Experimental and Computational Polycrystal Studies of Fatigue Damage and Crack Initiation

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1. Introduction

Studies on ‘two-dimensional’ polycrystals have been carried out both experimentally and computationally. In the experimental work, a directionally solidified nickel alloy has been used in which grains, with an average size of about 0.6 mm, are approximately prismatic through the test specimen depth. In this way, some of the very complicating features of three-dimensional microstructures have been eliminated. In addition, the comparatively large grain size simplifies microscopy. SEM with EBSD was used to determine grain morphology and crystallographic orientation. Three-point bend tests have been carried out on the material generating low cycle fatigue. Micro-crack initiation and growth have been examined.

In the computational work, time-independent crystal plasticity [1] has been used to model explicitly grain morphology and crystallographic orientation for a sixty-grain representative volume element (RVE) of a nickel alloy. The RVE has been subjected to conditions of low and high cycle fatigue, and comparisons of macro-stress strain prediction with experiments allowed the critical resolved shear stress for the material to be determined. In addition, because of the established link between the development of persistent slip bands and the initiation of fatigue cracks in both single and polycrystal materials, a simple crack initiation criterion based on accumulated plastic slip has been introduced. The initiation model relies on just one material property; namely, the critical accumulated plastic slip. When combined with the polycrystal RVE model, predictions of cycles to crack initiation can be made. The model results have been compared with macro-level empirical lifing methods such as that of Basquin for high cycle fatigue and Coffin-Manson for low cycle fatigue. Predictions have also been compared with low and high cycle fatigue test results [2].

2. Computational Investigations

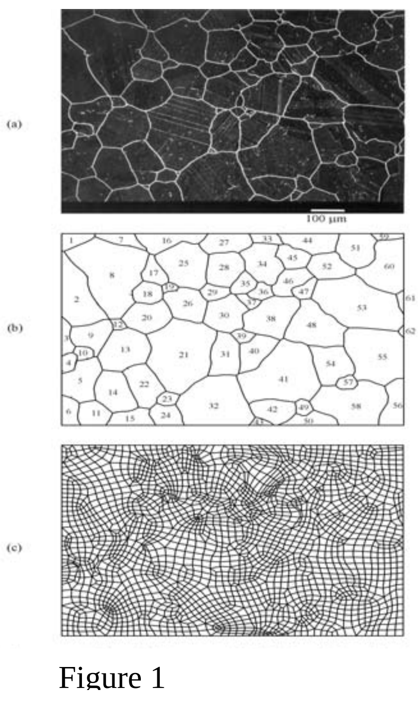

Figure 1

Figure 1(a) shows a typical microstructure of the nickel-base alloy C263. This is an fcc material with grains having a nominally random crystallographic orientation. The material's grain boundaries have been identified as shown in figure 1(b). Each grain has been meshed initially using four-noded plane strain elements as shown in figure 1(c). For the majority of the calculations reported here, plane strain elements are used. In the model, there are 62 grains and 2313 elements in total. The free edges were constrained to remain straight to represent a repeating unit of this typical microstructure. Under strain controlled fatigue simulation, the loading is applied using a displacement subroutine to specify the displacement on the top free edge. Under stress control, a uniformly distributed load is applied at the top free edge. The crystal plasticity constitutive equations were implemented into a user-defined material subroutine within the ABAQUS nonlinear finite element solver. Random crystallographic orientations for each grain were generated. All finite elements falling within a grain were therefore allocated the crystallographic orientation corresponding to that grain.

The experimental saturated LCF stress-strain hysteresis loops at 20^{o}C have been used to determine the plasticity material properties. Fully reversed, strain controlled, uniaxial tests with R ratio = -1 at strain amplitudes ±1.0, 0.5 and 0.37% were carried out, and the experimental saturated stress-strain loops are shown in figure 2 by the broken lines. The same strain controlled loading was applied to the finite element model shown in figure 1(c). The resulting macro-level stress is calculated, at any time, by summing the nodal reaction forces on the top edge, and dividing by the current cross-sectional area. The solid lines show the computed results, which saturate after just two cycles.

