



Simulated microstructure-sensitive extreme value probabilities for high cycle fatigue of duplex Ti–6Al–4V

Craig P. Przybyla^{a,b,*}, David L. McDowell^{b,c}

^a Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson AFB, OH, USA

^b Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia

^c George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia

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ABSTRACT

A newly developed microstructure-sensitive extreme value probabilistic framework to characterize the performance/variability for damage evolution processes is exercised to compare the driving forces for fatigue crack formation (nucleation and early growth) at room temperature for four different microstructure variants of a duplex Ti–6Al–4V alloy. The aforementioned probabilistic framework links certain extreme value fatigue response parameters with microstructure attributes at fatigue critical sites through the use of marked correlation functions. By applying this framework to study the driving forces for fatigue crack formation in these microstructure variants of Ti–6Al–4V, these microstructures can be ranked in terms of relative high cycle fatigue (HCF) performance and the correlated microstructure attributes that have the most influence on the predicted fatigue response can be identified. Nonlocal fatigue indicator parameters (FIPs) based on the cyclic plastic strain averaged over domains on the length scale of the microstructure attributes (e.g., grains, phases) are used to estimate the driving force(s) for fatigue crack formation at the grain scale. By simulating multiple statistical volume elements (SVEs) using crystal plasticity constitutive relations, extreme value distributions of the predicted driving forces for fatigue crack formation are estimated using these FIPs. This strategy of using multiple SVEs contrasts with simulation based on a single representative volume element (RVE), which is often untenably large when considering extreme value responses. The simulations demonstrate that microstructures with smaller relative primary α grain sizes and lower volume fractions of the primary α grains tend to exhibit less variability and smaller magnitudes of the driving forces for fatigue crack formation. The extreme value FIPs are predicted to most likely occur at clusters of primary α grains oriented for easy basal slip. Additionally, surrounding grains/phases with soft orientation shed load to less favorably oriented primary α grains, producing extreme value FIPs.

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1. Introduction

Variability of the fatigue life of engineered components arises from microstructure stochasticity. This is particularly true for the processes of fatigue crack nucleation and microstructurally small crack growth in ductile metallic material systems, which are driven by localized plasticity and the accumulation of dislocations against obstacles or the development of particular dislocation structures (e.g., persistent slip bands) (Suresh, 1998). In high cycle fatigue (HCF) of metals for which cyclic stress amplitudes are below the macroscopic yield stress, plasticity is quite heterogeneous and localized at microstructure

* Corresponding author at: Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson AFB, OH, USA.

E-mail addresses: cpri@gatech.edu, craig.przybyla@wpafb.af.mil (C.P. Przybyla).

attributes that raise the local stresses sufficiently to induce flow (McDowell, 1996), are favorably oriented for preferential yield, or both. Specific life limiting attributes can vary from specimen to specimen or from component to component due to the stochasticity of material microstructure. Thus, scatter in the HCF life of specimens or components depends on the extreme value probabilities of existing microstructure attributes that elevate the driving forces for fatigue crack formation, contributing to specimen and notch size effects.

1.1. Extreme value statistics and metal fatigue

Current methods that estimate fatigue resistance as a function of the extreme value statistics of microstructure are limited to distributions of a single microstructure attribute; these methods do not consider the effect of multiple interacting microstructure attributes on the extreme value response distributions (e.g., fatigue crack formation). For example, Atkinson and Shi (2003) reviewed various extreme value models that predict the fatigue resistance in clean steels based on the largest inclusions which control fatigue crack formation in these materials. The first class of models discussed is based on the log-normal distribution (or any standard distribution that considers the entire population) of inclusion size. Accuracy of these models, however, is limited by the experimental difficulty of correctly capturing the tails of the distribution for inclusion size because of the paucity of extreme value data. The second class of models discussed by Atkinson and Shi is based on the classical extreme value Gumbel (1958) distribution. For example, Beretta and Murakami (1998) used classical Gumbel extreme value statistics to estimate the size of the largest inclusion based on specimen volume, which was subsequently used to estimate fatigue strength. The third class of models is based on the generalized Pareto distribution. Atkinson and Shi argue that the generalized Pareto distribution is more effective than the two previously described methods because it incorporates a limit on the maximum inclusion size, whereas the extreme value Gumbel distribution predicts a monotonically increasing inclusion size for increasing volume of material sampled. However, it is very difficult to estimate the upper bound on this type of attribute. Additionally, all three model classes do not consider how interactions between the inclusion and surrounding matrix or microstructure affect fatigue performance. Although first order approaches based on a single microstructure attribute (e.g., inclusion size) may be sufficient for some material systems or applications, the process of fatigue crack formation in many advanced engineering alloys is often complex and depends on the influence of multiple interacting microstructure attributes. In some cases, multiple interacting microstructure attributes exert influence at different material length scales.

Some recent computational work has considered effects of multiple microstructure attributes on fatigue response. Liao (2009) used a Monte Carlo technique to instantiate volume elements of microstructure with distributions of particle size, grain size, and grain orientation that have been randomly sampled from experimental data with known distributions. These multiple microstructure instantiations are then used to simulate the variation in fatigue response in 2024-T351 aluminum sheets. The response was estimated using FEA with elastic constitutive laws. Fatigue-relevant attributes, including particle size, grain size and grain orientation, were identified in each simulated instantiation and the distribution of these attributes was considered. These fatigue-relevant attributes were selected a priori based on experiments. The results of this Monte Carlo method correlated well with methods based on extreme value statistics and with the experiments. However, as with the previous methods discussed, correlations between the important microstructure attributes relative to their influence on the driving forces for fatigue crack formation were neglected because each critical attribute was considered independent of the others.

1.2. Fatigue crack formation in duplex $\alpha + \beta$ Ti–6Al–4V

In this work, the processes of fatigue crack formation will be considered in duplex $\alpha + \beta$ Ti–6Al–4V. Experimental observations for Ti–6Al–4V support the hypothesis that fatigue crack formation in this material system is not adequately described by a distribution of any single microstructure attribute. Fatigue crack formation in $\alpha + \beta$ Ti alloys has been associated with slip as early as the 1960s by Wells and Sullivan (1969), who observed that cracks form along slip bands in the α phase of Ti–6Al–4V. However, confusion persists regarding mechanisms of fatigue crack formation in this material system. In short, it is not clear which specific microstructure attributes (or arrangements of attributes) is/are most important in the processes of fatigue crack formation. Relevant experiments that have investigated fatigue crack formation in $\alpha + \beta$ Ti alloys under typical cyclical loading conditions at room temperature are reviewed next.

In duplex $\alpha + \beta$ Ti alloys, the appearance of distinct facets in the primary α grains is commonly observed at sites of fatigue crack formation. In some cases, these facets are associated closely with basal planes oriented perpendicular to the uniaxial loading axis in Ti–6Al–4V (Bache and Evans, 2001; Bache et al., 2001). Bache (2003) argued that crack formation on basal planes in grains that are unfavorably oriented for slip is due to shear stresses induced by dislocation pileup on the grain boundary in adjacent grains oriented for easy slip. This mechanism, originally postulated by Strohh (1954), is thought to activate when a critical density of dislocations accumulate on the boundary such that the shear stresses in the adjacent grain (oriented for easy slip) are sufficient to induce slip on the hard oriented (i.e., nearly perpendicular to the loading direction) basal slip planes. Thus, under cyclic loading conditions a crack forms over many cycles in the hard oriented grain. This proposed mechanism is supported by the work of Baxter et al. (1996) who observed slip on basal planes oriented nearly perpendicular to the loading axis in IMI 834.

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