A statistical evaluation of micro-crack initiation and growth in thermally cut structural elements

M. Šori, S. Glodež, U. Fevžer

University of Maribor, Faculty of Natural Sciences and Mathematics, Koroška c. 160, 2000 Maribor, Slovenia <u>marko.sori@uni-mb.si</u> <u>srecko.glodez@uni-mb.si</u> <u>ufevzer@gmail.com</u>

ABSTRACT. In this paper a numerical simulation of micro-crack initiation is presented. The simulation is based on the Tanaka-Mura crack nucleation model and has three crucial improvements. Firstly, multiple slip bands are used in each grain. Second improvement deals with micro-crack coalescence by extending existing micro-cracks along grain boundaries and connecting them into a macro-crack. The third improvement is a segmentation of a micro-crack, meaning a micro-crack is not created in one step like in Tanaka-Mura model, but it is generated in multiple steps, which makes it far more sensitive to local stress gradients. Individual grains are randomly generated with Voronoi tessellation and different loadings are applied to the model. The computational results are then analyzed and evaluated to present the dependence between operating loading and number of stress cycles required for failure.

High cycle fatigue testing is also performed and showed a quite good correlation with the computational results. Since computational model is directed at simulating fatigue properties of thermally cut steel, edge properties of test specimens were additionally inspected in terms of surface roughness and micro-structural properties.

INTRODUCTION

Micro-crack behaviour is quite different from macro-crack behaviour [1, 2]. Researches had shown that micro-cracks occur on slip bands of grains and stretch across the whole grain [3]. Often used method to solve micro-crack initiation on the slip bands is Tanaka-Mura model [4]. This model predicts the number of stress cycles N_C required for micro-crack nucleation:

$$N_C = \frac{8GW_S}{\pi (1 - \nu)d(\Delta \tau_S - 2k)^2}$$
(1)

Eq. 1 shows that the number of stress cycles N_C for micro-crack nucleation is dependent on slip band length d and average shear stress range on the slip band $\Delta \tau_s$. Other constants (shear modulus G, specific fracture energy per unit area W_s , Poisson's ratio v and frictional stress of dislocations on the slip plane k) are material properties and can be found in specific literature (for martensite see reference [5]).

However, this model still has difficulties when micro-cracks occur in two neighbouring grains. It does not consider their coalescence as they may form a macrocrack. Furthermore the Tanaka-Mura model uses the average shear stress of entire slip band to determine micro-crack nucleation. In our previous attempts to simulate microcrack initiation [6], often happened that a particular grain already had a micro-crack and raised stress values of neighbouring grain quite substantially, but not enough to form a micro-crack as the average stress along entire slip band was still under the threshold to form a micro-crack. This problem becomes more severe when using lower loads, as in high cycle fatigue.

NUMERICAL MODEL

The selected specimen was a 5 mm thick, 110 mm wide and 200 mm high steel plate with a centred hole of 40 mm in diameter, subjected to different tension loadings. To simulate micro-crack nucleation considering complex loadings around crack nucleation area a multi-scale model was created (Fig. 1).

The macro-model (Fig. 1 – left-hand side) is constrained at the bottom and a line loading of various magnitudes is applied at the top, matching different nominal stress levels of 485, 500, 550 and 600 MPa. The finite element mesh is progressively concentrated at the inner edge, where stress is concentrated and a crack initiation is expected. Size of the finite elements on the macro-model is 5 by 5 millimetres at outer edges and 0.2 by 0.2 millimetres at the inner right-hand side edge.



Figure 1. FE-mesh of macro (left-hand side) and micro (right-hand side) model.

Stress distribution at inner hole is then applied to boundary edges of a micro-model (Fig. 1 – top, right and bottom edge on the right-had side). The size of a micro-model is chosen to be 0.3 by 0.3 millimetres and is meshed with approximately 10^5 finite elements of type CPS4R, giving size of a single finite element of about 1 micrometre.

Presuming crack nucleation occurs on a slip band in a particular grain, multiple grains had to be modelled (Fig. 2). This was done using randomly generated Voronoi tessellation, which represents a cell structure constructed from a random twodimensional distribution of points. These points are closed by areas, fulfilling the condition that all possible positions must be closer to the enclosed point than to any other point. The number of points is selected in such a way that the obtained grain size is as close as possible to the average grain size of used material. Each grain is then assumed to behave as a randomly oriented mono-crystal with anisotropic elasticity.

Because thermally cut steel components had been investigated, the cut edge properties had to be considered. Therefore cut edge roughness was modelled as a Bezier spline (Fig. 2 - left-hand side), which has an amplitude and period similar to the maximal measured roughness.

Numerical simulation of crack initiation was performed with commercially available software ABAQUS [7], where additional routines have been written for model generation, adaptation and evaluation. The code is written in Python language and uses ABAQUS Scripting Interface – ASI. ASI is an object-oriented extension library based on Python for advanced pre- and post-processing tasks in ABAQUS.



Figure 2. Grains in the micro-model.

Multiple slip bands and crack coalescence

Slip bands are created through grain centres and their orientation is kept constant within one particular grain. Additional slip bands are created with 2 μ m offset, covering the entire grain. However, grains at the edges (grey coloured) do not have slip bands and

serve as a buffer zone to minimize numerical mismatch at boundaries (top, right and bottom edge of Fig. 2), hence do not partake in micro-crack evaluation.

