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Microstructure-based fatigue modelling with residual stresses: Prediction of the fatigue life for various inclusion sizes

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Abstract: In this study, the calcium aluminate inclusion induced fatigue failure of a high-carbon martensitic steel was investigated. The results showed that the size of calcium aluminate inclusion observed near the fatigue crack initiation site ranges from 12.5 μm to 33.2 μm . Three typical calcium aluminate inclusions with sizes of 15 μm , 20 μm and 30 μm were investigated by a microstructure-based model, by considering the residual stress distribution induced by the cooling process before the fatigue loading. The S-N curves were predicted and validated with respect to calcium aluminate inclusions with different sizes, which were compared with the calculation neglecting the residual stress distribution around inclusions. The 10^9 -fatigue limits were also calculated by models with and without considering the residual stress. The S-N curves predicted by models considering residual stress showed a better agreement with the experiment data. Interestingly, the predicted 10^9 -fatigue limits concerning calcium aluminate inclusions with different sizes also showed more reliable dependence on the square root of inclusion area to $-1/6$ power. Furthermore, the relation between fatigue life, inclusion size and fatigue stress is built according to the predicted results.

Key words: Microstructure-sensitive modelling; Residual stress; Defects; Fatigue life; Inclusion size

- Nomenclature:**
- ε = the thermal strain
 - n = the material definition number
 - α_n is the thermal expansion coefficient
 - T_0 = the initial temperature
 - T = the current temperature
 - μ = mean value of grain size in log-normal distribution
 - δ = standard deviation of grain size in log-normal distribution
 - α_j = thermal expansion coefficient of material j
 - T_0 = initial temperature of inclusion/steel matrix system
 - T = current temperature of inclusion/steel matrix system
 - $\mathbf{F}$ = deformation gradient
 - $\mathbf{F}_e$ = elastic deformation gradient
 - $\mathbf{F}_p$ = plastic deformation gradient
 - $\dot{\mathbf{F}}_p$ = rate of the plastic deformation gradient
 - $\mathbf{L}_p$ = plastic deformation gradient
 - $\mathbf{S}^\alpha$ = Schmid tensor of the slip system α
 - $\mathbf{m}^\alpha$ = slip direction vectors of the slip system α
 - $\mathbf{n}^\alpha$ = plane normal vectors of the slip system α
 - N = total number of active slip systems
 - $\dot{\gamma}^\alpha$ = shear rate
 - $\dot{\gamma}_0$ = initial slip rate
 - τ^α = resolved shear stress
 - τ_c^α = critical resolved shear stress on slip system α
 - $1/m$ = strain rate sensitivity factor
 - χ^α = kinematic back stress on slip system α
 - χ^α = the back stress of slip system α
 - G_1 = material parameter
 - G_2 = material parameter
 - τ_0 = initial resolved shear stress
 - $q^{\alpha\beta}$ = latent hardening parameter matrix
 - h_0 = hardening parameter
 - τ_s = hardening parameter
 - a = hardening parameter
 - $\Delta\gamma^\beta$ = plastic slip increment of each slip system β
 - p_{acc} = value of local accumulated dislocation slip
 - P_{max} = maximum grain-level-averaged value
 - i = identifier of the finite element of the involved grain
 - N_E^{Gr} = number of elements within the grain
 - V_i^{Gr} = volume of the element i of the grain
 - m = the indicating number of stress amplitude
 - A_m, B_m = the distribution parameters of P_{max} under indicating number of stress amplitude m
 - $N_{inc,m}$ = cycle amount for crack incubation
 - $N_{f,m}$ = the fatigue life under indicating number of stress amplitude m

α_p = a fitting constant

d_{gr} = mean grain size

$\bar{P}_{max}$ = mean value of P_{max}

k = amount of RVEs

N = amount of cycles for P_{max}

u = fitting constant

σ_m = stress amplitude value under indicating number m

HV = Vickers hardness of the steel

$\sqrt{area}$ = square root of inclusion area

a' = position coefficient of the inclusion

σ_w = 10^7 -fatigue limit

σ'_w = 10^9 -fatigue limit

σ = fatigue stress amplitude

d = diameter of the inclusion

A, B₁ and B₂ = the fitting constants

1. Introduction

Inclusions, as unavoidable defects existing in steels, will decrease the steel quality from multiple aspects ¹⁻³. Over centuries, metallurgists have been making efforts on the removal of inclusions and the improvement of the purity of steels ⁴⁻⁶. However, there is still a certain amount of inclusions with multiple types in steels due to different melting and deoxidation methods during the production process. Most oxide inclusions, such as spinel, calcium aluminate, and silicate, are deoxidation products and generated in molten steels; most precipitate inclusions, such as titanium nitride and manganese sulphide, are generated during solidification ⁷⁻⁸.

All these inclusions with different features have effects on fatigue life of steel during cyclic loading. Spriestersbach et al. ⁹ reported that the inclusion type is related to the threshold value for the stress intensity factor in the very high cycle fatigue (VHCF) regime. Murakami et al. ¹⁰ claimed that closer distance of the inclusions to the specimen surface tends to lead to a lower fatigue life with a numerical model. Nevertheless, the most evident factor that affects fatigue property is the inclusion size. To clarify the effect of inclusion size on fatigue life, extensive research has been conducted. Lu et al. ¹¹ clarified that the shape of the S-N curve for subsurface inclusion-induced fracture depends on the inclusion size. Murakami et al. ¹² claimed that the fatigue limits are dependent on the inclusion sizes to the $-1/6^{\text{th}}$ power. Furuya et al. ¹³ confirmed the $-1/6^{\text{th}}$ relation between 10^9 -cycle fatigue limit and inclusions with a diameter larger than 15 μm . Zhu et al. ¹⁴ further developed the original model by Murakami et al. ¹⁵ with a parameter taking account of both the size and location of inclusions to estimate the fatigue limit.

