

論文の内容の要旨

論文題目 Microstructure-sensitive modeling for the prediction
of fatigue performances in structural steels
(構造用鋼の疲労性能予測のための微細構造を考慮した
モデリング)

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The work presented in the dissertation focuses on the fatigue behavior in low-carbon steels from a microstructure-sensitive point of view using the crystal plasticity finite element method.

A literature review on the fatigue problem in metallic single crystals and polycrystals is presented in the first chapter. The various sources of scattering in high-cycle fatigue as well as its statistical treatment, especially using the extreme value theory, are first discussed. The review continues by describing the mechanisms and existing models related to the formation and early propagation of fatigue cracks. The models are mainly based on the local mechanical fields at the grain scale (plastic strain, shear stress); microstructural and crystallographic attributes (grain size, twist and tilt angles). In this regard, the recent trend for the application of these models is based on microstructural mechanics through the explicit modeling of polycrystalline aggregates and the evaluation of mesoscopic field using finite element method coupled with crystal plasticity models for the elasto-plastic behavior at the crystal level. The evaluation of a fatigue criterion, often referred as fatigue indicator parameter (FIP) is mainly based on a critical plane approach in which the criterion on discrete crystallographic planes. The current limitations regarding the modeling of synthetic aggregates, crystal plasticity models and methods for the evaluation of FIPs are finally raised.

The second chapter focuses on the characterization and modeling of the materials studied in this work from a microstructural aspect. The chemical and metallurgical characteristics of the low-carbon steels are first presented. The microstructural attributes of the three steels numerically studied in the last chapter are

then extensively investigated by EBSD analyses. It is shown that polycrystals with a single scale of heterogeneity can be well characterized using an ellipse fitting process. However, EBSD measurement of multi-scale materials such as martensitic steels requires initial data processing to separate and accurately quantify the different scales of heterogeneity. Several original procedures are developed in this work to generate synthetic polycrystalline aggregates based on elliptic seeds and a novel anisotropic tessellation taking into account the shape and orientation of the grain. A framework is also described to generate martensitic microstructures based on sequential multi-scale tessellations. The reproduction of the crystallographic texture follows existing algorithms. The developed methods are finally validated by comparing experimental and synthetic EBSD image. It is shown that the anisotropic tessellation is capable of reproducing experimental grain boundary with a relatively high confidence and the proposed framework can generate synthetic aggregates statistically similar to the experimental ones.

The mechanical behavior of the different steels under cyclic conditions is experimentally investigated in the third chapter. At first, low-cycle fatigue experiments are conducted at constant applied strain amplitudes and fully reversed uniaxial tension-compression conditions. The cyclic stress response of most of the materials reveals three phases commonly reported in literature: cyclic hardening for ten to hundred cycles, softening up to half-life and a stabilization of the cyclic stress-strain curve until the final failure. The effect of the thermal treatment pattern is analyzed by studying the strain-life behavior and comparing the fracture surfaces of the different steels. It is found out that the first treatment pattern, leading to a significant increase in the grain size, reduces the cyclic ductility of the steels.

Numerical procedures based on homogenization and scale transition theories are then applied to calibrate the parameters of a phenomenological crystal plastic and an isotropic J_2 -plasticity model by inverse analysis on stabilized stress-strain hysteresis curves. A three-dimensional RVE constituted of 300 grains is modeled using Voronoi tessellation and cycled with the same conditions than in experiments, considering Periodic Boundary Conditions (PBC). As expected for similar parameters, the Taylor-Lin model overestimates the behavior of the materials as it represents the upper-bound of the average mechanical response.

