Cyclic behavior of 316L steel predicted by means of finite element computations

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Abstract

The cyclic behavior of 316L steels is predicted based on crystalline elastoplastic constitutive laws. Calculations are performed with the finite element software CAST3M, using a polycrystalline mesh where the individual grains are modeled as cubes, having random crystallographic orientations. At the grain scale, the constitutive law parameters are adjusted using single crystal cyclic stress strain curves (CSSCs) from literature. Calculations are performed for different loading conditions (uniaxial tension-compression, biaxial tension-compression and alternated torsion) and a large range of three remote plastic strain amplitudes. We obtained 3 close macroscopic CSSCs. Somewhat lower stresses are obtained in torsion, particularly at high plastic strain amplitude. Our results are in agreement with all the published experimental data. The mean plastic strain is computed in each grain, yielding a particular polycrystalline mean grain plastic strain distribution for each loading condition and remote plastic strain. The plastic strain scatter increases for decreasing macroscopic strains. The number of cycles to the first micro-crack initiation corresponding to the aforesaid plastic strain distributions is then calculated using a surface roughness based initiation criterion. The effect of the different loading conditions is finally discussed.

Keywords: PSBs; cyclic behavior; polycrystal; CSSCs; number of cycles to micro-crack initiation;

1. Introduction

One of the materials used in nuclear power plant piping system is the austenitic stainless steel 316L (chemical formula: Fe, <0.03% C, 16-18.5% Cr, 10-14% Ni, 2-3% Mo, <2% Mn, <1% Si, <0.045% P, <0.03% S). The piping system forms a set of circuits of hot water and cold water, inducing the phenomenon of thermal fatigue. Moreover, thermal fatigue is close to a bi-axial loading [1]. Under thermal fatigue, surface areas can show networks of cracks. In earlier papers [1] [2], predictions of micro-crack initiation were already proposed showing the interest of crystalline modeling. Never the less, a rather large number of adjustable parameters were often used. Our 3D simulations are based on crystalline cyclic elastic-plastic constitutive laws [3] which parameters are adjusted on only single crystal CSSCs and finite elements computations (software CAST3M). Finite element calculations based on crystalline cyclic plasticity are performed on the polycrystal
mesh using three types of loading: uni-axial tension-compression, bi-axial tension-compression and alternated torsion. At the macroscopic scale, the cyclic strain stress curves (CSSCs) are computed and plotted for the three types of loading. It is shown that the loading type influences only weakly the macroscopic material behavior. At the microscopic scale, the distributions of mean grain plastic strain amplitude are interpreted by plotting cumulated probability of the mean grain plastic strain. The different mean grain plastic strain distributions depend strongly on the macroscopic plastic strain amplitude. Furthermore, a micro crack initiation model [4] based on the extrusion of the persistent slip bands (PSBs) and depending on the cyclic mean grain plastic strain range is used for the prediction of the number of cycles to the first crack initiation.

2. Polycrystalline model hypothesis

2.1 Crystalline elastoplastic constitutive laws

The 316L steel is a face-centered cubic alloy. Each crystal/grain, contains twelve slip systems (\{111\}<110>). During a cyclic loading at low plastic strain amplitude, one of the twelve slip systems is activated firstly in well-oriented grains due to their higher Schmid factor values (close to 0.5). Others oriented for multiple slip (with a lower Schmid factor) still deform elastically. Crystal is considered as a single slip structure (only one slip system is allowed). In the model proposed by Sauzay and co-workers [3][13], the standard crystallographic triangle is divided in two domains using a simple criterion. If the ratio between the secondary and primary resolved shear stresses, \( \frac{\tau_2}{\tau_1} \), is lower than a critical value, \( r_{\text{crit}} \), the grain is considered as oriented for single slip (figure 1). A higher criterion value corresponds to grains oriented for multiple slip.

![Fig. 1. two domains of orientations corresponding to either single slip or multiple slip.](image)

A simple Armstrong-Fredericks kinematic hardening type law is used. It was indeed shown experimentally that cyclic hardening of single crystals is mainly caused by kinematic hardening [5]. On each slip system, the hardening law is written as:

\[
\dot{x}_i = C \left( \frac{2}{3} A \dot{\gamma}_i^p - x_i \dot{\gamma}_{\text{cum},i}^p \right)
\]

with \( x_i \) and \( \gamma_i^p \) the kinematic resolved shear stress and the plastic slip for the \( i^{th} \) slip system. For each orientation domain, two parameters, \( C \) and \( A \), should be adjusted as well as the initial critical shear stress, \( \tau_0 \) which is the same for the two domains. The parameters \( C \) et \( A \) (simple and multiple slip) can be easily adjusted using the single crystal CSSC obtained for either the single slip orientation \( \{1\bar{4}49\} \) or the multiple slip orientation \( \{1\bar{0}00\} \) at room temperature [3]. Activation of the \( i^{th} \) slip system occurs if:

\[
|\tau_i - x_i| = \tau_0
\]
with \( \tau_i \) the corresponding resolved shear stress. Finally, grains oriented for single slip should deform on a single slip system only and the critical ratio, \( r_{\text{crit}} \), is adjusted using dislocation arrangement maps [3].

2.2 Finite elements computations

A typical mesh of 125 cubes shown in figure 2(a) is used in our finite elements computations. The set of the 125 cubes forms a polycrystalline mesh of 125 grains. Random crystallographic orientations are distributed to the grains, and the same material parameters are used in all grains. According to the literature [3], this sample of 125 grains can properly model the whole polycrystal without any effect of the number of grains of FE. For computing grain crack initiation number of cycles, it is necessary to localize the positions of the surface grains. The numbering is shown in figure 2(b). Following the direction of the axe Z, each grain is named by a number as shown in figure 2(b).