Although it is evident that the inclusion is a non-negligible factor for fatigue life, there are still difficulties to analyse the numerical effects of them comprehensively with experimental

methods. Firstly, the time cost for fatigue tests in high cycle fatigue (HCF) and the VHCF regime leads to the low efficiency of data production. The traditional method for fatigue tests offers low frequency, usually from 1 Hz to 30 Hz, with which 10^7 cycles need about 4-116 days for one single test. Secondly, univariate analysis is not possible for actual material since different features of inclusions (size, type and shape) are always mixed up due to a complicated chemical reaction during metallurgical processes. Aiming at the aforementioned difficulties, the microstructure-based numerical models to correlate the fatigue life with microstructure has been developed. With the models, the time for fatigue tests is saved and the features of inclusions can be precisely controlled so that the numerical effects of inclusions can be studied thoroughly.

The microstructure-based modelling study for fatigue property was initially introduced by Dunne et al.¹⁶ and McDowell and Dunne¹⁷. It is further enriched in recent years in several studies. Musinski and McDowell¹⁸ estimated the fatigue crack initiation and early propagation in fatigue specimens with notches with the crystal plasticity finite element method. Przybyla and McDowell¹⁹ introduced a microstructure-sensitive extreme-value function and characterize the coupled crystallographic microstructure features which influence the fatigue indicator parameters. Przybyla et al.²⁰ proposed an algorithm for estimating the cumulative probability distribution of cycles for crack formation and growth from notches in HCF and VHCF regime with microstructure-sensitive simulation. Castelluccio and McDowell²¹ exercised a microstructure-sensitive model for smooth and through hole specimens and claimed that their three-dimensional small fatigue crack growth algorithms can quantify the most damaging loading conditions concerning strain ratios, multiaxial strain state and mean stress.

It is quite clear that most of these studies on the application of the microstructure-sensitive

modelling approach on fatigue problems are concerning the steel matrix; however, as it was emphasized in the previous section, inclusions play such a critical role in determining the microcrack initiation and the fatigue life. Therefore, Gu et al.²² extended the microstructure-based modelling approach to include the effect of inclusions as well as the residual stresses developed between the inclusions and the steel matrix.

In the new approach, inclusions observed in fatigue crack initiation was inserted with actual size, shape and type. The effect of the inclusion was analysed with the assistance of residual stress simulation around inclusions, which has been proved to vitiate with different features of inclusions²³ and have a non-negligible influence on the mechanical behaviour of materials²⁴⁻²⁶. However, a quantitative method to analyze the effect of the residual stresses on fatigue life is still missing. Furthermore, the effect of the inclusion size on the fatigue life with the microstructure-based modelling method is also missing, although some microscopic models are formulated. Zerbst et al.²⁷⁻²⁸ proposed a model for the fracture mechanics based prediction of the S-N curve of metallic components with large microstructural defects and validated the model with data from the literature.

In the present study, a certain type of inclusion, calcium aluminate, which contributes the most on the fatigue crack initiation, with different sizes were inserted in the developed microstructure-based model. Fatigue life and S-N curves were predicted accordingly. The numerical results were compared with model predictions neglecting residual stress and further validated by HCF and VHCF experimental results. As an extension of the previous study, the effect of calcium aluminate inclusions of various sizes on fatigue life was described and the accuracy of the fatigue life prediction model with residual stress was proved in this study.

2. Experiments

The material investigated in this study is high-carbon chromium bearing steel GB GCr15 (equivalent to SAE 52100). The main composition (mass percentage) is 1.03 C, 1.37Cr, 0.21 Si, 0.33 Mn, 0.0110 P, 0.0008 S, 0.0744 Cu, 0.0110 Al. This material was vacuum oil quenched after holding at 835°C for 20 minutes and tempered at 150°C for 120 minutes.

In total, 37 ultrasonic fatigue experiments under 20 kHz frequency were conducted in this study in HCF and VHCF regime. The specimen dimension is shown in **Fig. 1**. The loading condition was fully reversed tension-compression ($R = -1$). After the fatigue tests, all the crack initiations were analysed with scanning electronic microscopy-energy dispersive X-ray spectrometer (SEM-EDS).

Fig. 1. Geometry and dimensions of the fatigue test specimen, dimensions in mm.

3. Modelling strategy

The central four elements for the modelling strategy in the current study to predict the fatigue life are i) the generation of the representative digital microstructure of the material, ii) the simulation of the residual stress profiles during the cooling process, iii) the crystal plasticity model to describe the micro-deformation mechanisms and the parameter calibration and iv) the microcrack initiation and fatigue life prediction. The first three elements are described in detail in the previous studies ²²⁻²³. However, for the completeness of the description of the modelling approach, they are briefly reviewed below and the fourth element, which is the key contribution for the current study, is described in detail. Fig. 2 shows a general flow chart of how they are interacting with each other and how they are calibrated. The details are given individually in the following sections.

