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Microstructure based fatigue life prediction framework for polycrystalline nickel-base superalloys with emphasis on the role played by twin boundaries in crack initiation

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ABSTRACT

Fatigue crack initiation in polycrystalline materials is dependent on the local microstructure and the deformation mechanism, and can be attributed to various mechanistic and microstructural features acting in concert like the elastic stress anisotropy, plastic strain accumulation, slip-system length, and grain boundary character. In nickel-base superalloys, fatigue cracks tend to initiate near twin boundaries. The factors causing fatigue crack initiation depend on the material's microstructure, the variability of which results in the scatter observed in the fatigue life. In this work, a robust microstructure based fatigue framework is developed, which takes into account i) the statistical variability of the material's microstructure, ii) the continuum scale complex heterogeneous 3D stress and strain states within the microstructure, and iii) the atomistic mechanisms such as slip-grain boundary (GB) interactions, extrusion formations, and shearing of the matrix and precipitates due to slip. The quantitative information from crystal plasticity simulations and molecular dynamics is applied to define the energy of persistent slip bands (PSB). The energy of a critical PSB and its associated stability with respect to the dislocation motion is used as the failure criterion for crack initiation. This unified framework provides us with insights on why twin boundaries act as preferred sites for crack initiation. In addition to that, the computational framework links scatter observed in fatigue life to variability in material's microstructure.

1. Introduction

Fatigue scatter observed in components made of polycrystalline materials can be partly attributed to the variability of complex heterogeneities in the microstructure. These heterogeneities are responsible for the complex stress and strain fields developed under load, and govern where cracks could potentially nucleate. Empirical life prediction methods [1,2] cannot relate fatigue life to the variability in microstructure. Although there has been substantial work done in using advanced computational tools and experimental techniques to understand the driving forces for fatigue crack initiation, there is still a considerable amount of work to do in calculating fatigue scatter by explicitly taking into consideration the heterogeneities of a given material's microstructure and the complicated 3D stress and strain states that develop within the bulk of the material. The current work discusses a computational fatigue framework which fills this gap by linking virtual microstructures that resemble real material's microstructure in a statistical sense, to a fatigue life prediction model. This life prediction model within the fatigue framework defines crack initiation based on the stability of persistent slip bands (PSBs) as they interact with grain boundaries (GBs).

During fatigue loading, dislocations multiply and accumulate within the material resulting in an increased value of the dislocation density. These dislocations arrange themselves in the lowest energy configurations by forming clusters of dipoles [3–5]. As a consequence, strain is localized into thin slip bands called PSBs, which are precursors for crack initiation. In polycrystalline metals, PSBs consist of alternating high and low dislocation density zones, representing a ladder-like structure [6,7]. In precipitation hardened materials, like nickel-base superalloys, PSBs form as dislocations cut through the γ matrix and γ' precipitates in a planar slip manner

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[8,9]. Essman, Mughrabi, and co-workers have done extensive work in understanding strain localization in PSBs and establishing the formation of extrusions, intrusions, and microcracks due to interaction of PSBs with surfaces and GBs [6,7,10]. PSBs were observed to pass through low angle grain boundaries (LAGB) unhindered, where as they are impeded by high angle grain boundaries (HAGB). The PSB-HAGB interaction results in the formation of dislocation pile-ups, which increase stress concentrations at the PSB-GB interface, ultimately leading to the formation of microcracks [11]. The topic of PSB formation in polycrystalline metals and alloys has been discussed extensively in literature surveys [12–14]. The experimental observations pertaining to the structure of the PSB and its interaction with GBs are taken into consideration while formulating the energy of a PSB, whose stability will be used to define crack initiation in the fatigue framework discussed in the current study.

Microcracks were observed to nucleate at the twin boundaries (TBs) in certain FCC polycrystalline metals [11,15–17] and alloys [18–22]. Over the past three decades, studies have searched for an understanding of why TBs are preferred sites for fatigue crack initiation. Wang et al. used a finite element model on a bi-crystal with a TB and found that stress and slip enhancement is greatest in a small volume of material near the surface and close to the TB [23]. Peralta et al. calculated the compatibility stresses at TBs and varied the orientation of the loading axis to the TB [24]. They observed that the stress concentration at the TB is a maximum when the tensile axis is applied along a <111> direction. Neumann derived an analytical expression for the tractions at the intersection of a TB and a surface, and further emphasized that the observed slip activity and the crack initiation on planes parallel to the TB plane is not due to the compatibility stresses, but due to the logarithmic singular surface tractions that occur at the intersection of the surface with the TB [25]. In addition to simple bicrystal based models, which teach us about activity in the local neighborhood of a TB, high fidelity models that take into account heterogeneous deformation of twins and energetics of twin-slip interactions have also been developed.

