International Conference on Advances in Computational Modeling and Simulation

Microstructural modeling of fatigue crack initiation in austenitic steel 304L

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Abstract

A methodology for modeling realistic microstructures of metallic polycrystalline material is presented. This approach is applied to the prediction of cyclic behavior of austenitic steel 304L in order to study the role of microstructural effects on fatigue crack initiation. The microscope observations show crack initiation and microcrack propagation are dependent on crystallographic orientations, indicating the need for such modeling approach. A representative volume of the material corresponding to a realistic microstructure, containing about 200 grains, has been numerically modeled with the crystal plasticity approach. This model takes account of dislocation densities on the 12 slip systems, isotropic and kinematic hardening, grain sizes, crystal orientations and elastic anisotropy. The material parameters used in this model were obtained through experimental measurements and the literature or identified through an inverse procedure, which give good predictions of stress-strain response at the macroscale. The field results of local strain, stress, slip-based and energy-based initiation metrics are simulated at grain scale. The results show that some of these metrics are in good agreements with experiments and can be used in fatigue crack initiation criteria.

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Keywords: Fatigue; microcrack initiation; crystal plasticity; numerical simulation

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1 Introduction

Because the phase of fatigue crack initiation and the propagation of microstructurally short cracks represents most of the high cycle fatigue life of some technical component in high-strength materials, the study of crack initiation has attracted increasing attention recently, in contrast to the conventional research approaches where fatigue crack initiation and microcrack propagation path were ignored and only the life to failure of the specimen were concerned [1-8]. In classical fatigue life criteria the material is considered to be elastically and plastically isotropic and structure-less. However, in reality, most structural alloys show polycrystalline structure and large amounts of small grains with various orientations. When the polycrystalline material is subject to external loading, the stress/strain distribution from grain to grain should be inhomogeneous because of the elastic and plastic anisotropy. Some “hard” grains may show larger stress than average level while crystal plastic slip and accumulated plastic strain may lead to stress and strain concentration in grain or at grain boundaries, which is considered as one of the reasons for crack initiation. As the microcrack size is smaller than or comparable with the grain size, the inhomogeneous microstructure strongly affects the microcrack initiation and propagation behavior. There are many factors influencing the fatigue crack initiation such as material microstructure (grain size, microscopic flaws at grain boundaries, twin boundaries and inclusions) and loading conditions such as sequence and path effects (multiaxial fatigue, variable amplitude problem) etc [9-16]. Although the principal mechanisms leading to fatigue crack initiation were well studied and identified, the effect of microstructure and local stress/ deformation distribution on crack initiation remain unclear. In austenitic stainless steels, these cracks generally arise in the persistent slip bands (PSB) at the surface, along grain boundaries (GB) or between them (PSB-GB) [17, 18]. So in order to numerically study the effect of microstructure on the crack initiation, it is required that the model must be three dimensional and based on realistic microstructure to reflect the nature of crystal deformation behavior.

In this present work, the aim is to numerically simulate micromechanical behavior of 304L steel and to study the microstructure effect on fatigue crack initiation and evaluate the crack initiation predictive capabilities of some factors in fatigue criteria. By considering a representative volume of the material of 304L steel, a finite element model of polycrystal plasticity with details of realistic grain morphology and crystallographic orientation was developed in Abaqus. In this model, the dislocation densities on the 12 slip systems, isotropic and kinematic hardening, grain sizes, crystal orientations and elastic anisotropy were taken into account. The numerical results were compared with the experimental observation. The fatigue test and the corresponding numerical studies were performed under constant stress amplitude of ±220 MPa. The mechanical fields of local strain, stress, maximum shear strain amplitude on 12 slip systems and normal stress on the slip plane with maximum shear strain amplitude, the function value of Socie-Fatemi criterion, plastic strain energy were considered.

2 Low cycle fatigue test

2.1 Experiment procedure

The material used in this study is an austenitic stainless steel (AISI 304L) with an f.c.c structure which is widely used in nuclear industry. The average grain size is about 50μm. Chemical composition can be seen in Table 1.

