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A stored energy criterion for fatigue crack nucleation in polycrystals

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ABSTRACT

A series of microstructurally-differing, large-grained, notched, polycrystal BCC ferritic steel bend test samples have been analysed to extract the experimentally observed sites of fatigue crack nucleation together with the numbers of cycles to cause crack nucleation. The samples have been modelled with explicit representation of both grain morphologies and crystallographic orientations using crystal plasticity which has enabled a detailed assessment to be made of key microstructure-level quantities such as accumulated slip, slip rate, and densities of both statistically stored and geometrically necessary dislocations local to the experimentally observed sites of crack nucleation. These quantities when considered independently have not been found to correlate with experimentally observed cycles to nucleation.

A new criterion for fatigue crack nucleation has been introduced in which a critical stored energy density, G_c, is argued to be necessary in order for crack nucleation. The rate of stored energy density determined at the sites of crack nucleation has been shown to correlate well with experimental measurement of cycles to nucleation, and the number of cycles to cause fatigue crack nucleation, for the samples for which such measurements are available, is well predicted. The criterion enables prediction of cycles to crack nucleation for all of the experimental samples and has been shown to demarcate correctly the crack nucleation lives observed over the range of differing experimental microstructures.

1. Introduction

An area of fundamental importance in fatigue and fracture is the development of understanding to address the role of microstructural features in influencing, and in some cases determining, cycles to crack nucleation. Its importance in the prediction of fatigue limits of specimens and structures is discussed by, for example, Schijve [1]. Fatigue scatter is commonly witnessed in many experimental tests and recent examples include those in crack nucleation in AISI 310 stainless steel [2], in notched DZ951 DS Ni-based superalloy [3] and beyond 10^7 cycles to failure in Ni-based superalloy René 88DT [4]. The heterogeneities at the microstructural scale are now accepted as the key reason for the variation of fatigue life in alloys. For example, Sauzay and Jourdan [5] evaluated crack nucleation scatter from the influences of crystallographic orientation and anisotropy coefficient and argued that a key factor in the scatter originated from distribution of resolved shear stress. A whole range of fatigue indicator parameters (FIPs) and approaches have been studied to address crack nucleation and failure of polycrystal materials. These criteria include failure based on energy, stress or strain formulations and each of these approaches is assessed below. However, differing criteria are sometimes adopted depending upon the loading regime considered. Shi, Huang, Yang and Yu [6] used six different critical plane-based criteria to assess which of the individual criteria corresponded most closely to observed fatigue failure in their 2nd generation nickel-based superalloy (DD6).

Local stored energy is often adopted as a failure criterion, since it is argued that the formation of cracks is due to dislocation pile up and constrained plastic flow such that the stored energy eventually leads to the nucleation of a crack [7,8]. Early work addressing the development of slip and persistent slip band (PSB) formation, and their relationship with crack nucleation and free surface effects was addressed by Sauzay and Gilormini [9], and a detailed discussion of PSB formation as a precurser to crack nucleation and fatigue damage was reviewed in [10]. Sangid et al. [11–14] primarily consider an energy approach where PSB-grain boundary (GB) interaction in polycrystalline Ni was argued to govern fatigue crack nucleation. An atomistic-based energy barrier was introduced for slip transmission and dislocation nucleation along the GB, which evolves with increasing fatigue cycles. Slip and GB interaction were found to be focused in twin boundary regions where PSBs formed in large grains were found to play a more indicative

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role for predicting fatigue crack nucleation. It remains, however, a matter of discussion that PSB formation may, in some materials, require many cycles which may in fact form a significant fraction of the crack nucleation history.

Failure based on stress has long been considered at the macroscopic (i.e. without consideration of microstructural features) level. For example, the normal stress associated with a critical plane of maximum shear strain was considered by Fatemi and Socie [15]. The same approach considering maximum shear strain amplitude and maximum normal stress has also been assessed at the microstructural level in studies [16–19] which have shown that the shear-based parameter correlated well with multiaxial fatigue conditions, and sensitivity of crack nucleation for small crack growth in both low cycle fatigue (LCF) and high cycle fatigue (HCF) at the grain length scale. With this modelling approach, Wen and Zabaras [20] relied on four FIPs based on this criterion to assess a Ni-based superalloy subjected to cyclic loading. The focus was to address the significance of different particle features and their effects on the FIPs. Mughrabi [21] attempted to relate cyclic slip irreversibility with fatigue life, but through relations which incorporated two empirical fatigue ductility constants in their power law model. Normal components of traction were considered by Shanthraj and Zikry [22] at the microstructural level in which it was assumed that crack nucleation occurs once a critical fracture stress is achieved, based on the evolving orientation of cleavage planes. Their physically based model also considered the dislocation density evolution at the GB where transmission across it is dependent on block or pack boundaries, and random GB misorientation and microstructures were generated for arbitrary martensitic steel microstructures, but no direct comparisons with experimental observations were possible. Ghosh et al. [23,24] also used the normal traction component to quantify failure in their criterion for cold dwell fatigue in Ti-6242 alloy, but considered a mixed mode solution where the effective stress (on a grain badly orientated for slip) is also employed. The critical stress they incorporated is based upon the dislocation pile up which, it is argued, acts similarly to the presence of a crack that scales with the length of the pile up. The accumulation of dislocation pile up was associated with the fatigue cycles to nucleation, and predicted cycles to nucleation were found to be in good agreement with experimental observations. The criterion proved satisfactory for identifying fatigue crack nucleation sites and the corresponding number of cycles to nucleation in a polycrystalline aggregate material for wedge crack opening. Studies [25,26] based on this model showed that the critical crack nucleation parameter, which is calibrated from experimental data for failure, played a key role in correlating with experimental observations. The approach utilises an accelerated crystal plasticity FE method through use of wavelet transformation induced multi-time scaling.