Fig. 2. The flow chart of the microstructure-based model consisting of inclusions and residual stresses used in this

study.

3.1 Generation of representative volume element (RVE) for steel matrix and inclusions

For the construction of microstructure model, instead of using the real microstructure approach by digitalization the graphs obtained by metallography ²⁹, a statistical approach to generate the artificial microstructure reported by Vajragupta et al. ³⁰ was applied. The RVE generation is based on the electron backscatter diffraction (EBSD) data. The representative information of the statistical microstructure features was obtained and the grain size distribution was analyzed with Eq. (1) accordingly.

$$y = f(x | \mu, \delta) = \frac{1}{x\delta\sqrt{2\pi}} \exp\left(\frac{-(\ln x - \mu)^2}{2\delta^2}\right) \quad (1)$$

The fitted parameters μ and δ were set as the input of RVE generation. The RVEs were constructed by a well-developed MATLAB code and Python scripts under the random sequential addition (RSA) algorithm and weighted Voronoi tessellation technique. 60 different RVEs with the same input parameters were generated.

The addition of the inclusion into the RVE was based on the digitalization of it with MATLAB codes. After the failure of fatigue specimens, the morphologies of fractures were observed with SEM and the crack initiation sites were determined accordingly. If the fatigue crack initiation was induced by inclusion, the figure of the inclusion was set as an input of MATLAB. With the assistance of contrast recognition function of MATLAB, the boundaries of inclusions were output in terms of their coordinates. These digitalized coordinates of the real inclusion geometries were implemented to the centre of all RVEs. Then each RVE was meshed and contains at least 20,000 elements.

3.2 Residual stress simulation during the cooling process

The residual stress simulation was based on the RVEs containing inclusion geometries

generated in the previous step. The simulation was conducted in Abaqus/Standard and the mechanical properties of the inclusions and the matrix are assumed to be isotropic. Only elastic responses of the steel matrix are considered in this study. During fast cooling, residual stresses were generated between the inclusion and the steel matrix due to their different thermal expansion/contraction coefficients. The elastic deformation is calculated with Eq. (2):

$$\varepsilon = \alpha_n(T - T_0), \quad (2)$$

where ε is the thermal strain; n is the material definition number, which represents steel matrix and different inclusions; α_n is the thermal expansion coefficient; T_0 is the initial temperature, and T is the current temperature.

In this study, the cooling process during quenching (samples were cooled from 835°C to 20°C) was taken into consideration. The parameters of the calcium aluminate inclusion and the steel matrix needed in this simulation are shown in **Table 1**. The obtained residual stress profile is further mapped to each element in the fatigue simulation model in terms of the full stress tensor. For details of the modelling procedures as well as the residual stress profiles for various inclusions, the readers are referred to Gu et al. ²² and Gu et al. ²³, respectively.

Table 1 Mechanical properties of the steel matrix and the inclusions in the martensitic steel.

Material	Coefficient of linear expansion, α ($10^{-6} \cdot ^\circ\text{C}$)	Young's modulus, E (GPa)	Poisson's ratio, ν (-)
Calcium aluminate	5.0	113	0.23
Steel matrix	23.0	206	0.30

3.3 Crystal plasticity for the fatigue simulation and its parameter calibration

The mechanical behaviour of the microstructure under cyclic loading was rendered by the

crystal plasticity (CP) model. Since its implementation in the finite element method, crystal plasticity model has shown powerful applications in texture evolution prediction during forming³¹⁻³², hot and cold rolling³³⁻³⁴, as well as in the plastic anisotropy prediction for various metallic materials³⁵⁻³⁷, the residual stresses prediction³⁸⁻³⁹ and damage initiation prediction⁴⁰⁻⁴¹ during plastic deformation. A thorough review of the formulation and the recent development of the crystal plasticity models has been presented by Roters et al.⁴². The model formulation in the current study is based on the well-established phenomenological description of slip with an extension to include the kinematic hardening, which was presented in detail in our previous study⁴³. It was assumed that the dislocation slip in the model is the only plastic deformation mechanism. The deformation gradient $\mathbf{F}$ can be split up in an elastic and plastic part:

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p, \quad (3)$$

The rate of the plastic deformation gradient $\dot{\mathbf{F}}_p$ can be calculated by Eq. (2):

$$\dot{\mathbf{F}}_p = \mathbf{L}_p \mathbf{F}_p, \quad (4)$$

where $\mathbf{L}_p$ is the plastic velocity gradient, which is caused by the crystal slips⁴⁴:

$$\mathbf{L}_p = \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} = \sum_{\alpha=1}^N \dot{\gamma}^{\alpha} \mathbf{S}^{\alpha}, \quad (5)$$

$$\mathbf{S}^{\alpha} = \mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha} \quad (6)$$

where $\mathbf{S}^{\alpha}$ is the Schmid tensor of the slip system α ; $\mathbf{m}^{\alpha}$ and $\mathbf{n}^{\alpha}$ are the slip direction and plane normal vectors of the slip system α ; N is the total number of active slip systems and $\dot{\gamma}^{\alpha}$ is the shear rate and is to be formulated by the kinetic law of slip. The plastic reaction occurs locally in grains that are in the most suitable orientation to the direction of applied load:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left| \frac{\tau^{\alpha} - \chi^{\alpha}}{\tau_c^{\alpha}} \right|^{\frac{1}{m}} \text{sgn}(\tau^{\alpha} - \chi^{\alpha}), \quad (7)$$

