



# A combined grain scale elastic–plastic criterion for identification of fatigue crack initiation sites in a twin containing polycrystalline nickel-base superalloy



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## ABSTRACT

Damage initiation during cycling loading of polycrystalline metallic alloys involves localized damage at the scale of individual grains. To better understand damage processes and to build models for material behavior, there is a need for quantitative assessment of the microstructural configurations that favor fatigue crack initiation. In materials that form annealing twins during processing, these special interfaces are often locations of particular interest for their role in strain and damage accumulation. In the present study, fatigue experiments in the very high and low cycle fatigue regime on a René 88DT polycrystalline nickel-base superalloy were performed to statistically evaluate grain-scale features that favor crack initiation. Combined elastic and plastic criteria at the grain scale have been developed. A crack distribution function is defined to compare and assess the effect of the microstructural parameters for the two fatigue regimes.

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## 1. Introduction

Predicting fatigue crack initiation in polycrystalline engineering materials remains a major challenge due to the inherent sensitivity of the initiation process to the details of the microstructure. Under many realistic loading scenarios, the strain amplitude in fatigue cycling is relatively low, with the implications that (1) initiation consumes a large fraction of the overall cyclic life and (2) both the elastic and plastic properties of the material may strongly influence the initiation process. Furthermore, in materials that form annealing twins during processing (stainless steels and Ni, Cu, Al and Ag alloys), this feature of the microstructure is of special interest for its influence on fatigue damage development. Miao et al. [1,2] reported that cracks initiated in high Schmid factor grains with slip planes parallel to and slightly offset from coherent twin boundaries in the nickel-based alloy René 88DT under very high cycle fatigue loading. Crack initiation during cycling loading has been observed along twin boundaries for various other twin-containing materials including other nickel-base superalloys [1–3],

stainless steels [4] and copper [5,6]. Heinz and Neumann [7] first suggested that elastic anisotropy causes a local stress concentration that strongly enhances glide at twin boundaries. For the case of face centered cubic (fcc) coherent twins, the boundaries are always parallel to a slip plane, so dislocations can travel across the entire diameter of a grain, creating a stress concentration, particularly if the slip is localized on a single system. Heinz and Neumann [7] emphasized that these twins lead to stronger strain localization than a general grain boundary with oblique slip planes. Stein, Rollett, Ingraffea et al. [8,9] report very high stresses near twin boundaries when slip occurs parallel to twin boundaries using crystal plasticity models for superalloys. Stinville et al. [10], using sub-grain digital image correlation (DIC) measurements at the microscale, report local strain enhancement of a factor of 4–10 near these coherent twin boundaries during straining. A variety of microstructure parameters have been reported to contribute to cyclic strain localization and fatigue crack initiation at twin boundaries. Fatigue cracks have been found to initiate in grains at the high end of the grain size distribution in twin-containing materials during high cycle fatigue [1,2,11–13]. In addition, grains oriented favorably for slip (high resolved shear stress slip systems) are observed to initiate cracks [1,14,15]. Moreover, elastic anisotropy has been shown to induce significant stress heterogeneities from grain to grain [16,17],

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strongly influencing crack initiation, particularly at lower strain amplitudes [7]. Under low deformation amplitudes, Heinz and Neumann [7] have shown that fcc materials exhibiting relatively strong elastic anisotropy experience elevated shear stresses at twin boundaries, which ultimately triggers local plasticity and crack initiation. However, the contribution of each of these material features on the crack initiation process and their interplay remain unclear. A better understanding of the role of microstructural parameters in the development of fatigue damage in twin containing materials is crucial for the prediction of fatigue life and fatigue life variability.

The present study investigates the effects of microstructural configuration on fatigue crack initiation in a twin-containing material at room temperature for loading conditions in the low cycle and very high fatigue regime. Investigation of a large number of cracks initiating near twin boundaries has been performed with consideration of both microstructural and mechanical parameters. A combined elastic–plastic criterion at the grain scale is shown to predict locations of crack initiation near twin boundaries. In addition, a crack distribution function that statistically isolates grains most likely to initiate cracks is defined to compare and assess the effect of the microstructural parameters for the two fatigue regimes.

## 2. Experimental procedure

### 2.1. Material

The material tested in this study is the polycrystalline nickel-based superalloy, René 88DT. This production alloy is processed through a powder metallurgy route. The nominal alloy chemistry is: 13%Co, 16%Cr, 4%Mo, 4%W, 2.1%Al, 3.7%Ti, 0.7%Nb, 0.03%C, 0.015%B (weight percent) [18,19]. The microstructure of the alloy consists of a  $\gamma$  matrix and two populations of spherical gamma prime ( $\gamma'$ ) precipitates; including larger secondary  $\gamma'$  ( $\approx 100$ – $200$  nm in diameter) and nm-scale tertiary  $\gamma'$  (several nanometers in diameter). Due to the super-solvus nature of the solution anneal, the microstructure of René 88DT contains no sub-solvus  $\gamma'$ , which is usually termed primary [19]. The material possesses very weak crystallographic texture, a large population of  $\Sigma 3$  grain boundaries (58% of the total boundary fraction), and an average grain size of  $26 \mu\text{m}$ . Crystallographic features have been previously detailed (see Ref. [20]) using electron backscatter diffraction (EBSD) measurements.