Fig. 2. (a) mesh of a polycrystal made of 125 cubic grains. Each of them contains eight CUB8 finite elements (b) numbering of the grains (c) a sample for boundary conditions (see text).

The boundary conditions can be explained using Fig. 2(c). For the uni-axial tension-compression loading, the surface 1 is blocked in the X direction, while a negative or positive displacement along the X-axis imposed to the surface 2. For bi-axial tension-compression loading, the surface 1 is blocked in the X direction and the surface 4 is blocked in the Z direction, and similar displacements (the same positive or negative sign) are imposed to the surfaces 2 and 3 respectively. Finally for alternated torsion, the surface 1 is blocked in the X direction whereas the surface 4 is blocked in the Z direction, and a displacement along the X axis is imposed to the surface 2 and an opposite one along the direction Z for the surface 3. Additional node displacements are blocked in order to avoid any rigid body motion.

2.3 Model of micro crack initiation

The experimental studies related in the literature [6] show different sources of cracking and 75% of them are due to the extrusion of PSBs such as shown by Ma and Laird [7]. The crack is observed to be parallel to the PSB plane. The prediction of micro-crack initiation is based on the extrusion growth kinetics [8]. Dislocation Dynamics modelling is one of the methods for predicting extrusion growth [9]. The kinetics of individual extrusion growth can be computed analytically, based on many previous dislocation dynamics computations. The number of cycles to micro-crack initiation obtained can be expressed as:
where \( N_i \) is the number of cycles to micro-crack initiation in the considered grain, \( D_g \) the surface grain diameter, \( h_g \) the grain depth and \( \Delta \epsilon_p,eq \) is the mean grain equivalent plastic strain range. The dimensionless parameter \( K \), scales with the cumulated cross-slip probability per cycle and per unit of cyclic plastic strain. The ratio, \( D_g / h_g \) is equal to 1 because of the cubic grain geometry. The \( K \) value is obtain by Discrete Dislocation Dynamics calculations [6]: \( K \approx 0.5 \). The \( \gamma_{lim} \) value is the critical slip of the PSB leading to the initiation of micro crack, which can be expressed as:

\[
\gamma_{lim} = \frac{d_b}{h_b \cos(\alpha)}
\]

where \( d_b \) is the critical extrusion height leading to micro-crack initiation whatever the PSB orientation and \( h_b \) is the PSB thickness. \( \alpha \) is the angle between the Burgers vector and the direction perpendicular to the free surface. Following the experimental study based on atomic force microscopy: \( d_b \approx 250 \text{ nm} \) [8] and \( h_b \approx 500 \text{ nm} \) [10] for the 316L steel in air and at room temperature.

3. Results

3.1. Macroscopic CSSCs and mean grain plastic strain distributions for the three different cyclic loading types

The macroscopic behavior is first discussed. For each loading, various strain amplitudes are imposed in the computation for predicting the macroscopic CSSCs. Figure 3 (a) show the amplitude of macroscopic Von Mises stress as function of the amplitude of macroscopic Von Mises plastic strain for uni-axial tension-compression, bi-axial tension-compression and alternated torsion. The three CSSCs in figure 3(a) are rather close. And Figures 3(b),(c),(d) present comparisons between the calculated and the experimental CSSCs. Our calculations agree well with these data. For the same level of macroscopic stress amplitude, the torsion loading leads to the highest level of macroscopic plastic strain amplitude and the uni-axial tension-compression loading to be the lowest.

Then the cumulative probability as a function of the normalized mean grain plastic strain is presented in figure 4, which shows the mean grain plastic strain scatter. In figure 4 (a), the mean grain plastic strain scatter increases for decreasing macroscopic plastic strain amplitude. Considering the curves in figure 4 (b), the different standard deviation curves show that the distribution of the mean grain plastic amplitude in alternated torsion and bi-axial tension compression are more homogeneous than in the uni-axial tension-compression loading. In other words, after a uni-axial tension-compression loading test, relative higher levels of mean grain plastic strain amplitude are reached in some grains. Therefore uni-axial tension-compression loading is relatively unfavourable on the point of view of micro-crack initiation.
3.2 The number of cycles of the micro-crack initiation

The number of cycles to the first surface micro-crack initiation is obtained by combination of expressions (3) and (4). By the finite elements computations, the mean grain plastic strain range can be calculated, which is needed in our calculation procedure. The results are presented in figure 5, the number of cycles to the first surface micro-crack initiation decreases with the macroscopic plastic strain amplitude increasing for the three loading types. Especially, the three curves is almost similar at the higher plastic strain amplitude, but for a lower plastic strain amplitude, uni-axial tension compression loading leads to micro crack initiation firstly, bi-axial tension compression secondly and alternated torsion loading thirdly. The first micro-crack is initiated is grain N.72 for uni-axial tension-compression and bi-axial tension compression loading, and grain N.52 for torsion. Uni-axial tension-compression loading is relatively unfavourable. The results agree with the remark mentioned in 3.1.
4. Conclusion

The macroscopic plastic strain comparison is obtained by the CSSCs. Somewhere lower stresses are obtained in torsion, particularly at high plastic strain amplitude. The mean grain plastic strain scattering distribution is related to the macroscopic plastic strain level, the plastic strain scatter increases for decreasing macroscopic strains. Finally, the number of cycles to initiation micro-crack verifies the prediction at the macroscopic scale. But our results are greatly influenced by the grain orientation, for a comparable result, we chose homogeneously the grain orientations. Depended on our predictions, the uni-axial tension compression is the most relative unfavorable loading. Work is in progress for investigating the effect of a higher number of surface grains on crack initiation and crack network formation.

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References