where $\dot{\gamma}_0$ is initial slip rate; τ^{α} is resolved shear stress; τ_c^{α} is critical resolved shear stress on slip

system α ; $1/m$ is strain rate sensitivity factor and χ^α is kinematic back stress on slip system α . A nonlinear kinematic hardening rule initially proposed by Armstrong and Frederick ⁴⁵ and later implemented for austenite in a recent micromechanical fatigue analysis ⁴⁶ is employed in the current study:

$$\dot{\chi}^\alpha = G_1 \dot{\gamma}^\alpha - G_2 |\dot{\gamma}^\alpha| \chi^\alpha \quad (8)$$

where G_1 and G_2 are material parameters, which need to be calibrated.

The micromechanical interaction among different slip systems is empirically captured by the hardening evolution law of the slip system α :

$$\tau_c^\alpha = \tau_0 + \sum_{\beta=1}^N q^{\alpha\beta} \left[h_0 \left(1 - \frac{\tau_c^\beta}{\tau_s} \right)^a \right] |\Delta\gamma^\beta| \quad (9)$$

where τ_0 is initial resolved shear stress; $q^{\alpha\beta}$ is latent hardening matrix; h_0 , τ_s , and a are hardening parameters and $\Delta\gamma^\beta$ is the plastic slip increment of each slip system β .

The calibration of parameters in the crystal plasticity model is conducted with an iterative fitting of the hysteresis loops obtained by the RVE simulation to the low cycle fatigue (LCF) tests with the trial-and-error method. Two strain amplitudes of 1.1% and 1.2% were considered in the LCF tests. For both strain amplitudes, the stable strain-stress cycles were taken. The calibrated results are shown in **Table 2** ^{22, 47}.

Table 2 CP model parameters.

C_{11} : 193.9 GPa	C_{12} : 94.6 GPa	C_{44} : 92.2 GPa	$\dot{\gamma}_0$: 0.01
$1/m$: 100	τ_0 : 645 MPa	G_1 : 100000 MPa	G_2 : 2000
h_0 : 1000 MPa	a : 1.1	τ_s : 2500 MPa	

3.4 Microcrack initiation and fatigue life prediction

During the fatigue simulation process, a fully reversed tension-compression ($R = -1$) was applied under a frequency of 20 kHz, which is consistent with the fatigue experiments. The accumulated dislocation slip is considered as the fatigue indicator parameter (FIP) according to McDowell and Dunne ⁴⁸, since the persistent slip bands are a precursor to fatigue crack initiation ⁴⁹. To overcome the mesh effect, the grain-level-averaged accumulation dislocation slip is considered in the present study.

According to Gillner and Münstermann ⁴³, the increment of the locally accumulated dislocation slip p_{acc} keeps as a constant value after the first cycle. Therefore, the number of cycles can be any number larger than two for capturing the statistical distribution of the development of p_{acc} in different RVEs. In the present study, the cyclic loads of 6 cycles with different amplitudes are imposed on all the RVEs with inclusions. Afterwards, the distributions of p_{acc} and the maximum grain-level-averaged value P_{max} are calculated, see Eqs. (6) and (7).

$$p_{acc} = \int_0^t \sqrt{\frac{2}{3}} \mathbf{L}_p : \mathbf{L}_p dt \quad (10)$$

$$P_{max} = \max \left(\frac{1}{\sum_{i=1}^{N_E^{Gr}} V_i^{Gr}} \sum_{i=1}^{N_E^{Gr}} p_i V_i^{Gr} \right) \quad (11)$$

where the parameter i is the identifier of the finite element of the involved grain, N_E^{Gr} is the number of elements within the grain, and V_i^{Gr} is the volume of the element i of the grain.

The position of P_{max} in every RVE in the present study is recognized as the fatigue initiation site ¹⁶⁻¹⁷. Under each stress amplitude, the simulation to calculate P_{max} was conducted on all 60 RVEs.

To calculate the fatigue life, the extreme value distribution of P_{max} was firstly fitted according to Eq. (12):

$$f(x | A_m, B_m) = A_t \exp \left(\frac{x - B_m}{A_m^{-1}} \right) \exp \left[- \exp \left(\frac{x - B_m}{A_m^{-1}} \right) \right], \quad (12)$$

where m is the indicating number of stress amplitude; A_m and B_m are the distribution parameters of $P_{\max}$ under stress amplitude m . Shenoy et al.⁵⁰ calculated the cycle number for crack incubation:

$$N_{\text{inc},m} = \frac{\alpha_p}{d_{\text{gr}}(\bar{P}_{\max})^2}, \quad (13)$$

where α_p is a fitting constant, d_{gr} is the mean grain size and $\bar{P}_{\max}$ is the mean value of $P_{\max}$:

$$\bar{P}_{\max} = \frac{\sum_k P_{\max}}{kN}, \quad (14)$$

where k is the number of RVEs, which is 60 in this study. N is the number of cycles for $P_{\max}$.

