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Microstructure modeling and crystal plasticity simulations for the evaluation of fatigue crack initiation in α-iron specimen including an elliptic defect

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ABSTRACT

In this study, fatigue crack initiation in pure α-iron is investigated through a microstructure-sensitive framework. At first, synthetic microstructures are modeled based on an anisotropic tessellation that accounts for the information of the grains morphology extracted from electron backscatter diffraction (EBSD) analysis. Low-cycle fatigue experiments under strain-controlled conditions are conducted in order to calibrate a crystal plasticity model and a J_2 model including isotropic and kinematic hardening. A critical plane fatigue indicator parameter (FIP) based on the Tanaka-Mura model is then presented to evaluate the location and quantify the driving force for the formation of a crack. The FIP is averaged over several potential crack paths within each grain defined by the intersection between a given slip plane and the plane of the model thus accounting for both the lattice orientation and morphology of the grain. Several fatigue simulations at various stress amplitudes are conducted using a sub-modeling technique for the attribution of boundary conditions on the polycrystalline aggregate models including an elliptic defect. The influence of the microstructure attributes and stress level on the location and amplitude of the FIP are then quantified and discussed.

1. Introduction

High-cycle fatigue (HCF) life and its scattering in metallic materials are mainly attributable to the dependency of the formation, early growth and interactions of small cracks with microstructural features. For a smooth specimen, in the absence of second phase inclusions, defects or local stress raiser such as a notch, fatigue damage mainly originates from irreversible plastic deformation located in slip bands leading to the formation of intrusions/extrusions at the surface [1]. The propagation or non-propagation of the newly formed microstructurally short crack (MSC) under single shear dominated mechanism is strongly influenced by microstructural barriers such as grain or twin boundaries [2–5]. When the crack reaches a sufficient length where multiple slips occur, the effect of the microstructure decreases and the crack mainly grows under mode I opening, also known as the Paris' regime, where linear elastic fracture mechanics (LEFM) applies. In most cases, a significant number of experiments have to be conducted to correctly measure fatigue performances, its inherent variability and identify the mechanisms responsible for the failure. Alternatively, predicting these performances can significantly reduce such investment and has become the subject of many recent studies.

With the improvement in computer performances, the recent trend towards the prediction of local damage process involves the explicit modeling of polycrystalline aggregates in so-called microstructure-sensitive simulations [6]. The evaluation of mechanical fields at the grain scale is often performed through full-field simulations such as the finite element method (FEM) or more recently by fast Fourier transform (FFT) [7] combined with a crystal plasticity (CP) constitutive model to capture the local deformation at the crystal level [8]. This method provides a flexible approach for linking the far fields imposed by the macroscopic structure with the micromechanical response of the grains in an aggregate. Compared with traditional homogeneous models where macroscopic fields are mainly used as a predictor, this approach grants the usage of mesoscopic fields in predictive models that give an insight of the damage mechanisms in the material. In the field of fatigue, the notion of fatigue indicator parameters (FIP) was therefore introduced by McDowell and Dunne [9] to link mesoscopic mechanical fields with driving forces responsible for the nucleation and/or growth of fatigue cracks. These FIPs are mainly based on critical plane approaches that use mechanical fields on individual slip systems.

For instance, Shenoy et al. [10] conducted a numerical study on Ni-base superalloy polycrystals in which a FIP based on the Tanaka-Mura model [11] was used to evaluate the incubation life while a FIP based on the Fatemi-Socie [12] was proposed for the MSC growth regime. It was later pointed out by Castelluccio and McDowell [13] in cracked single crystal simulations that such FIP could be well correlated with

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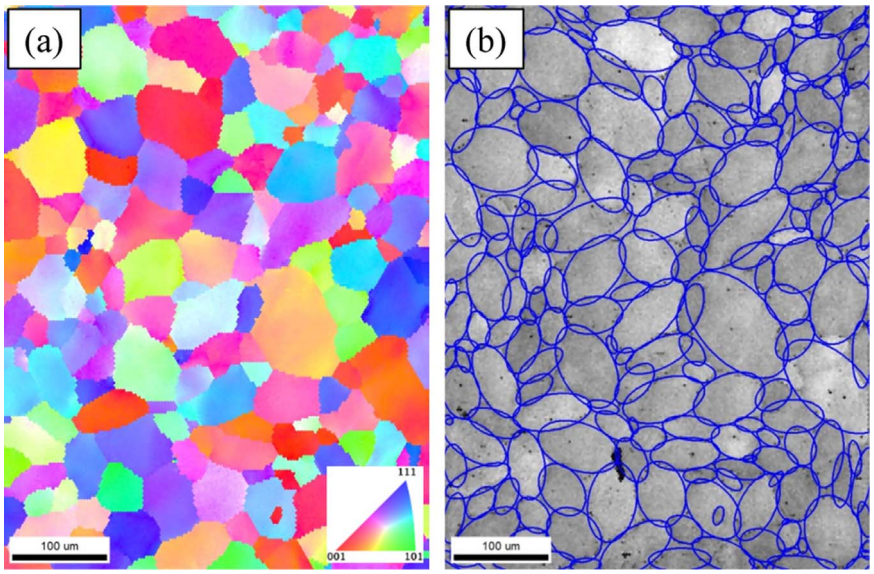