<table>
<thead>
<tr>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>S</th>
<th>P</th>
<th>Ni</th>
<th>Cr</th>
<th>Mo</th>
<th>Cu</th>
<th>N2</th>
</tr>
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<tbody>
<tr>
<td>0.029</td>
<td>1.86</td>
<td>0.37</td>
<td>0.004</td>
<td>0.029</td>
<td>10.00</td>
<td>18.00</td>
<td>0.04</td>
<td>0.02</td>
<td>0.056</td>
</tr>
</tbody>
</table>
The fatigue test under constant stress amplitude of ±220 MPa at a frequency of 2 Hz was conducted by MTS 810 servo-hydraulic system. In order to locate the crack initiation site, to make observation and measurement easier and to avoid the crack occur due to stress concentration at sharp corners, a quite smooth circular notch was machined. The specimen with a length of 44mm is designed according to required parameters of an in-situ machine used in SEM (Figure 1(a)). The specimen was mechanically polished before fatigue tests to satisfy the surface requirement of EBSD measurement and simultaneously improve optical observation of plastic deformation and crack initiation.

![Figure 1 (a) Specimen geometry for fatigue test under stress control (b) Observation zone (1mm × 3mm)](image)

This fatigue test was interrupted for observation. The central zone with 1mm × 3mm on the specimen (as shown in Figure 1(b)) was observed by microscope and SEM at 1000, 4000, 10000, 15000, 20000 and 35000 cycles. Fatigue test was terminated until 35000 cycles and at this moment some cracks were observed with the maximum length about 100 μm (Figure 2). As shown in Figure 2, the cracks mostly initiated in persistent slip bands and were dependent on crystallographic orientations. Then the specimen was cross-sectioned and polished to perform successive EBSD measurements on the same cracked area in order to reconstruct a three dimensional numerical aggregate.

![Figure 2 some cracks observed on the surface of the specimen after 35000 cycles under ±220 MPa stress amplitude](image)

### 3 Numerical simulation

The model of crystalline plasticity used in this work, CristalECP, is based on the large deformation theory and implemented in Abaqus. It has shown great capabilities to describe the characteristics of single and polycrystals deformation during monotonic and cyclic loadings with a good agreement between simulations and experiments [19-23].


3.1 Material constitutive laws

For 304L with an f.c.c structure, slip occurs respectively on the 12 systems \{111\} \langle110\>. The shear rate \(\dot{\gamma}^s\) on each slip system (s) is described by a viscoplastic law based on effective stress and threshold critical stress \(\tau^s\):

\[
\dot{\gamma}^s = \begin{cases} \\
\dot{\gamma}^0 \left(\frac{\tau^s - \tau^s}{\tau^s}\right)^n \times \text{sign}(\tau^s - \tau^s), & \text{if } \frac{\tau^s - \tau^s}{\tau^s} \geq 1 \\
0, & \text{if } \frac{\tau^s - \tau^s}{\tau^s} < 1 
\end{cases}
\]

(1)

The effective stress is the difference between the resolved shear stress and the kinematic back stress \(\tau^s\) on this slip system. \(\dot{\gamma}^0\) is a reference shear rate and n is a rate sensibility exponent.

The critical shear stress increases with the increase of the density of the dislocation forest and is given by [19]:

\[
\tau^s = \tau_0 + \mu b \sqrt{\sum_{i=1}^{\infty} a_i^2 \rho^i}
\]

(2)

where \(\tau_0\) is the friction stress, \(b\) is Burgers vector and \(\mu\) is the isotropic shear modulus. \(a^i\) is a hardening matrix whose terms depend on the type of elastic interactions between dislocation system (s) and all other dislocation systems (t), which includes self hardening. It consists of six coefficients which give a complete description of the hardening behavior at small strains [24-26]. The evolution of the dislocation density is taken according to the dislocation multiplication and annihilation mechanisms. It occurs in each slip system, and its rate can be written as:

\[
\dot{\rho}^s = \frac{1}{b} \left( \frac{1}{\lambda^s} - 2g_c \rho^s \right)
\]

(3)

where \(g_c\) is proportional to the annihilation distance of dislocation dipoles. \(\lambda^s = \frac{K}{\sqrt{2\pi} \rho^s}\) describes the mean free path of the mobile dislocations on slip system (s).

