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Published in: Procedia Structural Integrity

DOI: 10.1016/j.prostr.2018.12.210

Published: 01/01/2018

Document Version Publisher's PDF, also known as Version of record

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Please cite the original version:

Gu, C., Lian, J., Bao, Y., & Münstermann, S. (2018). A microstructure sensitive modeling approach for fatigue life prediction considering the residual stress effect from heat treatment. *Procedia Structural Integrity*, *13*, 2048-2052. https://doi.org/10.1016/j.prostr.2018.12.210

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Procedia Structural Integrity 13 (2018) 2048-2052



www.elsevier.com/locate/procedia

ECF22 - Loading and Environmental effects on Structural Integrity

A microstructure sensitive modeling approach for fatigue life prediction considering the residual stress effect from heat treatment

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Abstract

A multiscale numerical method to study the high cycle fatigue (HCF) and very high cycle fatigue (VHCF) properties of bearing steels is proposed in this study. The method is based on the microstructur sensitive modeling approach resulting from the integrated computational materials ensfginerrring concept, and further consider the effect of residual stress generated from the prior heat treatment processes. The microstructure features, including the grain size and shape distribution and inclusion size and shape description, are represented by the representative volume element (RVE) models. The matrix mechanical response to the cyclic loading is described by the crystal plasticity (CP) model. The CP material parameter set is calibrated inversely based on the strain-controlled low cycle fatigue tests. The results show that the residual stresses, especially those around the inclusion, have a great effect on the fatigue properties, which provides the key factor to give the correct prediction of the fatigue crack initiation site.

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Keywords: fatigue life; modeling; residual stress; microstructure

1. Introduction

Fatigue life is an important mechanical property to many kinds of materials, especially to those used in the safetyrelevant parts of engineering structures in various industrial sectors, e.g. automotive, aerospace, and railroad. To ensure the reliability and safety of these facilities, the demand on quality of materials has been steadily increased. Extensive

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studies have been carried on to investigate the mechanisms of fatigue fracture (Chai et al., 2016; Krewerth et al., 2016; Sakai et al., 2015). However, quantitative and microstructure informed study on the fatigue life, especially for HCF and VHCF, is still missing due to its extremely time-consuming investigation time. Therefore, developing a microstructure informed fatigue life prediction method is very important.

So far, some researchers have developed fatigue life prediction method based on the microstructure-sensitive simulation. The main constituents in the model are the material constitutive law and the statistical digital representation of the microstructure. For the material constitutive law, the crystal plasticity (CP) model is used to calculate dislocation reactions on slip systems. The initial crystal plasticity model was developed simply to accommodate the slip deformation on the discrete slip systems in a single crystal (Becker, 1991; Melchior and Delannay, 2006). Consideration of polycrystalline features, such as texture and grain orientation distribution, have increased the applicability of crystal plasticity models to address questions at a microstructural level (Eisenlohr and Roters, 2008). For the representation of the microstructure, the most straightforward approach is the immediate mapping of a micrograph in a geometric model, which suits the requirements of commercial simulation programs. As a benefit, the calculation leads to immediately matching simulation and experimental results (Özden et al., 2015). Furthermore, to enlarge the simulated material behavior, RVE is introduced.

However, these simulation methods are mainly concentrated in the matrix effect. The inclusions in material also significantly affect the fatigue life. Gillner et al. (Gillner et al., 2018) did a numerical study of inclusion parameters and their influence on fatigue lifetime based on FE models, but some results are not that accurate. To improve the accuracy of fatigue simulation models and the effect of inclusions on fatigue life, the present research provides a new fatigue life prediction method concerning the heat treatment process and the residual stress around inclusions.

2. Experiment

The material in the present study is a high-carbon martensitic bearing steel. The main chemical composition of this material is shown in Table 1.

	-	-					
С	Cr	Si	Mn	Р	S	Cu	Al
1.03	1.37	0.21	0.33	0.0110	0.0008	0.0744	0.0110

Table 1 Main chemical composition of the high-carbon martensitic bearing steel (mass contents in %).

The microstructure was investigated by electron backscatter diffraction technique (EBSD) for phase fraction and grain size analysis. The HCF and VHCF properties were measured under a resonance frequency of 20 kHz. The loading condition was a fully reversed tension-compression (R = -1). The hysteresis loops with a fixed strain 1.0% were also tested. After post-fracture scanning electron microscope (SEM) analysis of the fracture surface, it is evident that most of the fatigue crack initiations were caused by inclusions. Figure 1 shows the typical fatigue initiation site. As shown in figure 1(b), the main composition of the inclusion in the crack initiation site is Al-Ca-O-S, detected by the EDS, which is a commen type of inclusion in this steel grade (Gu et al. 2018).



Fig. 1 (a) SEM micrograph for a typical fatigue initiation site with inclusion and (b) the composition of the inclusion.

3. Modeling and parameter calibration

3.1. RVE generation

Based on the results of EBSD, the grain size of the matrix was fitted with log-normal distribution, see Eq (1):

$$y = f(x \mid \mu, \sigma) = \frac{1}{x\sigma\sqrt{2\pi}} exp(\frac{-(\ln x - \mu)^2}{2\sigma^2})$$
(1)

where μ is the mean value and σ is the standard deviation.

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The fitted parameters are shown in Table 2. The grain size distribution was set as an input of RVE generation. These two-dimensional microstructure models were generated by MATLAB code and Python scripts for the finite element (FE) software ABAQUS. The position of each grain was random in the model area. In this study, 80 RVEs were generated. These RVEs have periodic microstructures and the size is $70 \times 70 \ \mu\text{m}^2$. Each RVE contains approximately 200 grains.