With the parameters from Eq. (12)-(14), the fatigue life $N_{f,m}$ can be calculated by Eq. (15)⁴³:

$$N_{f,m} = N_{\text{inc},m} \left(1 + \frac{\sum_i^L (A_m B_m)^u \sigma_m}{(A_m B_m)^u \sum_m^L \sigma_m} \right). \quad (15)$$

where u , along with α_p , are fitting constants, which needs to be calibrated on at least two fatigue life data, and σ_m is the stress amplitude value under indicating number m .

4. Results and discussion

4.1 Fatigue crack initiation

According to the results of ultrasonic fatigue experiments, all the crack initiation sites in this study were inside the material. The fracture occurred due to both steel matrix inhomogeneity and non-metallic inclusions (**Fig. 2**). A small fraction of the fatigue crack initiation was found in the steel matrix⁵¹, which indicates a different fatigue mechanism⁵². The present study focuses on the fatigue initiation triggered by inclusions, which is the majority of the crack initiation mechanism of this steel. The non-metallic inclusion types observed in the crack initiation sites were calcium aluminate (Al-Ca-O-S), spinel (Mg-Al-O) and titanium nitride (TiN), among which the calcium aluminate inclusions contribute the most to the fatigue crack initiation. The S-N curves of the fatigue failure caused by the steel matrix and calcium aluminate inclusions differ from each other. In the next sections of this paper, only the effect of calcium aluminate inclusion was discussed due to the lack of data of spinel and titanium nitride inclusions.

Fig.2. S-N curves of the fatigue experiments sorted by the crack initiation sources. The points are indicating the individual experimental results, while the lines are linearly fitted curves based on the experimental data.

The typical morphologies of crack initiations with different types of inclusions are shown in **Fig. 3**. The fatigue cracks triggered by calcium aluminate and spinel are initiated from the steel matrix around inclusions with the inclusions unbroken, while the fatigue cracks triggered by titanium nitride are initiated from the inside of inclusions and extends to the steel matrix. The geometries of calcium aluminate inclusions are generally spherical due to the inclusion evolution mechanism in the smelting process. Therefore, in the present study, the size of calcium aluminate was expressed with diameter. The diameters of inclusions observed in the fatigue crack initiation sites were ranged from 12.5 μm to 33.2 μm and plotted with the method of statistics of extremes, as shown in **Fig. 4**. The detail of this method is given by Murakami and Beretta^{2, 12, 53}. It is often used for inclusion condition comparison for different materials or inclusion size estimation in certain component size. The return period T represents the multiple of the investigated area divided by the controlled area or the number of specimens. As shown in **Fig. 4**, the estimated maximum size of inclusions is 41 μm for 50 specimens and 49 μm for 200 specimens.

Fig. 3. Morphologies of crack surfaces with fisheye structures triggered by different types of inclusions with different sizes under various SEM magnifications: (a)-(c) calcium aluminate inclusion with diameter of 15 μm ; (d)-(f) calcium aluminate inclusion with diameter of 20 μm ; (g)-(i) calcium aluminate inclusion with diameter of 30 μm ; (j)-(l) titanium nitride inclusion; (m)-(o) spinel inclusion.

Fig. 4. Extreme value distribution of inclusion sizes observed in crack initiation sites.

4.2 Modelling of inclusions and the residual stress distribution

In the previous study of Gu et al.²², the inclusion shown in Fig. 3(f) was digitalized and inserted in all 60 RVEs, the corresponding residual stresses distribution in each RVE was simulated. In this study, the inclusions in Fig. 3(c) and Fig. 3(i) were also inserted in all RVEs.

Fig. 5 shows some examples of the geometry models of the three inclusions in the centre of different RVEs (the dark grey part represents the inclusion) and the simulated residual stress distributions. The maximum residual stress is on the boundary between the inclusion and steel matrix, and the inclusion size affects the value of the residual stress. In the residual stress simulation results of 60 RVEs for each calcium aluminate inclusion, the maximum value of the residual stress slightly increases with the increase of inclusion size, see **Fig. 6**.

Fig. 5. Different RVEs of the martensitic microstructure with the calcium aluminate inclusions of different sizes and the corresponding residual stress distributions: the inclusion in (a), (b) and (c) is shown in Fig. 3(c); the inclusion in (d), (e) and (f) is shown in Fig. 3(f); the inclusion in (g), (h) and (i) is shown in Fig. 3(i).

Fig. 6. The maximum residual stress simulation results of 60 RVEs with calcium aluminate inclusions of different sizes.

4.3 Fatigue life prediction without residual stress around calcium aluminate inclusion

The fatigue life prediction was conducted under three stress amplitudes: 1100 MPa, 1200 MPa and 1250 MPa. For comparison, the residual stress distribution around inclusions was

neglected in this section. Without residual stress, around 23-41% max grain-level-averaged accumulated dislocation slip $P_{\max}$ did not occur around the inclusion, which represents the inaccuracy prediction of fatigue crack initiation sites, as shown in **Fig. 7** (the white arrows point at the $P_{\max}$ positions). The ratios of $P_{\max}$ positions in all RVEs under different stress amplitudes with inclusions of different size are shown in **Fig. 8**. For RVEs with the inclusion of 15 μm , the ratio of $P_{\max}$ not occurring around inclusion is 41.1%; for RVEs with the inclusion of 20 μm , the ratio is 33.9%; for RVEs with the inclusion of 30 μm , the ratio is 23.2%. The ratio decreases with the increase of the inclusion size. When the inclusion size is smaller, the values of accumulated dislocation slip in the grains around inclusions decrease, which leads to the $P_{\max}$ away from inclusions. This condition tends to get alleviated with the increase of inclusion size. When $P_{\max}$ does not occur around the inclusion, the data cannot be considered in the next step of fatigue life prediction.

