Computational Materials Science 94 (2014) 258–272

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Modeling the microstructure influence on fatigue life variability in structural steels

M. Sharaf *, P. Kucharczyk, N. Vajragupta, S. Münstermann, A. Hartmaier, W. Bleck

RWTH Aachen University, IEHK Steel Institute, Intzestrasse 1, 52072 Aachen, Germany

ARTICLE INFO

Article history:
Received 3 January 2014
Received in revised form 29 April 2014
Accepted 26 May 2014
Available online 30 June 2014

Keywords:
Crystal plasticity
Microstructure-sensitive modeling
High-cycle fatigue
Extreme value statistics
EBSD
Kinematic hardening

ABSTRACT

The endurance and HCF lifetime of multiphase steel components depend mainly on the phase of fatigue microcrack initiation and early propagation. A numerical study, which quantitatively describes the influence of microstructural features on the initiation and growth of cyclic microcracks, is presented within the context of microstructure-sensitive modeling. The implementation of kinematic hardening on each slip system in a crystal plasticity model allows for capturing the local accumulation of plastic microdeformation representing slip irreversibility occurring in the crack incubation phase. A load increasing testing technique with continuous temperature measurement and interrupted cyclic bending experiments deliver information about the endurance strength of a structural steel and allow for metallographic observation of cyclic microcrack propagation and thereby provide the experimental basis for the numerical simulations. The material model is implemented in cyclic computations with statistically representative volume elements, which are based on experimental microstructure description using the electron backscatter diffraction technique (EBSD). The extreme value distributions of the computed accumulation of local dislocation slip are then correlated to the microstructure in an approach to assess and explore the validity extent of microstructure-sensitive modeling using fatigue indicator parameters (FIPs) to correlate to the endurance limit and fatigue life under high-cycle fatigue conditions. The eligibility of consideration of the stresses normal to the planes of localized plastic damage assisting fatigue crack formation into these FIPs is investigated.

1. Introduction

In metals, all failure modes can be attributed to only five micromechanisms and their combinations: cleavage, ductile fracture, creep, fatigue and corrosion. Available statistical studies performed during a long-term performance of engineering components and structures confirm that fatigue, including corrosion assistance, is a leading cause of material failures [1]. From the engineering point of view, fatigue is therefore the most important damage process. However, for many of modern high strength steels, which have been developed in the last three decades [2,3], the endurance fatigue limit could not be increased as much as the yield strength, so that the safety assessment for cyclic loading conditions becomes the limiting factor for lightweight design efforts for many applications in civil and mechanical engineering [4,5]. From the micromechanical point of view, the fatigue process can be decomposed into four subsequent stages: crack incubation, stable short crack propagation, stable long crack propagation and unstable fracture [5–10]. We intend therefore to carefully distinguish in this work between crack nucleation and early growth from growth in later stages.

The precise estimation of endurance fatigue limit of steel is difficult, since fatigue experimental data always exhibit wide scatter bands. This dispersion is attributable to the anomalous behavior of cyclic microcrack initiation and growth in polycrystalline microstructure relative to that of physically short and long fatigue cracks [8,9]. It was shown in many cases that microcracks can nucleate after a relatively small number of cycles but often come to a condition where they cannot overcome microstructural barriers, e.g. grain boundaries, even for several million cycles under constant remote loading amplitude close to the endurance strength of the material [4,11–16]. These observations indicate the need for quantitative models which can reflect the influence of microstructure configuration on the variability of fatigue response. The mechanism of fatigue on a microscopic scale has been extensively investigated in many research studies by Mughrabi et al. [17–23] about persistent slip bands and various dislocation structures. However, these studies are more or less qualitative and are still too limited to render possible quantitative solutions of practical engineering

* Corresponding author. Tel.: +49 176 5667 8668; fax: +49 241 80 22112.
E-mail address: mohamed.sharaf@iehk.rwth-aachen.de (M. Sharaf).

http://dx.doi.org/10.1016/j.commatsci.2014.05.059
0927-0256/

problems [4,7]. They nevertheless certainly provide descriptions which support the understanding and hence modeling of cyclic microdeformation and mechanisms of microcrack nucleation and early growth. Together with the studies of Socie et al. [24–28], they indeed form a range of approaches for multiaxial fatigue loading applied at the grain scale and possessing intimate potential link to fine scale driving forces for crack nucleation and early propagation. McDowell and Dunne [7,29] discussed the latter point and emphasized the importance of such mesoscopic simulations to quantify the role of microstructure from the perspective of a frequency distribution of driving forces within grains of a polycrystalline ensemble. One main goal of their work was to use simulations to bridge the gap between that fatigue-related research stream concerned with dislocation substructure, slip offsets and progressive crack formation and another distinct body of work utilizing smooth specimen testing for prediction of fatigue life of components under various loading conditions. They characterized this branch of study as microstructure-sensitive modeling of fatigue processes. In the current work, the microstructure-sensitive modeling approach is adopted and further developed in extent.