The nonlinear kinematic hardening rule initially proposed by Armstrong and Frederick [27] was chosen:

\[
\kappa^s = C \dot{\gamma}^s - D \dot{\gamma}^s |\dot{\gamma}^s| \tau^s
\]

(4)

where C, D are material parameters.

3.2 3D modeling method

A three dimensional numerical aggregate was constructed from four electron backscattered diffraction (EBSD) maps performed on successive cross-section polishing on the same cracked area from a sample of 304L steel. The microstructure of the aggregate was extruded from each layer through the third direction.
The EBSD maps were acquired with a resolution of 2µm on an area 500µm by 500µm which was chosen from observation zone mentioned above and including one crack. The distance between successive polished sections is 24µm thick. Figure 3(a) shows the results of EBSD mapping measurements.

Figure 3 (a) four layers EBSD maps used to reconstruct the numerical aggregate (b) 3D finite element aggregate constructed with the actual crystallographic orientation information (c) boundary conditions applied to the aggregate during the simulation

The actual crystallographic orientation information was added into the Abaqus program in order to get a fixed cubic meshed numerical aggregate including realistic microstructure as shown in Figure 3(b). The meshing is composed of C3D8R element (eight-node brick element with reduced integration) with the size of 4µm*4µm*8µm. Every 4 EBSD points (2x2) are assigned to one element. Each meshed element has a spatial position and orientation corresponding to the initial crystallographic constitutive properties obtained from EBSD. No particular element is taken into account for the grain boundaries.

Table 2 The parameters of the crystalline constitutive law identified for steel 304L

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>C11</td>
<td>197500</td>
</tr>
<tr>
<td>C12</td>
<td>125000</td>
</tr>
<tr>
<td>C44</td>
<td>122000</td>
</tr>
<tr>
<td>µ</td>
<td>61000</td>
</tr>
<tr>
<td>ε0</td>
<td>10</td>
</tr>
<tr>
<td>γ0</td>
<td>1.10^{-5}</td>
</tr>
<tr>
<td>n</td>
<td>49</td>
</tr>
<tr>
<td>a0</td>
<td>0.045</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>a1</td>
<td>0.625</td>
</tr>
<tr>
<td>a2</td>
<td>0.137</td>
</tr>
<tr>
<td>a3</td>
<td>0.122</td>
</tr>
<tr>
<td>a4</td>
<td>1.10^{-12}</td>
</tr>
<tr>
<td>b</td>
<td>0.254</td>
</tr>
<tr>
<td>K</td>
<td>1</td>
</tr>
<tr>
<td>g0</td>
<td>150</td>
</tr>
<tr>
<td>C</td>
<td>15300</td>
</tr>
<tr>
<td>D</td>
<td>430</td>
</tr>
</tbody>
</table>

The material parameters used in this model are given in Table 2. The boundary conditions were chosen to approximate the boundary conditions of an aggregate placed at the surface of a specimen Figure 3(c).

3.3 Simulation results

In this section, we consider some numerical simulation results aimed at drawing comparisons with experimental surface observation regarding the predictive capabilities of fatigue crack initiation metrics in fatigue criteria. One of the difficulties arising in this situation is the choice of “physical” metrics of crack initiation which is not in fact well established. Local stress and strain values are two important indicators in classical fatigue criteria and have great influence on fatigue life. Figure 4 shows simulation results of local strain ε22 and the stress σ22 field after 5 cycles (axis 2 is loading direction) which compared to the experimental surface observation. It can be seen that these two classical indicators almost cannot predict the possible position of the crack initiation, especially the local stress.
The Socie and Fatemi (SF) critical plane criterion was first proposed in 1988 as follows [28]:

$$\frac{1}{2} \Delta \gamma_{max} (t_1 - t_2) \left( 1 + k \frac{\sigma_n}{\tau_2} \right) = \frac{\delta f}{G} (2 \cdot N)^{\delta y} + \gamma^*(2 \cdot N)^{\delta y}$$  \hspace{1cm} (5)