### 2.2. Mechanical tests

Cyclic testing was performed in air at room temperature in the low cycle fatigue and very high cycle fatigue regimes. Low cycle fatigue tests were performed in a symmetric, uniaxial, push–pull mode on an electromechanical machine. Tests were carried out in stress control mode at maximum stress of 758 MPa, with a R-ratios of  $-1$  and  $0.1$  and a frequency of 1 Hz. Cylindrical specimens with a gauge diameter of 5 mm and gauge length of 16 mm were used in this study. Strain was measured by a mechanical extensometer positioned on the gauge. Interrupted tests were performed to enable crack density, crack size and sub-grain DIC measurements at different percentages of the lifetime. Very high cycle fatigue testing was conducted under fully reversed loading (R-ratio of  $-1$ ) using an ultrasonic fatigue instrument [36–40] operating at a frequency close to 20 kHz. Details of the ultrasonic fatigue testing technique can be found in Ref. [11]. Cylindrical ultrasonic fatigue specimens with a gauge diameter of 5 mm and a gauge length of 18 mm were used. After fatigue testing, specimen surfaces were examined using

scanning electron microscopy to identify regions exhibiting evidence of microcrack formation.

### 2.3. Sample preparation for EBSD, crack density and crack size measurements

EBSD measurements require the use of flat specimens. Therefore two flat areas, 2.5 mm in width and 8 mm in length, were machined on the gauge of selected fatigue specimens. The two flats were positioned on opposite sides of the specimen in the gauge section. Moreover, in order to obtain high quality back-scattered electron diffraction patterns, it was essential to remove any residual stresses in the surface layer due to sample preparation. This required removing a thin surface layer by electropolishing the samples in a solution of 10% of perchloric acid and 90% of ethylene glycol at 30 V. Finally, the gauge length of some specimens was etched with a Fe (III) chloride + HCL solution in order to produce a nm-scale speckle pattern which is favorable for sub-grain scanning electron microscopy digital image correlation (SEM-DIC) without interfering with EBSD measurements [21].

Crack density measurements were made on two flat surfaces with an investigated surface area of  $2.5 \times 8 \text{ mm}^2$  on each side of the specimen. Surface crack sizes were determined using secondary electron imaging and measuring the length of the entire path of the crack.

The geometry of the flat areas was designed to limit the potential stress concentration induced by the presence of edges produced during machining of the flat areas. In addition, careful mechanical polishing was performed to further reduce any local concentrations. This process resulted in crack densities and lifetimes that were indistinguishable in specimens with and without flat areas.

### 2.4. Sub-grain scanning electron microscopy digital image correlation

In-plane displacement fields at the microscopic scale were obtained using DIC open source software (OpenDIC) [22]. SEM (secondary electron microscopy) images ( $5120 \times 3840$  pixels) were divided into custom sized subsets of  $27 \times 27$  pixels regularly spaced by 17 pixels in both horizontal “X” and vertical “Y” directions. The correlation was based on the zero-normalized cross-correlation (ZNCC) criterion [23]. The correlation of each subset is fully independent from the correlation of neighboring subsets. Deformed images were interpolated by a factor 10 using a biquintic polynomial interpolation algorithm. The interpolation led to a theoretical resolution of 0.1 pixel ( $\approx 6.2 \text{ nm}$  at  $\times 1000$  magnification) for the displacements within each subset. A companion application was implemented in MatLab to calculate and plot the in-plane strain fields ( $\epsilon_{xx}$ ,  $\epsilon_{yy}$  and  $\epsilon_{xy}$ ) at each point of the image from the displacement fields,  $U_x$  and  $U_y$ , in the X (loading) direction and Y direction, respectively. The strain calculation was based on the isoparametric 2D finite element formalism using subset centers as nodes and introducing four Gauss bilinear interpolation points per element. Direct DIC measurements (cumulative) have been chosen, so the direct strain map is obtained by comparing after each deformation step the micrograph of the deformed specimen with the micrograph of the undeformed specimen. Details of the sub-grain SEM-DIC technique can be found in Ref. [17] and in Ref. [10].

## 3. Results

### 3.1. Low cycle fatigue regime

A total of 10 cyclic deformation tests were performed on cylindrical specimens in air under load control conditions at maximum stress of 758 MPa with a R-ratio of  $-1$  and a frequency of 1 Hz at

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