULATIONS OF DAMAGE ACCUMULATION UNDER FATIGUE LOADING

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Abstract

Mesoscopic simulations of damage accumulation under fatigue loading are based on understanding the processes of crack initiation, crack growth and crack coalescence. Analysing interacting cracks are still somewhat difficult whereas the initiation and extension behaviour of isolated small cracks is very well understood nowadays. Additional insight can be gained in the mechanisms of crack initiation if the local stress state is taken into account. The damage accumulation process can then be simulated on a random grain structure based on the real micro-structure or a stochastic model. Very good agreement can be achieved between experimentally observed crack patterns and simulated ones. The paper concludes with some remarks on how to infer damage accumulation laws from these crack patterns.

Introduction

There are two different scenarios for damage accumulation under fatigue loading: The first one occurs predominantly at low load levels and/or in materials with scare well-defined crack initiation sites. In this case small cracks are initiated at these initiation sites (e.g. inclusions, pores, PSBs) rather early in the lifetime of a specific component. These cracks are stopped by the first barrier in the microstructure, but will eventually start to grow in a subcritical manner: As long a given crack remains small compared to the characteristic length scale of the material it shows the well-known intermittent crack growth behaviour. When the microscopic barriers no longer act as obstacles for stable crack growth, cracks may start to interact and one dominant macrocrack is formed by stable crack extension and/or coalescence. This corresponds to the final stage of the component's lifetime.

The second scenario describes fatigue damage accumulation under high loading, in an adverse environment or at elevated temperatures. A high number of microcracks is formed at crack initiation sites such as slip planes grain boundaries etc., i.e. weak links in the microstructures which exist almost everywhere. Initiation time is a random variable which depends very much on the local deformation around the potential initiation site. A phase of intermittent crack growth will very often follow the initiation phase, but the time period of crack extension is very much reduced compared to the first scenario. The reason for this is crack interaction and coalescence which is much more frequent due to the high number of cracks per unit area.

The local deformation state at the crack initiation site is always needed in a mesoscopic simulation of damage accumulation under fatigue loading. This can be determined using a very coarse approximation such as the local stress/strain values in a continuum model or using a more refined model which takes the grain structure in to account. In this case, the material is locally anisotropic and the local orientation of the crystallographic axes plays an important role.

Damage in the first case is clearly related to the size of the worst crack. The failure probability after a specific number of load cycles, i.e. the lifetime distribution, is equal to the probability that the worst crack exceeds its critical size. This probability can be readily calculated from stress distribution in the component if suitable models for crack initiation and growth are available. The state of the art in this area is described in the first part of the paper.

The definition of a suitable damage variable is more involved for the second scenario. In some cases, the average number of cracks per unit area correlates well the lifetime, in others, the maximum crack length or the cumulated crack length seem to be more suitable. In all cases the damage accumulation law and the failure criterion is purely empirical and is derived from the microcrack patterns observed on the specimen surface. This implies that lifetime prediction is only possible if these crack patterns can be reproduced using a suitable mesoscopic simulation model. This problem is dealt with in the second part of this paper.

1. Probabilistic fracture mechanics

Probabilistic fracture mechanics deals with determining the lifetime distribution of components containing isolated cracks. The failure probability at load cycle N can be determined if a deterministic model for crack initiation and growth is available and a statistical model which describes quantitatively the scatter behaviour of the influence factors of the deterministic model. Starting from the early days of risk analysis of nuclear power plants, numerous probabilistic studies have been given in the literature with different degrees of sophistication in the deterministic as well as the statistical model.

A closed form expression for the failure probability can be derived using the following line of arguments. Let us first consider a crack which was initiated at load cycles N_i. The conditional probability that the initiation takes place at a specific crack initiation site at point $\vec{x}$ in the time interval $[N_i, N_i + dN_i]$ is given by

$$\lambda_i \, \mathrm{d}\, N_i = \frac{P(\text{initiation in } [N_i, N_i + dN_i])}{P(\text{no initiation before } N_i)} \tag{1}$$

and may depend on the local stress field $\sigma_{ij}(\vec{x})$. A crack initiated at load cycle N_i with size a_i will extend under cyclic loading until it reaches a critical size a_c. The probability that the crack size after N load cycles, $a(N)$ exceeds a_c, is denoted by

$$Q_1 = P(a(N) > a_c) \tag{2}$$

and depends on the nature and the parameters of the crack growth law, the initial crack size a_i, the initiation time N_i and the local stress field $\sigma_{ij}(\vec{x})$ which may also depend on the cycle number.

