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Simulating the effect of grain boundaries on microstructurally small fatigue crack growth from a focused ion beam notch through a three-dimensional array of grains

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ABSTRACT

Microstructurally small crack (MSC) growth strongly depends on local microstructure and often displays oscillatory character in terms of crack growth rate (da/dN) as a function of the conventional stress intensity range due to crack tip/grain boundary interactions of MSCs. A fatigue indicator parameter (FIP)-based MSC growth model is presented for high temperature MSC growth in polycrystalline Ni-base superalloy IN100 that takes into account crack tip/grain boundary interaction. An expression for FIP evolution is evoked based on a sequence of finite element simulations for stationary cracks. The MSC growth model was fit to experiments within the context of a simple 1D crack growth model and then applied to model 3D crack growth from a simulated focused ion beam (FIB) notch. Simulations showed that the MSC growth rate became less oscillatory as the MSC front sampled more grains, and eventually converged to the LEFM response with further crack extension.

1. Introduction

Microstructurally small crack (MSC) growth in fatigue depends strongly on local microstructure. MSCs typically exhibit oscillatory crack growth rate (da/dN) as a function of the conventional stress intensity range (ΔK), based on remote applied stress. The oscillatory behavior is often attributed to the episodic retardation of crack growth by grain boundaries [1–3]. The character of the grain boundary (e.g., misorientation, tilt and twist angle, etc.) can have a significant effect on whether a MSC will accelerate, decelerate, or arrest at the grain boundary. The probability that a MSC will propagate past a grain boundary becomes very important for determination of MSC thresholds and for the accurate fatigue life prediction in the high cycle fatigue (HCF) to very high cycle fatigue (VHCF) regimes. Previous experimental methods [3–5] indicate that GB character is the major driving force for fatigue crack growth. However, conclusions from such studies have been somewhat qualitative, i.e., higher angle grain boundaries tend to hinder or arrest fatigue crack growth. Consequently, most MSC growth analytical models have been phenomenological in nature. Many are fit to macroscopic mean fatigue crack growth behavior and are limited when trying to predict scatter in MSC growth behavior based on microstructural features. The incorporation of GB twist angles and GB misorientation by Wen and Zhai [6] and Castelluccio [7], respectively, show promise to inform physically-based MSC growth models at the mesoscale. To create a more physically-based MSC growth law, features such as the current crack length relative to grain size, grain size, crystallographic orientation, and distance of the crack from the grain boundary should be accounted for. The objective of this work is to account for microstructure influence via a more physically-based MSC growth law to quantify scatter in MSC growth rate and fatigue life response. The approach taken here is based on the computational analysis of cyclic plastic strain distribution of the initially uncracked body, considering realistic microstructure. These analyses are used to estimate driving forces for MSC growth in the first few grains, based on a trained mapping algorithm for FIP/stress redistribution due to crack growth which is calibrated to detailed finite element simulations. This framework is then applied to a MSC growing from a simulated focused ion beam (FIB) notch in a coarse grain Ni-base superalloy fatigued at elevated temperatures. It is noted that this mapping algorithm approximation affords efficiency and differs from the recent works of

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Castelluccio and McDowell [8–10], in which fields are successively recomputed as the crack front moves through each grain to allow for redistribution of the mechanical stress, strain, and plastic strain fields.

1.1. Multistage fatigue life approach

Microstructure-sensitive modeling of fatigue life using a hierarchical multistage approach has become very popular in recent years [11–14]. Often the total fatigue life, N_T, of a component is decomposed into stages of fatigue crack formation and growth by Refs. [11–14], i.e.,

$$\begin{aligned} N_T &= N_{form} + N_{MSC} + N_{PSC} + N_{LEFM} \\ &= N_{form} + N_{MSC/PSC} + N_{LEFM} \end{aligned} \quad (1)$$

where N_{form} is the number of cycles required to form a fatigue crack of length, a_i, on the order of microstructure scale (grain or phase size). In Equation (1), N_{MSC} represents the number of cycles required for the initially formed crack of length a_i to propagate through approximately 3–10 grain or second phase sizes/spacings [13,14]. In the HCF and VHCF regimes, the propagation or non-propagation of MSC cracks past the first few microstructural barriers controls the fatigue limit and contributes to fatigue life scatter. For HCF and VHCF, a large portion of life (>90% [15,16]) is spent in the fatigue crack formation and MSC growth regimes, $N_{form} + N_{MSC}$.

Following MSC propagation, physically small crack growth (N_{PSC}) is considered up until the crack is of sufficient size so that linear elastic fracture mechanics (LEFM) is applicable. Physically small crack growth is characterized by the growth of a crack that is long compared to microstructure scale, yet does not conform to conditions for similitude because the cyclic crack tip plastic zone is on the order of grain/phase size. When the crack reaches a sufficient size (typically several hundred microns and above [14]) where the cyclic crack tip plastic zone and damage process zone are large compared to microstructure scale and the conditions of small scale yielding and similitude are met, then long fatigue crack growth behavior is applicable. In this regime, LEFM can be used to determine the number of cycles, N_{LEFM}, required for the crack to grow from several hundred microns to failure.

