Fatigue 2010

Fatigue crack initiation modeling of 316LN steel based on non local plasticity theory

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Received 8 March 2010; revised 12 March 2010; accepted 15 March 2010

Abstract

Numerous studies have pointed out the major role of microstructural phenomena in the nucleation of intra-granular crack nucleation during low cycle fatigue tests. Complex dislocation arrangements and rearrangements have been observed and different dislocation structures such as vein, ladder and/or cell structures have been identified in cyclically loaded steel specimens. These dislocation structures are related to a heterogeneous localization of plastic strain which is mostly accommodated by ladder structure of dislocations, also named Persistent Slip Bands (PSBs). These regions of intensive slip generate on the material surface intrusions and extrusions called Persistent Slip Markings (PSMs). The emergence of this rough relief leads to the initiation of fatigue cracks and is commonly seen as the first sign of fatigue damage. For a better understanding of fatigue crack nucleation in 316LN stainless steel, interrupted low cycle fatigue tests with constant loading amplitude were carried out on cylindrical specimens with polished shallow notches. Observations have been made at different stages to monitor the specimen surface. Development of PSMs and the initiation of fatigue cracks were observed. In parallel a three-dimensional finite elements model of crystalline plasticity, named CristalECIP, has been developed in both ABAQUS\textsuperscript{TM} and CAST3M\textsuperscript{TM} finite elements codes. Compared to classical approaches, the hardening law has been modified to take into account a physically motivated measure of lattice incompatibility. This measure is introduced through Geometrically Necessary Dislocations (GNDs) which are directly related to the gradient of the lattice distortion and supposed to model the resistance to plastic flow provided partially by lattice defects and grain boundaries. The numerical studies performed on various polycrystalline aggregates of 316LN steel have shown that the inverse relationship between the macroscopic plastic flow stress and the grain size can be reproduced. An influence of the grain size on the localization of the computed mechanical fields has been observed.

Keywords: Low cycle fatigue; 316LN stainless steel; persistent slip bands; persistent slip markings; crystalline plasticity; lattice incompatibility; geometrically necessary dislocations

1. Introduction

Fatigue micro-crack process in crystalline materials has been a subject of research for more than a century. The first studies relating surface relief evolution during cyclic straining to fatigue damage is attributed to Ewing and
Humfrey [1]. Their observations performed with an optical microscope on polycrystalline iron loaded in reverse bending pointed out an inhomogeneous localization of surface damage within bands of intensive slip, later named Persistent Slip Bands (PSBs). During the last fifty years, numerous experimental studies have been conducted to understand the mechanisms evolved in fatigue crack initiation [2, 3, 4]. TEM observations enabled the identification of different dislocation structures (veins, ladder or cells structures) induced by cyclic straining. The ladder structures of dislocations that form PSBs are composed of dense walls of edge dislocations separated by dislocation free channels. They are believed to carry out approximately a hundred times higher plastic strain than the surrounding matrix vein structure and that principally due to the motion of screw dislocations within channels [5]. The detailed knowledge of these ladder structures yielded to well-known models of surface relief formation based on point defects formed by dislocation interactions in PSBs [6, 7]. Recent combination of modern techniques, such as SEM, EBSD and AFM, enabled precise crystallographic and topographic characterizations and quantitative analyses of surface relief evolution [8, 9, 10, 11]. Emergence of PSBs at the material surface induces extrusions and intrusions, called Persistent Slip Markings (PSMs), in which fatigue intra-granular fatigue cracks initiate. The appearance of PSMs on an initial flat surface of fatigued materials is commonly considered as the sign of fatigue damage.

Although the principal mechanisms leading to fatigue crack nucleation were identified, effects of microstructure (grain size and grain orientation for example) remain unclear. For a better understanding of surface damage in 316LN stainless steel, interrupted low cycle fatigue tests with a constant loading amplitude of $\Delta \varepsilon/2 = 0.5\%$ and 0.3% were carried out on cylindrical specimens with polished shallow notches. The surface relief evolution was monitored during cycling with the help of a long distance microscope and after cycling with SEM and EBSD analyses as well as AFM measurements. In this range of loading amplitude, fatigue cracks nucleate either in grains (within PSMs) or at grain boundaries, but preferentially in grains [11]. Thus, our experimental study focuses on the development of PSMs and intra-granular fatigue crack.