The role of accumulated plastic strain or discrete slip system measures through their relationship with PSB formation are known to be precursors to fatigue crack nucleation at the microstructural length scale. The criterion adopted in Manonukul and Dunne [27], which addressed slip accumulation in random fcc polycrystals using a crystal plasticity model, showed that experimentally-observed cycles to fatigue crack nucleation for both low and high cycle fatigue conditions could be captured. Dunne, Wilkinson and Allen [28] carried out a combined experimental and computational crystal plasticity study of a directionally solidified (fcc) nickel-based superalloy with columnar grains undergoing bending fatigue. It was found that the location of the highest accumulated slip corresponded to the experimentally observed sites of both plane strain and free-surface, plane stress fatigue crack nucleation and growth. Subsequent studies [29] in a body-centred cubic (bcc) ferritic steel subject to bending fatigue have demonstrated that accumulated slip, and particularly rate of slip accumulation, are good indicators of crack nucleation site in a set of ten independent and different experimentally characterised microstructures. Hochhalter et al. [30] incorporated three damage criteria based on accumulated slip into their elastic–viscoplastic polycrystal constitutive model. The criteria were used to study nucleation from second phase particles in aluminium alloy, prior to microstructurally small fatigue crack growth. Their model showed linear slip accumulation for up to five loading cycles in the aluminium alloy considered, but Sweeney et al. [29] have shown that slip accumulation may not be linear with cycles and that the rate of slip accumulation varies profoundly with spatial position in the microstructure. While Sweeney et al. [29] discussed the role of elastic anisotropy, length scale and crystallographic slip in determining the site of crack nucleation, they did not address the cycles necessary for fatigue crack nucleation and observed in their experimental matrix.

Atomistic, discrete dislocation and crystal plasticity modelling have played major roles in understanding the micromechanics of fatigue crack nucleation in polycrystalline metals, and details may be found in [31–33]. Across the range of criteria which include stress, energy or strain-based methods at the microstructural level, there remains the need for quantitative predictive analysis methods for cycles to fatigue crack nucleation. Techniques have been proposed [9,11–14] which follow an explicit full field modelling in the context of PSB formation as a precursor to crack nucleation, for which a crystal plasticity model framework in its own right is not always able to capture the full detail of slip localisation, and subsequent PSB formation, particularly where the slip bands are at sub-micron level. However, the studies by Sweeney et al. [29] demonstrate the facility with which gradient-enhanced crystal modelling successfully captures the site of fatigue crack nucleation in multiple, differing microstructures and, with suitable refinement of meshing, also captures significant slip localisation. It is therefore argued that the same approach has merit in the development of predictive capability for cycles to crack nucleation, taking full account of the key microstructural features, and this is the subject of this paper.

Hence, we revisit our gradient-enhanced crystal plasticity framework which enables grain by grain detail of slip, geometrically necessary (GND) and statistically stored (SSD) dislocation densities to be determined, and allows these quantities to be assessed in the context of a matrix of experimental observations of microstructurally sensitive fatigue crack nucleation and short crack growth. We assess the importance, or otherwise, of these quantities in relation to key microstructural features and specifically, the known sites of crack nucleation observed in an experimental study in which the fatigue scatter witnessed in ferritic steel bend samples forms the basis for the present study [29]. The experimental work also provides measurements of cycles to fatigue crack nucleation which, in combination with the grain by grain gradient crystal model comparisons, allows a variety of criteria to be assessed in ranking the observed fatigue nucleation lives. Hence, finally, we propose a stored energy criterion, which is informed by information on local slip accumulation, densities of statistically stored and geometrically necessary dislocations, and stress, for the prediction of both site of crack nucleation, and quantitative predictions of cycles to crack nucleation in microstructure-sensitive fatigue.

2. Experimental background and computational methodology

In this section, a brief description of the experimental programme reported in [29] and carried out by Nippon Steel Corp (NSC) on ferritic steel, four-point bend, notched-beam samples is given. A schematic representation of the experimental set-up is shown in Fig. 1 in which a notched beam undergoing four-point