From Eqs. (1), (2), the failure probability can be determined as

$$P_f(N) = 1 - \exp\left(-\frac{M}{V} \cdot \int_0^N \int_V \lambda_i \cdot Q_1 \, \mathrm{d}V \, \mathrm{d}\, N_i \right) \tag{3}$$

where M is the number of crack initiation sites in the component. Eq. (3) is applicable to those components in which there is no crack interaction, i.e. the number of crack initiation sites per unit volume is small or the crack initiaion rate is low.

Even though the fundamental relation for the failure probability is comparatively simple, the evaluation of the crack initiation rate and the probability Q_1 that a given crack exceeds its critical size is by no means straightforward, as suitble models of initiation, growth and failure of small cracks have to be developed.

1.1 Crack initiation rate

Cracks are initiated from micro-structural disturbances such as inclusions, pores, large grains or defective grain boundaries and from persistent slip bands which are formed during cyclic loading. In the first case, the crack is normally formed during the first few load cycles and starts to extent. Consequently there is virtually no physical crack initiation phase. The question whether or not a specific inclusion acts as an crack initiator depends very much on its meachnical properties and its geometrical shape. Quantitative results can be obtained using Finite Element methods (Kunow *et al.* [1]). Even if a crack is initiatied, it may then be stopped by some microstructural barrier which may be overcome after a certain number of load cycles. It is a matter of taste whether this part of the crack extension phase is included in the initiation phase or whether a model of intermittent crack growth is used to describe this part of the damage accumulation process.

Experimental proof of the absence of a crack initiation phase can be given by determining the crack growth law for a certain number of micro-cracks, e.g. by visual inspection of the cracks on the specimen surface using a sutiable microscopic device or using the marker load technique (Fischmeister *et al.* [2]). The crack growth law can be used to calculate the ficticious crack size a_{0e} at cycle $N = 0$. If a_{0e} is significantly smaller than the size of the crack initiator, then an initiation phase has to be taken into account. If, on the other hand, the size of the crack initiator significantly smaller than the extrapolated value a_{0e}, the crack shows a faster growth rate just after initiation which may be related to 3D effects or to small crack growth. With the reasoning it was concluded in [2] that cracks formed at inclusions start to extent immediately at the beginning of the cyclic loading.

In materials with no pre-defined crack initiation sites, microcracks are likely to be formed along persistent slip bands. The model proposed by Tanaka and Mura [3] is the classical model for dislocation pile-up and ensuing microcrack initiation. The number of cycles to crack initiation is related to the local value of the stress field by a simple power law:

$$N_i = \frac{8GW_c}{\pi(1-\nu)D(\Delta\tau_{res} - 2\tau_c)^2} \tag{4}$$

where τ_{res} is the resolved shear stress in the crack plane, τ_c, G, W_c and ν are material constants, and D is the grain size. Assuming that the grain size distribution is characterized by the probability density function $f_D(D)$ a closed-form expression for the probability density function $f_i(N_i)$ of the number of cycles to crack initiation can be derived:

$$f_i(N_i) = f_D(D(N_i)) \cdot \left| \frac{dD}{dN_i} \right| \tag{5}$$

$$= f_D\left(D = \frac{C_i}{N_i(\tau_{res} - \tau_C)^2} \right) \cdot \frac{C_i}{N_i^{\,2}(\tau_{res} - \tau_C)^2}$$

A typical example of an initiation rate λ_i derived from eq. (5) and the fundamental relation eq. (4) is shown in Fig. 1. There is incubation phase in which dislocations are formed and pile up along slip systems and a second phase which is characterized by an approximately constant initiation rate. After a certain period of time most grains are cracked and the initiation process dies out.