In parallel for a better understanding of strain and stress localization, a model of crystalline plasticity, based on large plastic deformation theory and named CristalECP, was developed and implemented in the finite elements codes ABAQUS® and CAST3M® [12, 13, 14]. The activation condition of the flow rule is given by the criterion of Schmid. The viscoplastic law, used in the model, is related to the theory of thermally activated dislocation glide. The hardening is introduced by describing the evolution of dislocation densities and dislocation interactions between the different slip systems. In this work, classical approaches [15] were extended to take into account Geometrically Necessary Dislocations (GNDs) directly related to the gradient of the lattice distortion. They correspond to a physical measure of lattice incompatibility and model the resistance to plastic flow partially provided by lattice defects and grain boundaries [16, 17]. Low cycle fatigue simulations were performed on different 3D polycrystalline aggregates.

2. Low cycle fatigue tests

2.1. Experimental details

The austenitic 316LN stainless steel was supplied in form of a $600 \times 250 \times 60\ mm^3$ rolled plate in the frame of the ANR project AFGRAP. The heat treatment consists of austenitization between $1050\ ^\circ\ C$ and $1150\ ^\circ\ C$ and water quenching. The chemical composition can be seen in Table 1. EBSD analyses showed an average grain size of 50 $\mu m$ (found using the area averaging method of the TSL-OIM® software), an isotropic texture and less than 0.1% of residual ferrite $\delta$.

In this work, results obtained during two interrupted low cycle fatigue tests are examined. The cylindrical specimens used have with a gauge diameter and a length of 8 mm and 16 mm, respectively. Two shallow notches were machined at both sides of the gauge by wire electrical discharged machining. Each notch area was mechanically and electromechanically polished to achieve a smooth surface and facilitate the surface relief observation. The specimens were cycled in a symmetrically push-pull cycle in strain control. For the first test, a strain amplitude of $\Delta \varepsilon/2 = 5 \times 10^{-3}$, equal to the half of the hysteresis loop width, was kept constant during the whole period of the fatigue test. For the second test, a strain amplitude of $\Delta \varepsilon/2 = 3 \times 10^{-3}$ was fixed. Both specimens were cycled under a constant rate of $5 \times 10^{-1}\ s^{-1}$. During straining, the surface of the shallow notches was monitored with the help of a long distance microscope QUESTAR QM200®. The fatigue test carried out at $\Delta \varepsilon/2 = 5 \times 10^{-3}$
was interrupted for observations at the end of the cyclic hardening, at the end of the cyclic softening, at 1/2 of the fatigue life and after specimen failure. It corresponds respectively to 20, 200, 3000 and 6000 cycles. The fatigue test carried out at $\Delta \varepsilon/2 = 5 \times 10^{-3}$ was interrupted for observations at the end of the cyclic hardening, at the end of the cyclic softening, at 1/3 and at 2/3 of the fatigue life. Before straining, the crystallographic orientations of the grains of a selected notch area were analyzed by EBSD measurements. After each interruption, these areas were investigated by using a high resolution SEM-FEG Leo\textsuperscript{TM} 1530 and an AFM Nano I (Pacific Nanotechnology).

### Table 1. Chemical composition of 316LN austenitic stainless steel.

<table>
<thead>
<tr>
<th>Element</th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cr</th>
<th>Ni</th>
<th>Mo</th>
<th>Nb</th>
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<th>Ti</th>
<th>Cu</th>
<th>B</th>
<th>Co</th>
<th>N</th>
<th>Fe</th>
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<td></td>
<td></td>
<td></td>
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<td></td>
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</tr>
<tr>
<td>Maximum wt. %</td>
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<td>2.0</td>
<td>0.5</td>
<td>0.025</td>
<td>0.01</td>
<td>18</td>
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<td>0.01</td>
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<td>0.05</td>
<td>0.08</td>
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</table>

#### 2.2. Observation of surface relief

In this paper, we will focus on the results of the EBSD measurements and SEM observations made on the specimen cycled with strain amplitude of $\Delta \varepsilon/2 = 5 \times 10^{-3}$. An EBSD analysis was carried out on a selected area of the polished shallow notch. The EBSD map has a size of $1400 \times 1400 \mu m^2$ (step size 1 $\mu m$) and contains 1169 grains. In this area, the development and the evolution of the PSMs in 12 chosen grains was analyzed via SEM observations. The observed PSMs have been compared to the plane traces associated to the 12 slip systems $\{111\} <110>$. The Schmid factors of these slip systems have been determined by considering each grain as ‘free’ single crystal and the activity of each slip system has been evaluated between the different straining sequences.