The experimental study follows by load-controlled high-cycle fatigue experiments under fully reversed ($R=-1$) and positive stress ratio ($R=0.1$). The experiments are conducted on specimens including an elliptical notch to measure the

crack initiation lives and short crack growth rate of the different steels without significantly affecting both the fatigue strength and limit. A procedure is developed to record the specimen surface at regular interval using optical microscope. In most specimens, crack initiated from the notch on a random angular position and not always at the location of highest stress concentration factor. The numbers of cycles for crack initiation are recorded and do not reveal any clear trend when decreasing the stress amplitude or compared with the number of cycles to failure. Overall, crack initiation is randomly scattered between 20 to 60% of the total fatigue life of the specimen. The crack length is then plotted against the number of cycle and the crack growth rate is computed based on a standard polynomial reduction method in order to reduce the measurement errors. The crack growth rate is represented against the crack length and confronted to a typical long crack growth model based on the computation of the stress intensity factor of a semi-circular crack. In most specimens, an oscillatory behavior of the crack growth rate is observed, more particularly for large notch specimen where the average grain size is several hundreds of microns. In small notch specimen, after two to three oscillations, the crack growth rate follows that of long crack, which is confirmed by the investigation of the fracture surface revealing striations at about three grain size from the notch. These observations are different for large notch specimens where the crack growth rate is still heavily fluctuating close to the final failure. It is also confirmed by the observation of the fracture surface.

To further deepen the evaluation of the influence of the microstructure on short crack growth a quantitative study of crack path with EBSD analysis is conducted. It reveals that cracks mainly propagate transgranularly with few intergranular propagation due to the presence of small grains. Comparisons of slip traces with crack orientation suggest that short crack propagation is mainly crystallographic. However, the propagation is not always found to be on the slip system with the highest Schmid factor, suggesting that the local stress near the crack tip may play a significant role in the activated slip system. Also estimations of the twist and tilt angles at the grain boundaries were not attempted due to the lack of information on the 3D nature of the grain boundaries.

The last chapter is dedicated to the numerical simulation of polycrystalline aggregates under fatigue conditions. At first, FIPs for crack initiation, propagation and retardation based on empirical and theoretical models and methods for their evaluation are presented. To assess the predictive capabilities of the different criteria, three distinct numerical studies are conducted.

The first study is concerned with the evaluation of the possible influence of grain morphology and cold rolling texture on fatigue crack initiation. It is found out that describing a microstructure only in term of average grain size is insufficient as the grain size distribution can significantly affect the scattering in crack initiation lives. Accordingly, accurately reproducing a certain grain size distribution appears to be necessary to reliably assess the scattering in fatigue life. Also, the morphology of the grains as well as the cold rolling texture tend to improve the crack initiation lives and decrease its variability. Finally, the twist and tilt angles at the tips of the predicted cracks are evaluated. It is observed that while cold rolling texture provides better orientations against crack initiation, the low disorientation between neighbor grains may induce a lower resistance to crack propagation compared with random texture.

The second study aims to reproduce the geometry and boundary conditions of the fatigue experiments conducted in the third chapter by simulating notched polycrystalline aggregates representing α -iron and DP steel. The numerical models based on sub-modeling technique are first presented. Two types of simulation are conducted: with and without an initial crack. It is found out that even in presence of a notch, the microstructure is still strongly affected the mechanical response as grains far from the notch can experience similar or even higher strain than the ones in contact with the notch. This observation may explain why in some experiments, crack initiated outside the notch, especially when the grain size is much larger than the notch. The comparison of the inverse FIP for the two materials provides a relatively good prediction compared with experimental results. The simulation of cracked microstructures reveals that crack propagation is mainly predicted to occur on slip systems with relatively low twist angle and high plastic strain. A comparison of the inverse FIP for initiation and blocking time suggests that the number of cycles to overcome the first microstructural barrier may be of the same order of magnitude or even higher than for the nucleation of initial crack. An attempt is made to calibrate the FIPs with experimental results. It is concluded that predictions for high stress amplitudes are not conservative.

The last study focuses on the investigation of the strain localization in martensitic steel by simulating multi-scale polycrystals with and without block boundaries. It is noted that the amplitude of the plastic strain is similar in both cases due to the absence of size effect in the phenomenological crystal plasticity model. However, the distribution of plastic strain are significantly different suggesting that block boundaries should be considered in order to reproduce strain partitioning within martensitic grains.