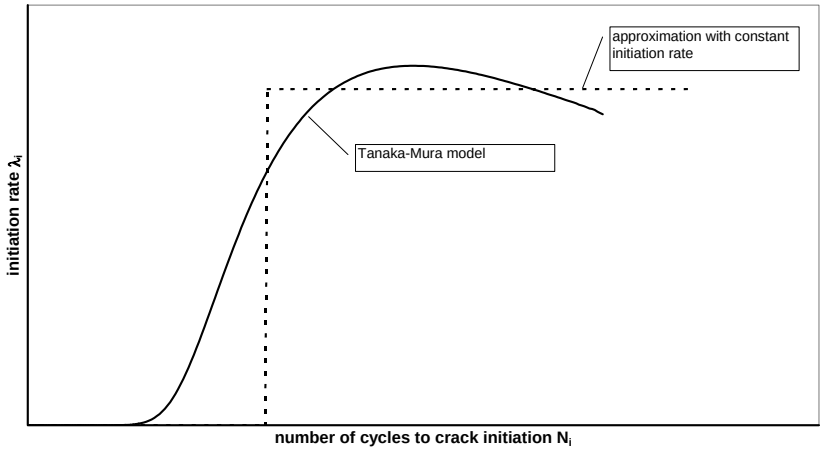

FIGURE 1: Initiation rate calculated from eq.(5)

1.2 Crack growth phase

Microcracks may be stopped at micro-structural barriers [4] leading to intermittent crack growth. This behaviour was observed in numerous experimental investigations. The classical model for intermittent crack growth was proposed by Navarro and de los Rios [5]. This model is completely deterministic for a given grain structure. This implies that once the spatial distribution of the grains is given, the number of cycles to failure of a specific microcrack can be calculated directly. Even though closed form expressions for the failure probability Q_1 in eq. (2) cannot be derived, a straightforward simulation for a given grain structure can easily be performed. This yields the number of cycles to failure for a specific microcrack. Lifetime predictions can be based on theses simulations and the Tanaka-Mura model.

The starting point of such a mesoscopic simulation is a random grain structure representing the microstructure of the material in question. Then a grain is selected as a candidate for microcrack initiation. A random orientation is attributed to this grain which determines the most favourable slip system for crack initiation. The Tanaka-Mura model is then used to determine the number of cycles N_i to crack initiation, whereas the number of cycles to fracture N_B follows by applying the Navarro – de los Rios relations to this specific micro-crack. The lifetime N_f is then given by $N_f = N_i + N_B$. Repeating this simulation step for different grain structures and different grains acting as initiation sites finally leads lifetime distributions which can be compared to experiment (e.g. Ahmadi and Zenner [6]). The agreement is quite good in those cases in which micro-crack initiation is a rare event in a statistical sense, i.e. there is no interaction between micro-cracks.

Apparently the drawbacks of the model such as neglecting the influence of the microstructure on the local stress state and neglecting the local plastic deformation do not play a decisive role and deviations in the lifetime predictions are averaged out. Obviously, these models cannot be applied to those cases in which micro-cracks are initiated from

inclusions (Tanaka-Mura model and/or Navarro – de los Rios model not applicable) or to materials in which crack coalescence is an important damage mechanism under fatigue loading.

2. Mesoscopic simulation with crack interaction

Under high loading or in an adverse environment, the number of cracks per unit area may become comparatively high even at the beginning of the component's lifetime. Crack coalescence becomes likely especially if the micro-structural barriers are strong enough to prevent individual crack from growing. Crack initiation may be influenced by local unloading caused by already existing cracks in the vicinity of the crack initiation site. The lifetime is related to the likelihood that one fatal crack is formed by crack coalescence and/or crack growth which, in turn, depends on the probability of having neighbouring long cracks. Consequently, the state of damage has to be characterized by a quantity which takes both the number of cracks per unit area and the length of the cracks into account.