At the end of the cyclic hardening (20 cycles), thin PSMs are present in the 12 studied grains. They are located either near grain or twin boundaries (grain 2 in Fig. 1) or in the grain interior (grain 1 in Fig. 1). Their orientation corresponds exactly with the plane trace of one I2 slip systems $\{111\} <110>$ (Fig. 1). Among the 12 grains, 9 exhibit only PSMs with one unique orientation. In 7 of them, the orientation of the PSMs corresponds with the plane trace containing the slip system with the highest Schmid factor. In 3 of them, PSMs are located near grain or twin boundaries and in the 4 other grains they are localized in the middle of the grain. Two grains exhibit PSMs with an orientation which corresponds to the plane trace containing the slip system with the second highest Schmid factor. In these two grains, the PSMs are localized at grain or twin boundaries. 3 grains show two different activated slip systems. The orientation of PSMs corresponds to the plane trace containing the slip systems with the two highest Schmid factors. Those associated to the primary system are located near grain or twin boundaries in two grains and in the interior of the grain in the other. Those associated with the secondary slip system are located near twin or grain boundaries. On the micrographs, the observed PSMs seem to have some features in common with the slip steps observable after unidirectional straining. The AFM measurement performed on these studied grains after 20 cycles confirmed a clear tendency for hilly extrusions. These results are in agreement with those obtained by Man et al. [9, 10]. The in situ observations made during the first cycle with the long distance microscope showed the development of thin dark lines in some studied grains at those locations where the hilly extrusions were later observed. This phenomenon was also observed in our previous study [13, 14] and shows that PSMs are formed at the very beginning of fatigue life. Hunsche et al. [18] identified on fatigued copper single crystals tensile and compressive slip steps where hilly extrusions developed later. These observations are in good agreement with the thin lines identified with the long distance microscope during the first cycle and the similarities between the PSMs observed after 20 cycles and the slip steps observed after unidirectional straining.

During the cyclic softening (after 200 cycles), PSMs have increased in size and number but still exhibit for most of them features of slip steps characteristic of unidirectional straining. PSMs already present at 20 cycles in the middle of a grain and associated to a primary slip system increase in width and height and spread in the whole grain (grain 2 in Fig. 1). These PSMs associated with a primary slip but only present near twin or grain boundaries after 20 cycles show the same tendency. The PSMs associated to the secondary slip system and present near twin or grain boundaries at 20 cycles can either have a very small activity or develop in size and number but in this case their activity is limited to the region close to the grain or twin boundary where they first appeared.
At the half of fatigue life (after 3000 cycles), PSMs are well developed and cover the whole grain. Most of them are equidistantly spaced and the width varies from about 100 nm to about 1 μm. The PSMs which developed during the cyclic softening continue their extension (grain 1 and 2 in Fig. 1). In the grains only marked by PSMs associated with a primary slip system, a secondary slip system can be activated near grain or twin boundaries forming new PSMs. It must be noticed well developed PSMs associated to different slip systems and present in the same grain are located in two distinct regions of the grain. In the 12 studied grains, only one or two slip systems are activated, except for one grain well oriented for multiple slip. This grain was marked by embryonic PSMs associated to the secondary slip system and located at a grain boundary. After 3000 cycles, it exhibits PSMs which correspond to three different plane traces. SEM observations also show that PSMs can have a tendency to agglomerate forming region of intensive slip of a few micrometers width. These regions are marked with intrusions and extrusions whose orientation corresponds to the plane trace associated to the slip system with the highest Schmid factor. Two initiated fatigue cracks have been identified in the studied area. These cracks are mixed cracks. They are initiated either at twin or grain boundaries and propagate in PSMs or in PSMs and propagate at twin or grain boundaries.