The notion of statistically representative volume element (RVE) has been considered in many studies where bridging length scales was intended [30,31]. Here, Voronoi tessellation [32] was often employed for the construction of RVEs for micromechanical simulations [33,34]. Christ et al. [35] have recently generated duplex microstructures by a Voronoi-algorithm and analyzed the influence of the arrangement of phases on short fatigue crack propagation on the basis of boundary element computations. McDowell et al. utilized Voronoi tessellation within the framework of microstructure-sensitive modeling and could thereby quantify the effects of interactions between various microstructure attributes on fatigue life in the high-cycle fatigue (HCF) regime [36,37]. To our knowledge, the latter studies are distinctive and quite promising with regard to enhancing the depth of understanding the role of microstructure in minimum life of steels. However, although the microstructure investigated in most of the aforementioned works was highly heterogeneous and contained multiple phases, the statistical data used in the implemented Voronoi-algorithms did not distinguish between the different phases so that the statistical parameters of each individual phase cannot be altered. We point out the fact that the degree of heterogeneity of microstructure under study is to be sufficiently captured in the statistical distribution input to the algorithm generating its virtual representations, particularly when they are to be used for evaluation of the HCF response. In other words, even the higher order moments of the statistical distribution of microstructure attributes (e.g. grain size distribution of each phase) are to be represented by a RVE, not just the lowest order moments. In this aspect, we attempt a trial to construct the virtual microstructures used in the current study implementing the multiplicatively weighted Voronoi tessellation [38,39] and hence considering the statistical distribution of each phase of a ferritic–pearlitic microstructure.

For the simulation of microdeformations in the subgrain scale, the use of a material model that describes crystalline anisotropy, activation and evolution of crystallographic deformation mechanisms (dislocations, twins, etc.) as well as their interdependences becomes inevitable. There exist innumerable continuum-based variational formulations for describing the elastoplastic deformation of anisotropic heterogeneous crystalline matter. In a previous study, we presented an implementation of the extended finite element method (XFEM) to phenomenologically describe cyclic ferrite cracking [40] and pointed out the limitation of such an approach with respect to microstructure-sensitive analysis and the need for including a constitutive definition of crystal plasticity. A thorough review of available crystal plasticity FE models has recently been presented by Raabe et al. [41,42]. Buchheit et al. [43] investigated the limits of conventional crystal plasticity (e.g. incorporating grain boundaries, mesh sensitivity, absence of length scale effects) and discussed important issues regarding the choice of slip system hardening laws. Shenoy et al. [44,45] conducted a careful implementation of crystal plasticity for fatigue research and showed its applicability to microstructure-sensitive modeling. We apply in the current study a crystal plasticity model with kinematic hardening and present a procedure for calibration of its parameters via cyclic loading experiments.

For HCF loading conditions, the first few microstructural barriers control the fatigue limit and the scatter of life time. The modeling of microstructurally small crack growth is complicated by the physics of barrier interactions and the mechanics of addressing geometric and computational aspects of 3D cracks in complex microstructures [46]. In general, the irreversibility of dislocation slip has been shown to be the main driving force for fatigue crack formation (nucleation and limited microstructurally small crack growth) in metallic materials [17–23]. Fortunately, the use of a microdeformation mechanism-descriptive material model enables the computation of mesoscopic fatigue indicator parameters (FIPs) that reflect this driving force [7] and thereby facilitates the analysis of fatigue sensitivity to microstructure. These FIPs invariably appeal to the notion of slip irreversibility in linking to fatigue damage [7]. For example, the accumulated equivalent plastic slip has been shown to correlate well to experimentally observed microcrack initiation sites and directions as well as crack growth in a fcc nickel-base superalloy under plane stress low-cycle fatigue (LCF) conditions [47]. Furthermore, it can be argued that crack incubation and microstructurally small crack growth depend on local energy dissipation, as shown in some studies [48,49]. Fatemi and Socie [24] introduced an energy-like, shear-based parameter and showed a very good correlation to multiaxial fatigue crack initiation at the grain scale and above, in both LCF and HCF regimes. Li [50] has most recently confirmed the potential of the Fatemi–Socie parameter in qualitative crystal plasticity simulations using carefully conducted cyclic cracking experiments in which the 3D crack geometry was imaged by X-ray tomography. In our study, a comparison between the accumulated dislocation slip and a new local energy-like parameter is presented and the significance of the differences resulting from additional consideration of the stresses normal to the planes of localized plastic damage compared to slip accumulation as a FIP is discussed.

The strategy for computational HCF modeling should focus on extreme value statistics of potential sites for microplastic deformation localization since the target probability of failure is quite low (<1%) in most fatigue design scenarios [7]. HCF is consequently a localization problem of extreme value type. In contrast to the case for experimental characterization, it has been pointed out in previous fatigue-related studies [36,37,46] that the most relevant distribution of rare events of fatigue crack formation can be much more easily addressed through extreme value statistics of FIPs. In the current study, we adopt the ideas of extreme value sampling from classical extreme value statistics of Gumbel [51] and present fits of extreme value fatigue indicator parameter distributions.

The main target of the work presented in the current paper is to numerically predict the endurance limit of a ferritic–pearlitic structural steel in a microstructure-sensitive modeling framework and to assess and further develop the validity of this framework in correlation to fatigue life in the HCF regime. The authors intend to use this study as the basis for following quantification studies of the influence of the grain size distributions of each phase of the steel on the capability of its microstructure to develop cyclic microcracks. Thereby, the concept of microstructure-sensitive modeling of fatigue crack formation, extensively reviewed in McDowell's work [7,36], is applied. The metallographic analysis of the material under study as well as the characterization of its