Table 2 Fitting parameters of grain size distribution.		
μ	σ	
1 00/18	0.4758	

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3.2. CP parameter calibration

The mechanical behavior to the cyclic stress of this material is based on the CP model, which is described with equations in Table 3. The calibration of parameters in the CP model is conducted with an iterative fitting of the RVE simulation to the hysteresis loops obtained from low cycle fatigue tests with a strain amplitude of 1.0%. As shown in Figure 2, a good agreement between the experiment and simulation is achieved with the optimized set of parameters.

Table 3 Equations of the CP model.

	$\dot{\gamma}^{\alpha} = \dot{\gamma}_{0} \left \frac{\tau^{\alpha} - \chi^{\alpha}}{\tau^{\alpha}_{c}} \right ^{1/m} sgn(\tau^{\alpha} - \chi^{\alpha})$	(2)
	$\dot{\gamma}^{lpha}$: slip rate along the slip system $lpha$;	
	${\dot \gamma}_0$: initial slip rate;	
constitutive equation	$ au^{lpha}$: resolved shear stress;	
	χ^{lpha} : backstress on slip system $lpha$;	
	τ_c^{α} : critical resolved shear stress on slip system α ,	
	1/m: strain rate sensitivity factor.	
	$\tau^{\alpha} = \boldsymbol{S} \cdot (\boldsymbol{m}^{\alpha} \otimes \boldsymbol{n}^{\alpha})$	(3)
	t^{a}	
Calculation of shear stress	ι : resolved shear stress along a slip system α ;	
	n^{a} : normal to the slip plane;	
	m^{lpha} : slip direction;	
	S: second Piola-Kirchhoff stress tensor.	
	$ au_{c}^{lpha}= au_{i}+\sum_{eta=1}^{N}q^{lphaeta}\left[h_{0}\left(1-rac{ au_{c}^{eta}}{ au_{s}} ight)^{a} ight]\left arDelta\gamma^{eta} ight $	(4)
Isotropic bardoning law	$ au_i$: initial resolved shear stress;	
isotropic nardening law	$q^{lphaeta}$: latent hardening parameter;	
	h_0 , τ_s , a : hardening parameter;	
	$\Delta \gamma^{\beta}$: plastic slip increment of each slip system $\boldsymbol{\theta}$.	
	$\dot{\chi}^{\alpha} = G_1 \dot{\gamma}^{\alpha} - G_2 \dot{\gamma}^{\alpha} \boldsymbol{\chi}^{\alpha}$	(5)
Kinematic hardening	G_1, G_2 : kinematic hardening constant;	
	χ^{α} : backstress tensor of slip system α .	

3.3. Inclusions and residual stresses

Based on the results of HCF and VHCF tests, inclusions play an important role in the fatigue life. When the material is subjected to heat treatments, residual stresses will be generated especially around inclusions during the cooling process (Brooksbank, 1969; Brooksbank and Andrews, 1968; Ma and CUI, 2011), which should be considered in fatigue simulation.



Fig. 2 Parameter calibration of the CP model based on the experimental and numerical results on the hysteresis loops.

In the present study, the shape of the inclusion in the fatigue crack initiation site was drawn and inserted in every RVE, as shown in Figure 3(a). Residual stresses during cooling were also calculated in ABAQUS. Parameters used in this calculation is shown in Table 4 (Brooksbank 1969; Brooksbank and Andrews 1968). For simplicity, only elastic deformation is assumed. The obtained residual stress profile is further node-to-node mapped to the CP simulation for the fatigue prediciton.

Table 4 Mechanical parameters and coefficients of thermal expansion.

Material	Coefficient of linear expansion, $\alpha / (10^{-6.\circ}C)$	Young's modulus, E / GPa	Poisson's ratio, v
Inclusion	5.0	113	0.234
Matrix	23.0	210	0.300



Fig. 3. (a) RVE with an inclusion; (b) residual stress distribution around the inclusion.

3.4. Fatigue indicator parameter

Under a pre-defined stress level, six cycles were simulated. During simulation, the highest value of the grain-level averaged accumulated plastic slip P was calculated, which is the indicator of the tendency for a fatigue crack to incubate.

4. Results and discussion

Figure 4 shows the comparison of P distribution in RVE area. The area, where the white arrow points at is the location of the maximum P, which indicates the location of fatigue crack initiation. When the residual stress distribution was not included in the fatigue simulation, the maximum P is located in the matrix, as shown in Fig. 4 (a).

When the residual stress distribution was considered, the crack initation site is correctly predicted around the inclusion, see Fig. 4(b).

When we discuss the effect of inclusions on fatigue, the crack should site around inclusions, which implies that the fatigue simulation without residual stress distribution is not accurate. When different inclusions are considered, residual stress distribution will change, which contributes to the effect of inclusion type, size and shape on the fatigue life.



Fig. 4 Comparison of RVE reactions (a) with residual stress and (b) without residual stress.

5. Conclusions

In this paper, a new method to improve the accuracy of the fatigue life prediction related to inclusions based on FE models is provided. In this model, the effect of inclusion on the fatigue life is considered with the contribution of the residual stress distribution resulting from the prior heat treatment process. With this method, the fatigue crack initiation site is correctly predicted by the simulation.

Acknowledgements

This work was financially supported by China Scholarship Council.

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