![Fig. 1. Evolution of PSMs during low cycle fatigue test at a straining amplitude of Δε/2 = 5 × 10⁻³. The crystalline orientations were measured by EBSD before cycling and PSMs were observed at 20, 200, 3000 and 6000 cycles (embryonic PSMs identified at 20 cycles are marked with white lines for both studied grain).](image-url)
Specimen failure occurred nearly 6000 cycles. The principal crack is located within the gauge length but just beside the polished notch. Between the half of fatigue life and the specimen failure, PSMs present in the 12 studied grains have increased in width but the surface density of PSMs has remained quite stable. These observations are in agreement with the observations of Polak et al. [8]. Their study of PSMs evolution in 316L stainless steel cycled with different plastic loading amplitudes revealed that the majority of the PSMs are formed during the first 20% of the fatigue life. During the rest of the fatigue life the surface density of PSMs remain more or less unchanged. They showed that the majority of the PSMs are formed during the first 20% of the fatigue life. After failure, the initiated fatigue cracks present on the surface of the whole polished shallow notch were studied by SEM. Most of cracks observed are well developed mixed cracks. 4 regions were identified as regions where fatigue cracks nucleate preferentially. These regions are PSMs located within a grain, grain or twin boundaries, PSMs present near grain or twin boundaries and growing tangentially to the boundaries and grain regions delimiting areas marked by PSMs associated to two distinct slip planes.

3. Modeling

3.1. Model description

3.1.1. Description of the basic model

The model of crystalline plasticity CristalECP is based on the large deformation theory proposed by Pierce et al. [19] and uses the modified hardening rules proposed by Teodosiu et al. [15]. Implemented in the finite elements codes ABAQUSTM and CAST3MTM, this model has shown great abilities to capture the characteristics of single and polycrystals deformation during monotonic and cyclic loadings with a good agreement between computation and experiments [12]. The numerical scheme used is an explicit forward gradient procedure which provides a sufficient accuracy and a high integration speed. The model was implemented for BCC, FCC and SC lattice structures.

For FCC crystals, which are the crystals of interest, slip occurs respectively on the 12 systems \( \{111\} <110> \). The glide velocity \( \dot{\gamma}^s \) for each slip system (s) is expressed with a classic viscoplastic rule based on of the resolved shear stress \( \tau^s \) and the critical resolved shear stress \( \tau^c_\varepsilon \):

\[
\dot{\gamma}^s = \dot{\gamma}_0 \left( \frac{\tau^s}{\tau^c_\varepsilon} \right)^n \text{ if } \left| \dot{\gamma}^s \right| \geq \tau^c_\varepsilon, \quad \dot{\gamma}^s = 0 \text{ otherwise.}
\]

(1)

Where \( \dot{\gamma}_0 \) is a reference shear rate and n is a rate sensibility exponent. The activation condition of this viscoplastic law is given by the criterion of Schmid. As long as slip occurs, hardening is caused by the interaction between different active or latent slip systems. This is modeled by the following phenomenological relationship between the critical shear stress increment on a slip system and all the slip increments weighted by the hardening matrix \( h^{\alpha} \):

\[
\tau^c_\varepsilon = \sum_{\alpha} h^{\alpha} |\dot{\gamma}^\alpha|.
\]

(2)

The \( h^{\alpha} \) terms are derived from relationship accounting for physical aspects of plasticity and based on internal variables such as dislocation densities on each slip systems. On a particular slip system, the dislocation density \( \rho^s \) is governed by a production term derived from Orowan’s relationship and balanced by an annihilation term which takes into account the dynamic recovery during deformation:

\[
\dot{\rho}^s = \left| \frac{\dot{\gamma}^s}{b} \right| \left( \frac{\sum \rho^s}{K} + \frac{1}{D - g_\varepsilon}, \rho^s \right) \text{ with } \rho^s (t = 0) = \rho_0.
\]

(3)
Where $b$ is the Burgers vector magnitude, $g_c$ is proportional to the annihilation distance of dislocation dipole, $K$ is a material parameter and $D$ grain average size. The critical resolve shear stress can be related to the dislocation densities by the following hardening rule:

$$\tau_c^* = \tau_0 + \mu b \sqrt{\sum_i \alpha_i^c \rho_i^c}.$$  \hspace{1cm} (4)

Where $\tau_0$ is a lattice friction stress and $\mu$ the isotropic shear modulus and $\alpha_i^c$ is a hardening matrix whose terms depend on the type of elastic interactions between dislocation families $(s)$ and $(t)$.