Fig. 1. (a) EBSD map of the pure α-Fe materials with IPF color coding. (b) IQ map of the pure α-Fe with ellipse fitted to each grain. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

the crack tip displacement range (ΔCTD) and therefore might circumvent the need to include an explicit crack in the microstructure in order to study MSC growth problems. In a more recent study, Castelluccio and McDowell [14] evaluated the influence of mesh refinement and averaging method to evaluate the Fatemi-Socie FIP. Three types of averaging methods were studied: local maximum, slip band averaging and grain volume averaging. It was concluded that volume averaging allows reducing the mesh dependency and need of refinement. Averaging over a certain slip band thickness appeared to be an interesting compromise providing additional information about the crack direction and sensitivity of intra-granular heterogeneity of local fields. Such a method is used in our study, transposed to two-dimensional models. From the observation that nucleation and small crack growth are not driven by average macroscopic field but by extremal values of local fields at the grain scale, Przybyla and McDowell [15–17] proposed the use extreme value theory. The Gumbel distribution was shown to fit with high confidence the Fatemi-Socie FIP even with as few as 25 simulations.

As opposed to homogenization studies whose aim is the average response of a representative volume element (RVE) to assess the macroscopic properties, microstructure-sensitive simulations are focused on the extreme variations of mesoscopic mechanical fields that will form the tail of a probability function of a given FIP. Therefore, the common strategy to assess the variability of a fatigue criterion requires the realization of a large set of polycrystalline aggregates that are said to be statistically representative of a material (SVE). In this regard, the reliability of the scattering prediction is directly affected by the quality of the models and their accuracy to represent a microstructure. While most of the realistic approaches rely on a direct importation of reconstructed microstructure from experimental measurements, it is maladjusted for fatigue simulations as several instantiations representing a given material are necessary to obtain statistical data. Accordingly, the use of procedurally constructed microstructures is still needed. Standard techniques to artificially generate a polycrystalline aggregate are often based on the use of simple polygons [18] or the tessellation of a surface or volume into geometric shapes that will represent the grains. Among them, the Voronoi tessellation is widely applied [19]. It is based on the partitioning of the space by the bisectors of a given set of seeds. The resulting cells present regular convex shapes with unique linear vertices between two adjacent cells. Poisson point process (PPP) that controls the positioning of seeds were shown successful to generate Voronoi tessellations with an objective of size distribution [20,21] but fails to catch higher order moment of statistical distribution of grain morphology [22]. Groeber et al. [23] proposed the use of multiple sequenced Voronoi tessellations where grains would consist of several adjacent cells. Alternatively, weighted tessellations such as the multiplicatively weighted Voronoi (MW-Voronoi) tessellation [24,25] or the Johnson-Mehl tessellation [26] directly consider the grain size objective by attributing a different weight to each kernel. The resulting cells are curved as opposed with the standard Voronoi diagram, with convex and concave edges. While the use of different weight ensures a correct grain size distribution, it was pointed out that the isotropy of the weight generates cells with high roundness so that they fail to reproduce the true morphology of the microstructure, especially when grains are elongated [27,28].

The proposed work is devoted to evaluate the fatigue crack initiation in pure α-iron specimen including an elliptic defect based on a microstructure-sensitive framework. The paper is organized as follows. In Section 2, a method to construct two-dimensional synthetic microstructures based on electron back scattering diffraction (EBSD) data and an anisotropic tessellation is presented. This method is proposed to circumvent the limitations found by previous researchers [27,28]. The constitutive models, low-cycle fatigue experiments, and material parameter identification are described in Section 3. The FIP based on the Tanaka-Mura model and the procedure for its evaluation is explained in Section 4. Finally, in Section 5, fatigue simulations are conducted on a set of microstructures including and elliptic defect and the FIP is evaluated. The predictive capabilities of the approach, as well as the influence of microstructural features on the FIP, are discussed.

2. Microstructure characterization and modeling

2.1. Microstructure characterization

The material investigated in this study is a high purity (99.5%) commercially-produced α-iron. To characterize the material in term of grain morphology and crystallographic orientations, SEM observations including EBSD analysis are conducted. A sample is cut, mechanically polished, ion beam cross polished and EBSD analysis is performed on an approximately $450 \times 600\ \mu m^2$ area with a sampling step size of 3 μm. Fig. 1(a) displays the EBSD map in inverse pole figure (IPF) color coding.