Sangid et al. using molecular dynamics (MD) simulations, showed that coherent TB offers the lowest interface energy and highest barrier to dislocation nucleation and transmission, thus providing a significant strengthening contribution [26]. Further, Sangid et al. developed a microstructure-based model to predict fatigue crack nucleation in a nickel-base superalloy, U720, consisting of a high density of coherent TBs [22,27,28]. Their model, which takes into account the energetics of GBs and the interaction of PSBs with GBs, predicted that most often cracks nucleated at TBs in U720, which was also observed in experiments [22]. By calculating a fatigue indicator parameter in a crystal plasticity framework, Castelluccio and McDowell showed that large annealing twins are more detrimental than thinner deformation twins and stressed their importance [29]. Further, Cerrone et al. used gradient crystal plasticity in a finite element model of an experimentally measured 3D microstructure wherein a microcrack nucleated along a coherent TB in a nickel-base superalloy, LSHR [30]. From the crystal plasticity simulations, they hypothesized that high elastic anisotropy and coplanarity of the boundary plane with a {111} slip plane were responsible for the accumulation of slip and subsequently for the microcrack nucleation event at the TB. Each of the aforementioned analytical and computational models provide valuable insights into the role played by TBs on fatigue crack initiation in polycrystalline materials. But understanding why fatigue cracks initiate at twins from a lengthscale point of view is still lacking. The fatigue framework presented in the current study takes into account, the energetics of slip-twin interaction (calculated using MD), and the quantitative information from the complicated stress/strain states developed within the twin (obtained from crystal plasticity simulations) and uses this information in a failure prediction model. A focus of the current study (which explicitly considers TBs in the microstructure) is to understand the effect of elastic anisotropy, plastic strain accumulation and normal stress on crack initiation at twins.

Fatigue crack nucleation is a microstructure and deformation mechanism based phenomenon and a robust fatigue prediction model should consider contributions from various length scales. Although there has been substantial and important work done using crystal plasticity based models and MD simulations, the present work develops a framework, which unifies length scales (by considering both atomistic and continuum level contributions) with explicit consideration of microstructures. Such a high fidelity model helps us gain more insight into the most critical factors that contribute to crack nucleation and also link microstructure variability to scatter observed in fatigue life. This framework takes quantitative information of the heterogeneous deformation from crystal plasticity simulations pertaining to microstructure descriptions of 3D stresses and strains, energetics of slip-GB interaction, stacking fault and anti-phase boundary energies from atomistic calculations, to predict where cracks could potentially nucleate. Further, this framework explicitly includes twins in statistically equivalent microstructures (SEMs) that are built on the morphological and crystallographic statistics obtained from the real material's microstructure data. The present work also delivers insights on the evolution of elastic anisotropy and plastic strain accumulation at the GBs. The development of SEMs based on the microstructure of the material of interest is discussed in Section 2. Section 3 discusses the formulation of the PSB energy based, microstructure dependent fatigue framework. The integration of the results from crystal plasticity based simulations and the fatigue model of PSBs are discussed in this section. Section 4 includes results and discussion. Conclusions are presented in Section 5.

2. Material characterization and statistically equivalent microstructure (SEM)

A nickel-base superalloy, RR1000, developed by Rolls-Royce plc is used in this study. The material produced using powder metallurgy process underwent forging and was heat-treated above the γ' solvus (at 1170 °C) for 5 h [21]. RR1000 is a precipitation hardened material and the ordered γ' precipitates present in the material provide a strengthening mechanism and stability at elevated temperatures. The heterogeneities present in the microstructure are quantified based on experimental electron backscatter diffraction (EBSD) data. These complex heterogeneities govern strain localization within the material and affect fatigue life. Quantitative characterization of the microstructure provides information on grain size distribution, orientation distribution (to understand texture of the material), misorientation distribution (to spatially understand the neighbor orientations) and grain boundary character distribution of special type of GBs called coincident site lattice (CSL) GBs. Such a characterization not only helps in linking microstructure to properties but also provides benchmark statistics based on which statistically equivalent microstructures (SEMs) can be generated. SEMs are virtual microstructures, built to statistically represent the (morphological and crystallographic) heterogeneities of the microstructure of the material, as closely as possible, as well as the strength properties of the material (but not necessarily the extreme values for fatigue as discussed in Section 4).

In order to enhance the predictive capabilities of the microstructure based failure prediction model, the representation of the microstructure must capture the variability observed in the material. For this purpose, the statistics of the different morphological