### 3.1.2. Introduction of GNDs

A great number of non-local theories have recently been formulated to address strain gradient and grain size effects, mostly based on continuum mechanics concepts. Significant numerical studies based on treatment of the solid as a Cosserat continuum were carried out by Muhlhaus et al. [20] and Forrest et al. [21]. In these models, material flow stress is assumed to be controlled not only by the slip rate but also partially by the material curvature. Gradient theories involving higher order stresses were developed by Fleck et al., Gurtin et al. or Lele et al. [22, 23, 24]. These formulations require, in addition to the introduction of higher order stresses, appropriate boundary conditions which leads to rather complex boundary value problems. Our work is based on the continuum crystal plasticity theory developed by Acharya et al. [16]. As they pointed out, the lattice distortion is not in general compatible with a deformation while it is capable of representing certain lattice imperfection associated with GNDs. The measure of lattice incompatibility was introduced in our previously described model by adding a GND density in the evolution law of dislocation density like Beaudoin et al. [17].

The total deformation gradient $F$ can be decomposed into elastic part $F^e$ and plastic part $F^p$.

$$F = F^e + F^p.$$  \hspace{1cm} (5)

If we consider a closed, continuous lattice circuit $C$ enclosing the area $A$ on a slip plane with normal $n^i$ in the current configuration, we can define the cumulative Burgers vector $b^c$ which represent the closure failure associated with this circuit in the reference lattice as:

$$b^c = \oint_C (F^{-1})^{-1} dS = \iint_A \text{curl}(F^{-1}) \vec{n}^i dS = \iint_A \Lambda \vec{n}^i dS.$$  \hspace{1cm} (6)

Where $A$ is Nye’s GND density tensor [25]. In their work, Acharya et al. [16] have clearly linked $A$ to a measure of lattice incompatibility. Another approach can also be adopted by expressing lattice incompatibility through the spatial derivative of $F^p$ (Busso et al. [26]). Cermelli et al. [27] have shown that both approaches are equivalent. Considering that elastic stretching is small, $A$ can easily be simplified:

$$\Lambda = \text{curl}(F^{-1}) = \text{curl}(R^e).$$  \hspace{1cm} (7)

Where $R^e$ corresponds to the elastic rotation. Nye’s tensor $A$ can then be projected on each slip system $(s)$. The results of this projection are new sources of GND density $\lambda^r$ for each slip system $(s)$, representing the slip plane lattice incompatibility. $\lambda^r$ is then introduced in the evolution of dislocation density Eq. (3):

$$\rho^r = \frac{\rho^s}{b} \left( k_0 \lambda^r + \frac{1}{L^r} g_c \rho^r \right) \quad \text{with} \quad \lambda^r = \sqrt{\left(\Lambda \vec{n}^i\right):\left(\Lambda \vec{n}^i\right)} \quad \text{and} \quad \rho^r(t = 0) = \rho_{0r}.$$  \hspace{1cm} (8)

Where $k_0$ is a material parameter to determine. This parameter is called the non local parameter the following.

### 3.1.3. Computation of GNDs

The simulations have been performed with 8-node linear elements with full integration (in ABAQUS™ C3D8 elements). At the end of each time increment, an explicit procedure computes Nye’s tensor $A$ from Eq. (7) for the
next time increment. The elastic rotation $R^e$ is extrapolated to the corner nodes by using linear shape functions associated to the type of element chosen here. $A$ is then computed back to the integration points from the spatial derivatives of the shape functions. The GNDs density $\lambda$ associated to each slip system $(s)$ is finally determined from Eq. (8) by projecting Nye’s tensor $A$ on each slip systems.

3.2. Application

3.2.1. Simulation procedure

The simulations results described in the following section were obtained with computations performed on 3D aggregates realized with an EBSD map of $900 \times 900 \mu m^2$ containing 732 grains (Fig. 2 (a)). This EBSD map corresponds to a part of the EBSD map realized before cycling on the shallow notch of the specimen cycled with $\Delta e/2 = 5 \times 10^{-3}$ studied in the previous section. The aggregates are meshed, as mentioned previously, with 8-node linear elements with full integration and respect the real texture and morphology of the material. The material parameters used are given in Table 2 and were identified by Medina Almazán [28]. The boundary conditions were chosen to approximate the boundary conditions of an aggregate contained on the surface of the shallow notch of a specimen (Fig. 2b).

To evaluate the impact of GNDs on the mechanical field localization, 3 aggregates were built. The first aggregate respects the original grain size ($GS = 50 \mu m$) of the material. The EBSD map was meshed with an element size of $4 \times 4 \times 4 \mu m^3$ and the aggregate is composed of a piling of 4 same meshed EBSD maps. The second and the third aggregate were built in the same way but their sizes were multiplied and divided by 10 leading respectively to aggregate grain size of $GS = 500 \mu m$ and $GS = 5 \mu m$. For the 3 aggregates, the ratio element size / aggregate size remains constant. The simulations were carried with a non local parameter equal to 0 to neglect the effect of GNDs and $1 000 000$ to take into account the effect of GNDs (this second value was arbitrarily chosen).