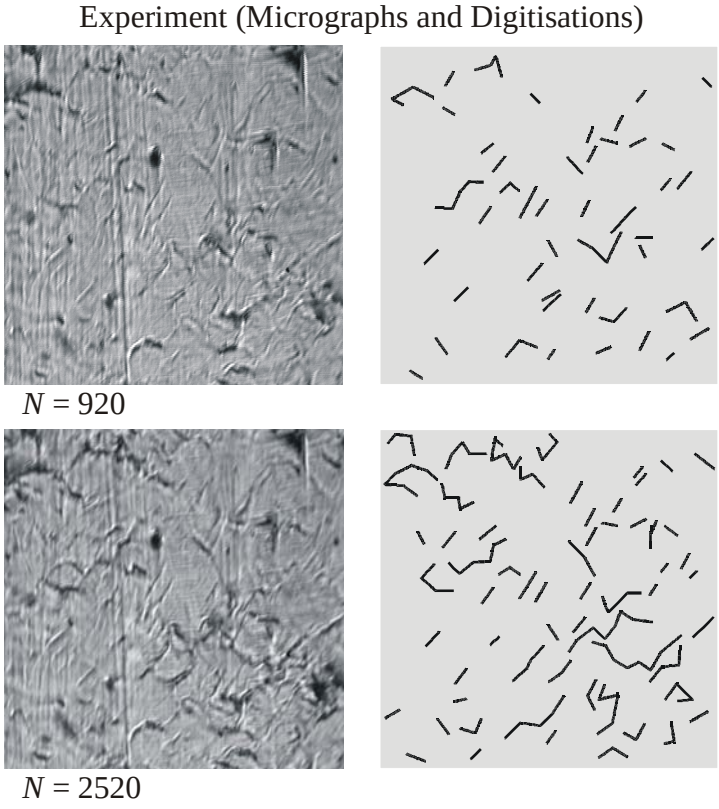

FIGURE 2: Crack patterns observed on the surface of a martensitc steel (original micrograph and filtered and digitised crack pattern)

2.1 Crack initiation

In general, crack initiation in an individual grain can be described by the Tanaka-Mura model summarised in section 1 of this paper. Additionally a crack initiation rate λ_i can be derived directly from experiment if the crack patterns on the surface are observed during the experiment. An example of such an analysis was given by Meyer *et al*. [7]. Specimens of a martensitic steel with a square hollow cross section were subjected to fatigue loading. At fixed load cycles the surface in the gauge section was scanned with a long range microscope.

This allowed to closely monitor the process of microcrack initiation, growth and coalescence. Typical examples of the crack patterns observed are shown in Fig.2. The micro-cracks can be categorized depending on their geometrical shape:

- One-segment cracks are cracks with no kinks. These cracks correspond to one fractured grain and are the database for studying the process of crack initiation.
- Two-segment cracks are cracks with one kink. Such a shape is formed if a microcrack in one grain overcomes the micro-structural barrier at the grain boundary and grows into the adjacent grain.
- Cracks with three or more kinks can be formed by crack coalescence or crack growth. In the case described here, very few two segment cracks were observed, i.e. crack growth is very unlikely and the majority of the three-segment cracks is formed by crack coalescence.

A crack initiation rate λ_i can be derived by counting the number of one-segment cracks on the specimen surface:

$$\lambda_i \cdot \Delta N = \frac{\text{Number of one segment cracks formed between two scans}}{\text{Number of non - fractured grains in observation area}} \qquad (6)$$

where ΔN is the number of fatigue cycles between two scans of the gauge section. A typical result of this analysis is shown in Fig. 3. The crack initiation rate was found to depend on the load amplitude, the orientation of the potential crack path to the load axis and the length of the potential crack.

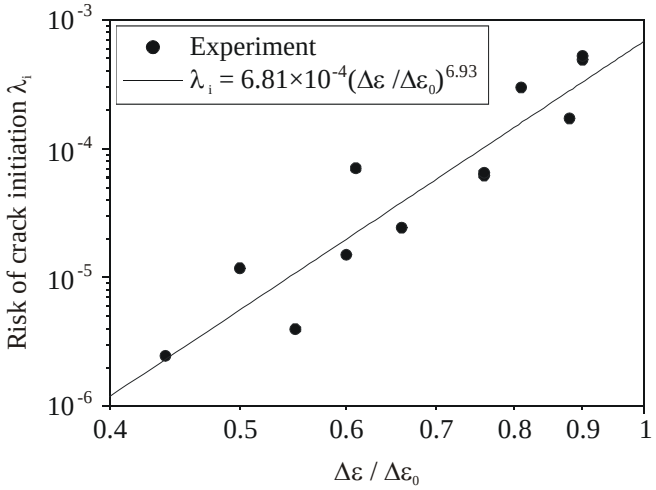

FIGURE 3: Crack initiation rate in a martensitic steel

A mesoscopic simulation of damage accumulation by crack initiation can be performed. The starting point is a grain structure which is either directly taken from experiment or defined by some stochastic model such as the Voronoi tessellation. An orientation value is attributed to each grain which follows either from some stochastic model or from EBSD results. This value, in turn, defines the slip system along which a potential micro-crack is initiated. If the Tanaka-Mura model is used, the local load amplitude has to be determined in order to calculated the resolved shear stress. This value may be quite different from amplitude of the applied load as the local anisotropy of the grains leads to a fairly inhomogeneous stress field (see Fig. 4a-d). On the other hand, the probability of crack initiation derived from a statistical analysis of the crack pattern depends only on the applied