Fig. 7. The p_{acc} contour distributions of steel matrix in typical RVEs with calcium inclusions of different sizes after six cycle simulation of tension-compression fatigue stress neglecting the residual stress generated during cooling process: (a) the inclusion shown in Fig. 3(c); (b) the inclusion shown in Fig. 3(f); (c) the inclusion shown in Fig. 3(i).

Fig. 8. The ratio that the position of $P_{\max}$ is around inclusions and not around inclusions.

After the data screening, the distribution parameters A_i , B_i and the max grain size averaged accumulated dislocation slip $P_{\max}$ under three stress amplitudes with inclusions of different sizes neglecting residual stress distribution are shown in **Table 3**. Inclusion 15 represents the inclusion in Fig. 3(c) with size of 15 μm . Inclusion 20 represents the inclusion in Fig. 3(f) with size of 20 μm . Inclusion 30 represents the inclusion in Fig. 3(i) with size of 30 μm . The values of $P_{\max}$ are larger for larger stresses and inclusions.

Table 3 Distribution parameters and the max grain size averaged accumulated dislocation slip under different conditions without residual stress around inclusions.

Stress amplitude (MPa)	Inclusion 15			Inclusion 20			Inclusion 30		
	A_i	B_i	$P_{\max}$	A_i	B_i	$P_{\max}$	A_i	B_i	$P_{\max}$
1250	2.47×10^{-9}	1.49×10^{-10}	1.18×10^{-11}	3.58×10^{-9}	1.08×10^{-9}	6.08×10^{-11}	4.21×10^{-9}	2.31×10^{-9}	1.78×10^{-10}
1200	2.39×10^{-10}	1.44×10^{-10}	9.18×10^{-12}	2.30×10^{-9}	1.06×10^{-9}	4.61×10^{-11}	4.13×10^{-9}	2.26×10^{-9}	1.38×10^{-10}
1100	1.17×10^{-10}	9.04×10^{-11}	6.19×10^{-12}	1.09×10^{-9}	4.96×10^{-10}	2.19×10^{-11}	1.92×10^{-10}	1.06×10^{-11}	6.88×10^{-11}

The parameters α_p and u were calibrated by three fatigue life data with inclusions of diameter 20 μm in the crack initiation site ($\sigma = 1248 \text{ MPa}$, $N_f = 3.47 \times 10^7$; $\sigma = 1209 \text{ MPa}$, $N_f = 4.85 \times 10^7$; $\sigma = 1178 \text{ MPa}$, $N_f = 7.72 \times 10^7$). The fitting constants α_p and u control the position and gradient of S-N curve, see **Fig. 9**. The increase of α_p will lead to a right shift of S-N curve. The increase of u will lead to a decrease of gradient of S-N curve. With $\alpha_p = 2 \times 10^{-13}$ and $u = 0.02$, the simulation result was best fitted.

Fig. 9. Calibration results with different parameters α_p and u for the model without residual stress based on the RVE with the calcium aluminate inclusion shown in Fig. 3(d).

With this set of parameters, the S-N curve predictions with inclusions of 15 μm , 20 μm and 30 μm were presented in **Fig. 10**. From the simulation results, the calculated fatigue life is longer for smaller inclusion, which is quite reasonable. However, the simulation results are not quite consistent with the experimental results. In Fig. 9, all the fatigue experiment results are sorted by inclusion size. The blue solid dots correspond to samples with inclusions not larger than 15 μm . The red half squares represent the inclusions of size between 15 and 30 μm . The black hollow

rhombuses represent the inclusion of size not smaller than 30 μm . As shown in the figure, all the blue dots are in the left side of the blue dashed line and two black hollow rhombuses are in the left side of blue dot line, which is against the experiment results. In the model neglecting residual stress around inclusions, the sensitivity of fatigue life to inclusion size variation is too large compared with experiment data. This inaccuracy is alleviated when residual stress distribution is considered, which will be discussed in the next section.

Fig. 10. The comparison between simulation S-N curves without residual stress and the experimental fatigue data sorted by the sizes of calcium aluminate inclusions observed in the crack initiation sites.

4.4 Fatigue life prediction with residual stress around calcium aluminate inclusion

The fatigue life prediction process described in Section 4.2 was repeated in this section with the residual stress distribution inserted. Under this condition, all max grain size averaged accumulated dislocation slips occurred around inclusions. **Fig. 11** shows the p_{acc} contour distributions of steel matrix in typical RVEs with the calcium inclusions of different sizes and the P_{max} positions (pointed out by the white arrows) considering residual stress. The distribution

parameters A_i , B_i and the max grain size averaged accumulated dislocation slip $P_{\max}$ are shown in **Table 4**. The values of $P_{\max}$ show an obvious increase in comparison with the results without residual stress, which is caused by larger stress concentration on the crack initiation site lead by residual stress. Besides of the stress concentration, better plasticity of material can also lead to a larger value of $P_{\max}$, which usually occurs in different material or different phase.