Table 2 Material parameters of 316LN austenitic stainless steel [28].

<table>
<thead>
<tr>
<th>$C_{11}$ [GPa]</th>
<th>$C_{12}$ [GPa]</th>
<th>$C_{44}$ [GPa]</th>
<th>$a_0$</th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
<th>$\gamma_s$ [s$^{-1}$]</th>
<th>$n$</th>
<th>$g_c$ [nm]</th>
<th>$\tau_0$ [MPa]</th>
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<th>$D$ [nm]</th>
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<td>80</td>
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<td>7</td>
<td>45</td>
<td>$10^{12}$</td>
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</table>

Fig. 2. (a) aggregate of 316LN steel made with EBSD measurement performed on the studied area of the specimen cycled with a straining amplitude of $\Delta e/2 = 5 \times 10^{-3}$; (b) boundary conditions applied to the aggregate during the simulation.

3.2.2. Simulation results

Fig. 3 (a) represents the stress/strain curves of the 5th cycle for the different simulations performed. With $k_0 = 0$, no grain size effect is visible. With $k_0 = 1 000 000$, a clear inverse relationship between the macroscopic plastic flow stress and the grain size can be seen. The impact of GNDs inducing these grain size effects is all the more visible as grain size decreases. Between the simulations performed with $GS = 500 \mu m$ and $GS = 50 \mu m$, only a slight increase in hardening is visible on the stress/strain curve. Between the simulations performed with $GS = 50 \mu m$ and...
GS = 5 μm, the increase in hardening is more significant. As it can be seen on Fig. 3 (a), the stress/strain curves obtained with $k_0 = 0$ are similar to the stress/strain curve resulting from the simulation in which the GNDs have the less influence, i.e. the simulation performed with $k_0 = 1 \times 10^6$ and GS = 500 μm. More generally, Fig. 3 (a) shows that the shapes of the hysteresis loops obtained per simulation are quite similar to the experimental one even though the stress is overestimated and the entry in the plastic domain occurs earlier for the specimen than for the aggregates. This phenomenon can be easily explained. Since no kinematic hardening is implemented in CristalECP, the model cannot reproduce the Baushinger effect to which the material is subjected. By passing, the material parameters used here can be adjusted for a better fit because they were identified for a 316L stainless steel which exhibits a quite different mechanical behavior.

When the aggregate grain size varies, the impact of GNDs can also been seen on the strain and stress distributions. A decrease in the aggregate grain size leads not only to an increase in the stress mean value as it can be seen on the stress/strain curves (Fig. 3 (a)), but also to an increase in stress heterogeneity (Fig. 3 (b)). When GS = 500 μm, the mean value of $\sigma_{11}$ is equal to 403 MPa after 5 cycles and the standard deviation is equal to 123 MPa. When GS = 5 μm, they reach respectively 485 MPa and 131 MPa. The influence of GNDs is less evident for the strain distributions. However, a reduction of the aggregate grain size leads to a decrease of strain heterogeneity (Fig. 3 (c)). The standard deviations of $\epsilon_{11}$ after 5 cycles are respectively equal to 0.00181 and to 0.00167 for GS = 500 μm and GS = 5 μm. These tendencies are in good agreement with the fact that for a fixed strain level, fine grains exhibit higher stresses than coarse grains. If GNDs are neglected, an increase or a decrease of aggregate grain size has no influence on the distribution curves (Fig. 3 (b)-(c)).

Fig. 3 (b) and (c) also show the influence of the non local parameter when the aggregate grain size is fixed. An increase in the value of $k_0$ leads to an increase in stress mean values and stress heterogeneity. For GS = 5 μm and $k_0 = 0$, the stress mean value of $\sigma_{11}$ is equal to 403 MPa and the standard deviation to 122 MPa after 5 cycles. When $k_0 = 1 \times 10^6$, they reach respectively 485 MPa and 131 MPa. Concerning stress fields, an increase in the value of $k_0$ leads to a decrease in strain heterogeneity. For GS = 5 μm, the standard deviations of $\epsilon_{11}$ after 5 cycles are respectively equal to 0.00181 and 0.00168 for $k_0 = 0$ and $k_0 = 1 \times 10^6$.