load; local deviations are taken into account by using a probabilistic criterion for crack initiation. However, the predictive capacity of such an empirical model is of course inferior to that of a mesoscopic simulation based on a micro-mechancial model.

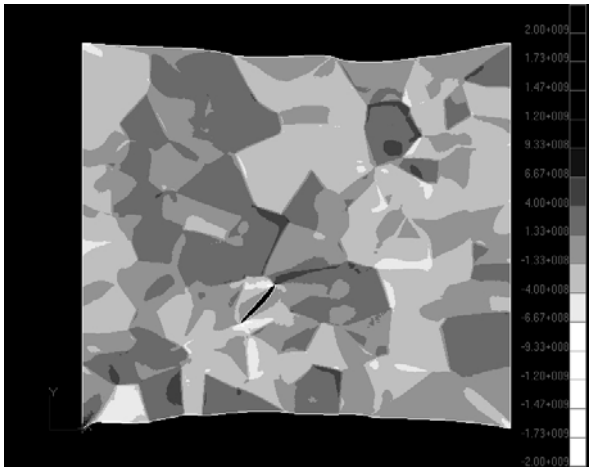

FIGURE 4a: Grain structure with 1 crack

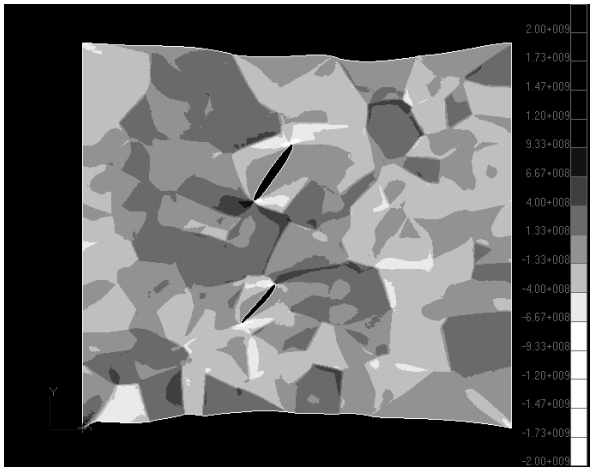

FIGURE 4b: Grain structure with 2 cracks

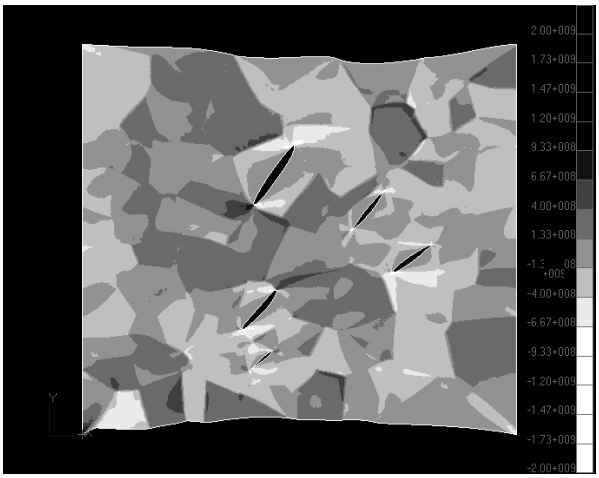

FIGURE 4c: Grain structure with 5 cracks

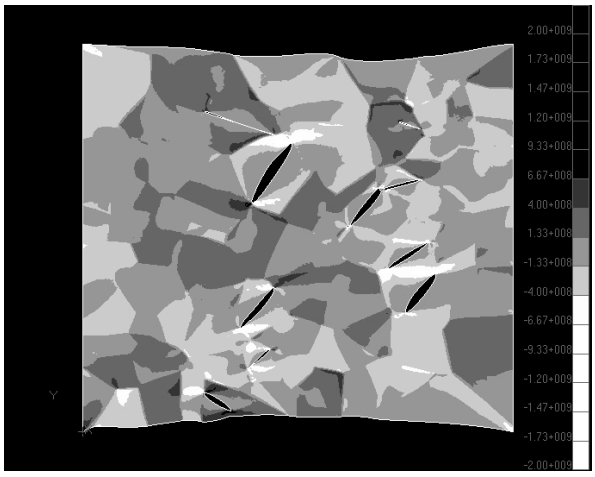

FIGURE 4d: Grain structure with 10 cracks

In a Tanaka-Mura-type of simulation the first crack will be initiated in the grain with the lowest value of N_i, i.e. in a grain with a comparatively long crack path and a high value of the resolved shear stress in the direction of this path. Local unloading will occur once this crack is formed and a new stress field has to be determined. Damage accumulation by crack initiation can be simulated by stepwise identifying the grains with the lowest value of N_i and calculating the stress field after crack initiation.

Two different types of results are obtained: First typical crack patterns can be generated which can be compared to experimental findings, if the specimen surface is continuously monitored in the fatigue experiment. An example of a simulated crack pattern is shown in Fig. 4a-4d. It is found that experiment and simulation agree quite well. Characteristic strata of parallel cracks were observed in both cases. These can be attributed to the re-distribution of the load after crack initiation and were not found in a similar calculation based on the empirical crack initiation rate [7].