In this criterion, two indicators, maximum shear strain amplitude on 12 slip systems $\Delta \gamma_{max}$ and normal stress on the slip plane with maximum shear strain amplitude $\sigma_n$ are taken into account. The right hand side in equation (5) contains the number of cycles to crack initiation, $N$, and some material dependent constants: $\delta f$ is the shear fatigue strength coefficient; $\delta y$ is the shear fatigue strength exponent; $\gamma^*$ is the shear fatigue ductility coefficient; $\delta y$ is the shear fatigue ductility exponent; $G$ is the shear modulus.

Figure 5(b and c) give the simulation fields of maximum shear strain amplitude on 12 slip systems $\Delta \gamma_{max}$ and normal stress on the corresponding slip plane. They are compared to experimental surface (Figure 5(a)). The results show that the real fatigue crack initiated at the sites where significant maximum shear strain amplitude takes place. This can partly verify that micromechanical shear strain amplitude is essential for crack initiation and high values in the grain may lead to the crack initiation. Meanwhile, we can see from Figure 5(c) the crack can initiate at the position where normal stress is not quite significant. However, from the crystal plasticity point of view, it is clear that a positive normal stress can increase the distance between the atomic planes in the structure, which facilitates the shear loading to cause damage.
Furthermore, formulating the fatigue criterion with the value taken at the maximum extreme points in the cycle may present a limitation. The same extreme points can correspond to different families of fatigue loops which have distinctly different shape and area. So in some recently proposed energy-based fatigue criteria [29-32], plastic strain energy as an important metrics is taken into account, which depends on the deformation history including the combination of shear stress and shear strain values at all points in the stabilized loop:

\[
W(x)_{cycle} = \sum_{\tau} \int_{cycle} \tau : \gamma^2 dt
\]

where \( T \) is the total number of active slip systems, \( \tau_s \) is the current critical resolved shear stress on the s slip system, \( \dot{\gamma}_s \) is the shear strain rate, \( dt \) is the duration of load increment, and \( x \) refers to the location (integration point).

Figure 6 (b and c) show the functional values corresponding to SF criterion and plastic strain energy based criteria. By comparison with the surface observations (Figure 6(a)), it is clear that the points where crack initiation takes place are significantly associated with increased plastic strain energy and functional value of SF criterion. This result means that the slip-based and energy-based metrics would both be expected to have good predictive capabilities for crack initiation. It can also be noticed that these high local values are associated with strong gradients in crystal deformation, depending on local crystal orientation.

4 Conclusions

A polycrystal finite element model with realistic microstructures of 304L steel is applied under cyclic loading to study microstructural effects on fatigue crack initiation and to evaluate predictive capabilities of some micromechanical factors that can control the crack initiation in the grains. The local stress and strain, maximum shear strain amplitude on 12 slip systems, normal stress on the corresponding slip plane, plastic strain energy and functional value in SF criterion were calculated and analyzed in terms of their
suitability as the indicators for prediction of the crack initiation. The numerical field results were compared with the observation of specimen surface. Under constant ±220 MPa stress amplitude, among these simulated micromechanical factors, maximum shear strain amplitude and microscopic plastic strain energy were found to provide comparable level of predictive ability. The SF criterion also showed good correlation and sensitivity to experimental crack initiation site.

Acknowledgements

This research is supported financially by Carnot C3S and CSC. The authors would like to thank EDF research center for supplying the materials studied in this work. The assistance of N. Roubier during the fatigue tests and the help of F. Garnier for SEM observation and EBSD measurements are gratefully acknowledged.

References