Fig. 11. The p_{acc} contour distributions of steel matrix in typical RVEs with calcium inclusions of different sizes after six cycle simulation of tension-compression fatigue stress considering the residual stress generated during the cooling process: (a) the inclusion shown in Fig. 3(c); (b) the inclusion shown in Fig. 3(f); (c) the inclusion shown in Fig. 3(i).

Table 4 Distribution parameters and the max grain size averaged accumulated dislocation slip under different conditions with residual stress around inclusions.

Stress	Inclusion 15			Inclusion 20			Inclusion 30		
amplitude (MPa)	A_i	B_i	$P_{\max}$	A_i	B_i	$P_{\max}$	A_i	B_i	$P_{\max}$
1250	5.20×10^{-5}	2.10×10^{-5}	1.89×10^{-6}	7.11×10^{-5}	6.30×10^{-5}	3.25×10^{-6}	6.69×10^{-5}	8.24×10^{-5}	5.33×10^{-6}
1200	3.60×10^{-5}	1.40×10^{-5}	1.54×10^{-6}	5.12×10^{-5}	4.09×10^{-5}	3.00×10^{-6}	5.55×10^{-5}	6.12×10^{-5}	5.29×10^{-6}
1100	1.00×10^{-5}	4.17×10^{-6}	7.46×10^{-7}	3.22×10^{-5}	2.31×10^{-5}	1.67×10^{-6}	3.52×10^{-5}	3.01×10^{-5}	3.14×10^{-6}

Based on the values of A_i , B_i and $P_{\max}$ in Table 4, the parameters α_p and u were also calibrated with the same fatigue life data in Section 4.2. **Fig. 12** shows the calibration results with different values of α_p and u . With $\alpha_p = 7.5 \times 10^{-4}$ and $u = 0.6$, the calculated $S-N$ curve with the inclusion of diameter 20 μm was well fitted with experiment data. The value of α_p , in this case, is larger than that in the case neglecting residual stress, which is mainly caused by the larger value of $P_{\max}$. The value of u is also larger, while it is in the same order of magnitude with the value of u in the case neglecting residual stress. A larger value of u is needed to correct the large effect of stress amplitude on fatigue life. **Fig. 13** shows the $S-N$ curves with the 20 μm inclusion predicted by the models considering residual stress and neglecting residual stress under the same value of parameter u ($u = 0.6$). The obviously larger slope of the $S-N$ curve predicted by the model with residual stress is shown in the figure, indicating that the effect of stress amplitude on fatigue life variation is larger. When the residual stress is considered, the stress on the whole RVE during the fatigue process consists of the residual stress and fatigue stress. When the fatigue stress changes, the residual stress, which is generated during heat treatment, remains constant after the relaxation in the first cycle²². This constant part of stress leads to smaller change of fatigue life with the same variation of fatigue stress. However, when the residual stress is not considered, the stress on the whole RVE is only made up by the fatigue stress. Without the constant part, the fatigue life changes larger with the same variation of fatigue stress.

Fig. 12. Calibration results with different parameters α_p and u for the model with residual stress based on the RVE

with the calcium aluminate inclusion shown in Fig. 3(f).

Fig. 13. The S-N curves with the 20 μm inclusion predicted by the models considering residual stress and neglecting residual stress under the same value of parameter u .

The simulated S-N curves of different inclusion size predicted by the model considering residual stress were also compared with the fatigue experiment results sorted by inclusion size (Fig. 14). As shown in Fig. 14, the sensitivity of fatigue life on inclusion size obviously decreases

in comparison with the model neglecting residual stress, which also leads to a better agreement between simulation results and experiment results. Although the simulated S-N curves are more consistent with the experimental data, the predicted fatigue life in terms of the inclusion of 15 μm is still slightly larger (there is still one blue dot in the left side of the blue dotted line in Fig. 14). This inaccuracy indicates that there are still limitations of the model with residual stress even if it offers more accurate predicted S-N curves than the model without residual stress, for example, the local voids around the inclusions, which have been observed in the present study and some other researches⁵⁴⁻⁵⁵, were neglected for simplicity.

Fig. 14. The comparison between simulation S-N curves with residual stress and the experimental fatigue data sorted by the sizes of calcium aluminate inclusions observed in the crack initiation sites.

4.5 Comparison of the accuracy of models considering and neglecting residual stress on fatigue life prediction

According to the research of Murakami¹², the 10^7 -fatigue limit σ_w for stress ratio, $R = -1$, depends on the square root of inclusion area to $-1/6$ power, see Eq. (16):

$$\sigma_w = a'(HV + 120)/(\sqrt{area})^{1/6}, \quad (16)$$

where HV is the Vickers hardness of the steel; $\sqrt{area}$ is the square root of the inclusion area, μm ;

a' is the position coefficient of the inclusion, $a' = 1.43$ for surface inclusions, $a' = 1.41$ for inclusions in contact with the sample surface, $a' = 1.56$ for internal inclusions.

During the research on HCF and VHCF properties of high-strength steel, Furuya¹³ reported that the 10^9 -fatigue limit σ_w' also obeyed this $-1/6$ -power rule for inclusions larger than $15 \mu\text{m}$. To compare the fatigue life prediction results of the models considering residual stress and neglecting residual stress, the 10^9 -fatigue limits concerning calcium aluminate inclusions with different sizes predicted by these two models were calculated. **Fig. 15** shows the calculation results plotted on a logarithmic scale. It is obvious that the slope of the relation between 10^9 -fatigue limits and square roots of inclusion areas calculated with the model considering residual stress is closer to $-1/6$, which also proves the improved accuracy of the fatigue life prediction model with residual stress.