Second the simulated crack initiation rate can be determined using eq.(6) and the simulated crack patterns. This value can be directly compared to the statistical analysis of the experimentally observed crack patterns. Agreement between experiment and simulation can be looked at as a verification of the Tanaka-Mura model or, alternatively, as a method to determine the parameters of the Tanaka-Mura model. Fig 5 shows results obtained with a martensitc steel in the experiments described above. The simulation was performed with parameters of the Tanaka-Mura model taken from the literature. There was only one fitting parameter in the simulation model, namely the average grain size. Experiment and simulation agree surprisingly well.

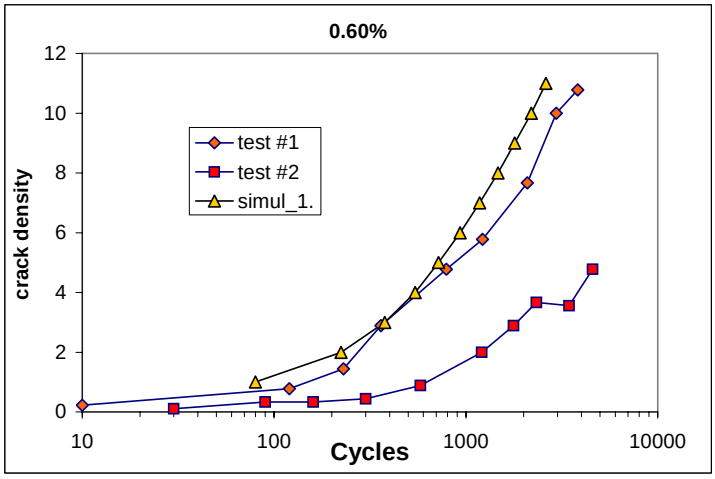

FIGURE 5: Number of one-segment cracks in observation area; experiment and simulation with Tanaka-Mura model

2.2 Crack growth and crack coalescence

Crack growth and crack coalescence can also be analysed both with the experimentally observed crack patterns and a simulation model. Due to the complexity of the problem, a rather coarse approximation seems to be more promising than a detailed analysis in which the re-distribution of the load is taken into account This implies that the mesocopic simulations of crack growth and crack coalescence described below are based on the value of the applied load at the crack site, and the influence of local anisotropy and local unloading due to other cracks is neglected.

As in the case of crack initiation, mesoscopic simulation of damage accumulation can be based on two different models. The first one is a theoretical model such as the Navarro-de los Rios model which defines the crack growth rate for a given crack. In this case the simulation procedure for crack growth is very similar to that described in the first section of this paper for isolated cracks, except that a suitable shielding criterion has to be introduced in order to prevent the cracks from crossing their paths. The second model is a probabilistic one and relies on a statistical analysis of the two-segment cracks (Meyer *et al.* [8]).