Fig. 3 shows a case where the first micro-crack was nucleated in the left grain and influenced its neighbouring grain on the right, so that a micro-crack in it nucleated far from the grain centre, close to the first micro-crack. The proximity of nucleated micro-cracks also enables easier micro-crack coalescence than in a model where micro-cracks are formed through grain centres only [5, 8].





When considering crack coalescence a conservative approach was taken. Each time a new micro-crack was nucleated near existing one, the area between these micro-cracks was checked if the stress values were surpassing yield stress. If this was the case, a new seam was added on the line between two micro-cracks efficiently converting two micro-cracks into one single crack (Fig. 3). When adding a seam between two cracks no stress cycles were calculated, therefore the transition between Fig. 3a and Fig. 3b happens instantaneous. Consequently total stress number of cycles for crack initiation period is equal to the sum of stress cycles needed for each micro-crack to nucleate.

Segmented micro-cracks

Fig. 4 shows the shear stress range $\Delta \tau_{bs}$ (solid black line) along a slip band through a single grain shown in the Fig. 5a. Note significant stress concentration at the left-hand side of the slip band. This is caused by a crack in a neighbouring grain. Using Tanaka-Mura model this would not cause a micro-crack to nucleate, because average shear stress range $\Delta \overline{\tau_s}$ (dotted black line) is lower than the required threshold 2k (solid grey line). This problem was solved with segmentation of slip bands into four segments and observing average shear stress range in every segment separately $\Delta \overline{\tau_{bs}}$ (dashed black line). Note average shear stress in leftmost segment is surpassing the required threshold. Therefore a seam is created in the next iteration (Fig. 5b).



Figure 4. Shear stress through slip band position (Fig. 5a).



Figure 5. Shear stress distribution before (a) and after (b) micro-crack nucleation.

STATISTICAL EVALUATION

Several computational analyses were done for each loading to determine the influence of grain orientation on the crack initiation period. For statistical representation of given computational results it is assumed that N_i (i = 1 to n) is the number of loading cycles required for crack initiation, where n is the number of computational analyses on the same load level. The mean value \overline{N} and the standard deviation σ^2 can be determined with standard statistical equations [9]:

$$\overline{N} = \frac{1}{n} \sum_{i=1}^{n} N_i \tag{2}$$

$$\sigma^2 = \frac{1}{n} \sum_{i=1}^n \left(N_i - \overline{N} \right)^2 \tag{3}$$

The chosen frequency function f(N), used for the determination of interval $[N_1, N_2]$ in which crack will be initiated with the probability P(N), should satisfy the following conditions [9]:

$$f(N) \ge 0$$
 for every N (4.a)

$$\int_{-\infty}^{\infty} f(N) dN = 1$$
(4.b)

$$\int_{N_{1}}^{N_{2}} f(N) dN = P(N_{1} \le N \le N_{2})$$
(4.c)

Practical considerations of the fatigue analyses show that the Weibull and lognormal distributions are best suited for this type of problems. In this paper the lognormal distribution is utilised. In this case, the variable (the number of loading cycles N) can take values in the interval $[0, \infty)$, which is applicable to the fatigue problem. The frequency function is defined as [9]:

$$f(N) = \frac{1}{N\sigma^* \sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{\ln N - \overline{N}^*}{\sigma^*}\right)\right]$$
(5)

where \bar{N}^* and σ^* are defined as follows:

$$\overline{N}^* = \ln \frac{\overline{N}^2}{\sqrt{\sigma^2 + \overline{N}^2}}$$
(6)

$$\sigma^* = \sqrt{\ln\left(1 + \frac{\sigma^2}{\overline{N}^2}\right)} \tag{7}$$

The interval $[N_1, N_2]$ in which the crack is initiated with the probability P(N) can then be estimated by using Eqs 4 and 5. Example for probability P = 0.9 is shown in the Fig. 6.



Fig. 6. Numerical and experimental results in S-N graph.

As multiple calculations were preformed, multiple crack paths were pursued. In Fig. 7 there are three different crack paths from three different calculations for loading level 550 MPa after $4 \cdot 10^5$ cycles. Fig. 7 shows only the path of the crack front; other occurred micro-cracks are not indicated. Multiple calculations showed, that micro-cracks start to form individually and then tend to form clusters. Connecting clusters then forms a macro-crack. Testing showed numerical calculation is more stable if macro-crack starts to grow from the free edge inwards.



Fig. 7. Three different crack paths and their averaged path for loading level 550 MPa after $4 \cdot 10^5$ cycles.

CONCLUSION

Fatigue crack initiation in dynamically loaded machine parts and structures becomes increasingly important in high cycle fatigue (HCF), as it can amount to 90% or more of the complete service life of the component. Minute features like microstructure and surface roughness can significantly affect the crack initiation period. Tanaka-Mura approach represents quite good solution when solving micro-crack nucleation, but it is not taking into account crack coalescence and significant stress gradients caused by existing micro-cracks in neighbouring grains. This problem is solved by connecting two cracks into one and by segmentation of slip bands. The solutions are then statistically evaluated and compared with experiments, showing quite good correlation.

On the other hand, this method still has some deficiencies. Combining of microcracks is solved very conservatively and mainly manually, adding a subjective error to the calculation. Some method should be applied to determine number of cycles needed for crack to extend along grain boundary. Additional testing also showed the number of segments on a slip band influences the rate of micro-crack nucleation. Possibly not all segments should be treated equally susceptible to micro-crack nucleation, because the proximity of grain boundaries may inhibit the rate at which micro-crack nucleate.

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