Since the variability in N_{form} and MSC growth contributes to the marked variability/scatter in fatigue life in the HCF and VHCF regimes, the main focus of this work is to develop a MSC growth law that takes into account microstructural barrier (specifically, grain boundary) effect on MSC growth. In the next section, we review previously proposed MSC growth laws.

1.2. MSC growth laws

In the MSC growth regime, microstructure effects dominate small crack growth. As cracks grow, the effect of microstructure on fatigue crack growth decreases and the MSC and elastic-plastic fracture mechanics (EPFM) regimes tend to merge into the LEFM growth curve when a condition of growth similitude is reached [17,18].

A sampling of simple phenomenological and micromechanical MSC growth expressions is shown in Table 1. For brevity, the commonalities of these expressions are discussed here and a more detailed consideration of each expression is covered in Ref. [19]. Regardless of the form, each MSC expression has several elements in common. First, a driving force for fatigue crack extension is expressed via the crack length (a in Eq. (2)), applied cyclic shear strain range ($\Delta\gamma$), applied normal stress range (σ_a^n), applied range of stress intensity factor (ΔK), or applied range of crack tip displacement ($\Delta CTSD$). Next, an expression for driving force intensification with crack extension is employed by application of a material-dependent exponent to the driving force or by multiplying the driving force by the crack length. Crack growth deceleration at grain boundaries is accounted for in Equations (2) and (3) by the ($d-a$) term where d is a microstructural parameter depending on the dominant microstructural barrier resisting MSC growth. Likewise, the bracketed expression in Equation (6) accounts for grain boundary deceleration of the MSC, where D is the grain diameter, X is the distance of the crack tip from the nearest grain boundary, m is a constant, and τ_A and τ_B are the resolved shear stresses in grains A (containing crack) and B (neighboring grain). The second term in Equation (7), $\eta b \approx \Delta CTD_{th}$, designates the threshold range of crack tip displacement below which irreversible crack tip extension does not occur, with η on the order of unity and b equal to the magnitude of the Burgers vector. Finally, each expression has a number of material constants denoted by capital letters A, B, C, and EPFM threshold D_{th}.

While these basic phenomenological MSC models (Equations (2)–(6)) can be used to correlate the mean small crack growth behavior, they cannot predict the scatter in MSC growth evidenced in experiments. Micromechanical MSC growth models (for example Equation (7)) can be used to predict the scatter in MSC growth, but require a means to compute local micromechanical forces driving crack extension. Hence, these micromechanical MSC growth models can be further enhanced with the crystal plasticity finite element method (CPFEM). Simonovski et al. [20–22] used 2D CPFEM simulations to determine the crack tip opening displacement (CTOD) ahead of the crack tip and found that crystallographic orientation has a significant effect on CTOD. Castelluccio and McDowell [7,8] used CPFEM to simulate a crack within a single crystal Cu subjected to mixed mode loading, with emphasis on the cyclic crack tip sliding displacement as a driving forces for Stage I MSC growth. They found that computed multiaxial Fatigue Indicator Parameters [12] (FIPs) were directly proportional to the cyclic crack tip sliding displacement, and hence can be used as a surrogate local driving force for fatigue crack propagation. These nonlocal FIPs are preferred since they are easily computed within a CPFEM scheme with sub-grain scale refinement. Musinski and McDowell [23] used CPFEM to estimate fatigue crack initiation and early propagation within smooth and notched IN100 specimens. The total fatigue life was estimated as the summation of crack formation life (N_{form}), MSC propagation life ($N_{prop,MSC}$) and LEFM propagation life (N_{LEFM}). Similar frameworks for mesoscale modeling of MSC growth in polycrystalline materials using CPFEM have been adopted by Castelluccio and McDowell [8–10]. This hierarchical model [8–10,23] is adopted and modified here to include grain boundary effects on MSC growth.

1.3. Fatigue crack growth in Ni-base superalloys

A brief discussion of fatigue crack growth mechanisms in Ni-base superalloys is presented first, as these mechanisms inform the manner in which fatigue crack formation and early growth processes are modeled in this work. A more detailed review of fatigue crack growth mechanisms in Ni-base superalloys can be found elsewhere [19].

The mode by which Ni-base superalloys fail in fatigue is primarily affected by temperature, grain size, the crack tip cyclic plastic zone size, environment, and the loading frequency. In general, the fracture surface tends toward more transgranular than intergranular character for lower homologous temperatures, larger grain sizes, smaller cyclic plastic zone (or crack) size, an environment with lower oxygen partial pressure, and higher (or no hold time) testing frequencies.