Crack coalescence is very likely in materials containing micro-cracks separated by a few undamaged grains. Coalescence criteria are very often based on a geometrical model or a fracture mechanics model or a combination of both. A typical example is the one given by Weiss *et al*. [9]. Their coalescence criterion is based on an estimate of the extension of the plastic zone for each micro-crack. Coalescence occurs if the plastic zones of two cracks start to overlap. A more advanced fracture mechanics model was used Meyer *et al.* [10, 11]. Here

the J-integral of interacting cracks was estimated on the basis of an extended Finite-Element study. It was shown that the probability of crack coalescence correlates well with the corresponding value of the J-integral.

2.3 Definition of damage

In the case of isolated cracks the remaining lifetime can be calculated once the size of the most dangerous crack, i.e. the longest crack in an area of high stress, is known. Even though this concept should be also applicable to interacting cracks, it is not a simple task to identify the most dangerous crack. Comparatively small cracks in areas of moderate stress may coalesce thus forming a very long crack which extends rapidly. Hence it is obvious that the both the size of the existing cracks and the number of cracks per unit area play an important role for the remaining lifetime.

Several damage accumulation laws were proposed in the literature. Obrtlik *et al.* [12] and Vasek and Polak [13] introduce an equivalent crack which is the maximum crack length in the area of interest and try to infer a crack growth law for this crack on the basis of experimental observation. investigations. The characteristic behaviour of this crack is shown in Fig. 6a. At the beginning of the components lifetime, this crack increases in length. Later it attains a more or less stationary value. This is due to shielding effects by the surrounding cracks. At the end of the component's lifetime coalescence occurs and this equivalent crack extends rapidly and finally reaches its critical length.

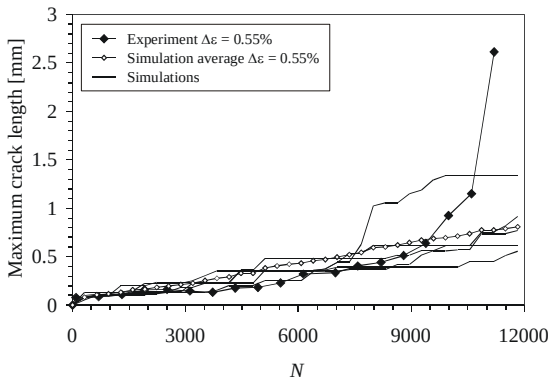

FIGURE 6a: Maximum crack length as observed in fatigue experiments with a martensitic steel

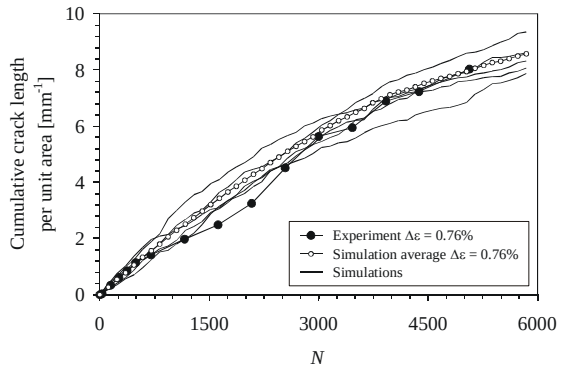

FIGURE 6b: Cumulated crack length as observed in fatigue experiments with a martensitic steel

An alternative approach is to characterize damage by the cumulated crack length (Winkler *et al*. [14], Gao [15]. This is the sum of the length of all cracks visible in the observation area divided by the area. Fig. 6b shows a typical example [11]. The cumulated crack length increase steadily until the end of the component's lifetime and is consequently a good candidate as a damage parameter. However, the critical value appears to increase with the load amplitude as more cracks are initiated for high loads. Hence there is no load independent critical value of this parameter. The results obtained in [11] suggest that the cumulated crack length should be normalized by the strain amplitude is an approximately load-independent

damage variable. It remains to be seen whether a similar quantity can be defined for other materials.

3. Conclusion

Mesoscopic simulation of the damage accumulation process ha advanced considerably during the last years. Combining microscopic observations, micro-mechanical models and quantitative analysis of the local stress state gives new insights in the process of fatigue. This is especially true in the crack initiation phase. Eventually, the models developed have to be summarized in damage accumulation laws. There is still a certain lack of knowledge in this area, and additional work is needed in order to derive tools for lifetime prediction of components.

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