![Fig. 3. (a) stress/strain curves of the 5th cycle obtained with the different simulations performed (the stress/strain curve of specimen cycled with a straining amplitude of Δε/2 = 5 × 10⁻⁵ was plotted as reference); (b) distribution of the strain $\epsilon_{11}$ of the surface element layer after 5 simulated cycles; (c) distribution of the stress $\sigma_{11}$ of the surface element layer after 5 simulated cycles.](image)

The results of the finite elements simulations show a strong heterogeneity of the computed mechanical fields. A comparison of the stress field $\sigma_{11}$ of the surface element layer between the simulations performed with the aggregate having a grain size of 500 μm and 5 μm, and a non local parameter equal to 1 × 10⁶ is presented in Fig. 4 (a). The strain field $\epsilon_{11}$ computed after 5 cycles for the surface element layer of the aggregate with GS = 50 μm and $k_0 = 1 \times 10^6$ can be seen in Fig. 4 (b).

After 5 cycles, i.e. after a same imposed deformation, the aggregate with GS = 5 μm exhibits clearly higher and more heterogeneous stress concentrations than the one with GS = 500 μm. These results are in good agreement with the analysis of stress distribution curves. For GS = 5 μm, the stress values $\sigma_{11}$ of the aggregate surface layer spread
between 110 and 1130 MPa while they lay between 40 and 990 MPa for GS = 500 μm. As previously pointed out, grain size effects are also less visible for strains. However, aggregates with coarse grains exhibit slightly more heterogeneous and more localized strain fields than aggregates with fine grains.

Fig. 4. (a) comparison of the stress field $\sigma_{ij}$ of the surface element layer after the 5th cycle between the simulations performed with $k_0 = 1\,000\,000$ on the aggregate with a grain size of $GS = 500$ μm (left) and the aggregate with a grain size of $GS = 5$ μm (right); (b) strain field $\epsilon_{ij}$ of the surface element layer after the 5th cycle for the simulation performed with $k_0 = 1\,000\,000$ on the aggregate with a grain size of 50 μm (the development strain concentrations forming bands of deformation in some grains are visible in the black boxes).

In our previous studies, aggregate grains exhibit after 10 cycles strain localizations in bands [13, 14]. This phenomenon can also be observed after 5 cycles when GNDs are taken into account. It is definitely less visible due to the smaller number of simulated cycles but strains begin to concentrate in some grains forming bands of deformation.

4. Conclusions

The observation of 316LN stainless steel surface during interrupted low cycle fatigue tests enabled the monitoring of PSM formation and development. The markings caused by the emergence of PSBs at the specimen surface corresponds to the trace plane of the $\{111\} <110>$ slip systems. In most of the studied grains, the PSMs present are attributed to the activation of one or two slip systems, the two systems having highest Schmid factors, except for one grain well oriented for multiple slip. PSMs are formed at the very begin of the low cycle fatigue tests. They increase in size and number during the 3000th cycle. But their density seems to be quite stable during the rest of the fatigue life. PSMs associated with the primary slip system generally extend during cycling and tend to cover the whole grain. Those associated with the secondary slip system are present near grain or twin boundaries. The activation of these slip systems can be attributed to the influence of the surrounding grains.

Concerning the simulations, the introduction of GNDs in CristalECP enables a great reproduction of grain size effects. The model shows a great ability in recreating an inverse relationship between the macroscopic plastic flow stress and the grain size. Moreover aggregates with fine grains exhibit more higher and more heterogeneous stress field localizations and more homogeneous strain localizations than aggregates with coarse grains. More generally, after 5 cycles, a strong heterogeneous localization of the computed mechanical fields can be observed with or without GNDs. Strain concentration begins forming deformation bands in some grains.

Acknowledgements

The authors would like to express their thanks to Dr. F. Curtit and Dr. J. M. Stephan from MMC department of EDF research center Les Renardières and ANR project AFGRAP for supplying the material used in this work. The assistance of N. Roubier from LMSSMat (École Centrale Paris) during the low cycle fatigue tests is gratefully acknowledged. A special thank goes to F. Garnier and J. De Jaeger from LMSSMat (École Centrale Paris) for their help during the SEM-FEG observations and the EBSD measurements. The authors are also indebted to CEA research center of Saclay and ANR project AFGRAP for financial support.
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