Fig. 15. The relation between 10^9 -fatigue limit and $\sqrt{area}$ of calcium aluminate inclusions calculated with models considering residual stress and neglecting residual stress on logarithmic scales.

4.6 A formulation of fatigue life with respect to stress amplitude and inclusions size

After the correlation between a specific fatigue strength and inclusion size, a 3D analytical equation between fatigue life, stress amplitude and inclusion size in VHCF regime ($10^7 \leq N_f \leq 10^9$) is proposed in this section. This analytical description of these three elements can be of great importance for the fatigue life prediction based on microstructure information in practice. Following the equation by Murakami¹² and Furuya¹³, the effect of inclusions size on fatigue life is fitted with the power-law relation. In addition, the relation between the stress amplitude and the fatigue life is also simply expressed in a power-law equation. Therefore, based on the systematic results by the residual stress enriched model, the following equation is proposed and the fitted 3D surface is also compared with the experimental and numerical data as shown in **Fig. 16**.

$$\lg(N_f) = F_1 \times \sigma^{F_2} \times (\sqrt{area})^{F_3} \quad (17)$$

where σ represents the stress amplitude in MPa; $\sqrt{area}$ represents the square root of the inclusion area in μm ; and F_1 , F_2 and F_3 are the fitting constants, where $F_1 = 15402 \text{ MPa}^{0.98} \cdot \mu\text{m}^{1/4.7}$, $F_2 = -0.98$ and $F_3 = -1/4.7$.

The comparison on the effect of inclusions sizes on the fatigue limit at different fatigue life cycles are shown in **Fig. 17**. A good estimation is reached by the proposed general correlation when $\sqrt{area}$ is in the range of 13.3-26.6 μm . It is also noted that for an overall good fitting at various fatigue life cycles, the exponent is no longer 1/6 as reported by Murakami¹² and Furuya¹³. To further represent the effect of inclusion size and stress amplitude on fatigue life, the relation between N_f and $\sqrt{area}$ under various stress amplitudes is shown in **Fig. 18**. N_f decreases with the decrease of $\sqrt{area}$ and σ . The correlation between the fatigue life and the applied stress

amplitudes for specific inclusion size is also illustrated, see **Fig. 19**, which also gives a good estimation of the numerical simulation results.

It should be emphasized that the proposed analytical equation is not intending to be a universal one for all the materials. Instead, its applicability is limited to the current investigated steel and the inclusions type, as the simulation data to feed the fitting is derived based on these material properties. A current on-going work is to extend the investigation to more types of inclusions as well as different steel matrixes. As a result, the intrinsic nature of the materials could be implemented to the equation with more data.

Fig. 16. The fitted surface of the effects of the stress amplitude and the inclusion diameter on the fatigue life and the comparison between the fitted surface and experiment results.

Fig. 17. The relation between 10^9 -fatigue limit and $\sqrt{area}$ of calcium aluminate inclusions based on the fitted surface shown in Fig. 16 on logarithmic scales.

Fig. 18. The effects of the inclusion diameter on the fatigue life under consistent stress amplitude based on the fitted surface shown in Fig. 16.

Fig. 19. The effects of the stress amplitude on the fatigue life under consistent inclusion diameter based on the

fitted surface shown in Fig. 16.

5. Conclusions

In this study, the effect of calcium aluminate inclusion sizes on the fatigue life was investigated experimentally and numerically. Based on the inclusions observed in the crack initiation sites, the fatigue life and S-N curves were predicted with a microstructure-based model by considering residual stresses between the inclusions and matrix induced by cooling process before the fatigue loading. The modelling results were validated using the corresponding experimental data. The following conclusions are drawn:

- (1) The sizes of calcium aluminate inclusions observed in the crack initiation sites in the investigated high carbon bearing steel were ranged from 12.5 μm to 33.2 μm . The S-N curves of fatigue data caused by calcium aluminate inclusions and steel matrix differ from each other.
- (2) The microstructure-based fatigue model with residual stresses correctly predict the effect of the calcium aluminate inclusion on fatigue life. The calculated S-N curves show good agreement with the experiment data in terms of inclusion size.
- (3) When the residual stress is neglected in this model, the calculated S-N curves are not consistent with experiment data. The effect of inclusion size on fatigue life is significantly overestimated.
- (4) The 10^9 -fatigue limits concerning calcium aluminate inclusions with different sizes calculated by models considering residual stress and neglecting residual stress were compared and the former depends more closely on the square root of inclusion area to $-1/6$ power.
- (5) Based on the systematic simulation with the fatigue modeling approach, a general 3D analytical correlation for the martensitic high carbon chromium bearing steel in this study in VHCF regime is proposed between the fatigue life, stress amplitude and inclusion size. The

analytical solution provides a good estimation compared to the numerical simulation results.

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Highlights

- The S-N curves caused by inclusions with different sizes are accurately predicted by a microstructure-based fatigue model.
- To include the residual stresses between the inclusions and matrix is critical for the fatigue life prediction.
- The effect of the inclusions size on fatigue strength is quantitatively analysed.
- A general 3D analytical solution is proposed to describe the relation between fatigue life, stress amplitude and inclusion size.