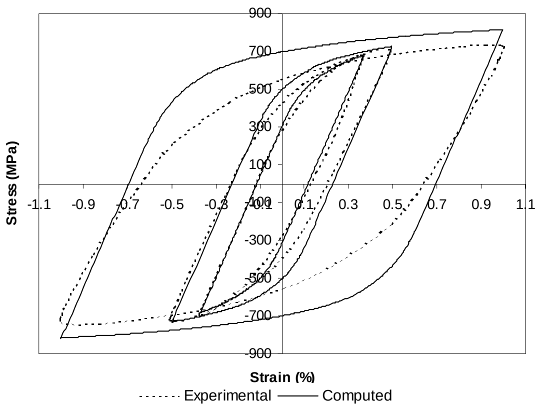

Figure 2

2.1 Fatigue Crack Initiation in LCF and HCF

The plastic velocity gradient, $\underline{L}^p$, is defined by

$$\underline{L}^p = \sum_{\alpha=1}^{n} \dot{\gamma}^\alpha \, \underset{\sim}{s}^\alpha \, \underset{\sim}{n}^{\alpha T}$$

An effective plastic slip rate, $\dot{p}$, is defined as

$$\dot{p} = \left(\frac{2}{3} \underline{L}^p : \underline{L}^p \right)^{1/2} .$$

Because in all the analyses carried out here, the rigid body rotations are small, $\dot{p}$ is the effective plastic slip rate. A fundamental quantity at the micro-level must be the accumulated (plastic) slip which, like strain, is a dimensionless quantity, and can be calculated for every point in the finite element model as

$$p = \int_0^t \dot{p} dt$$

A simple initiation criterion is proposed, applicable to both HCF and LCF, based on (plastic) slip, which is written

$$p = p_{crit}.$$

Figure 3 shows the field variation of p after two cycles of fully reversed LCF at 300^{o}C with strain amplitude 0.5%. It can be seen how localised this quantity is, with the peak values occuring at just one or two grain boundaries. The higher values of accumulated slip in general follow the grain boundaries, but it can be seen that the highest values occur at, or close, to grain triple points. It can also be seen that the accumulated slip is localised even within individual grains, leading to the formation of intense bands of slip - persistent slip bands. These are often also associated with triple points. The average grain size is about 100μm, so the width of the slip bands lies within the range 1 - 20µm.

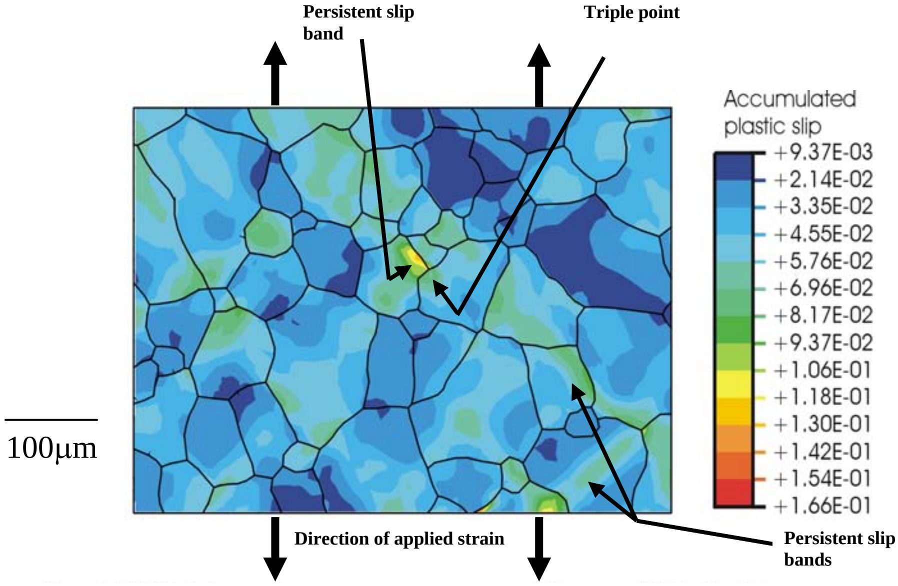

Figure 3

Predictions of low cycle fatigue life for nickel alloy C263 at 300°C, are shown in figure 4 for R-ratios of -1 (with plastic strain amplitudes between 0.32 - 0.63%) and 0 (with plastic strain amplitudes between 0.29 and 0.68%). Good agreement is seen, and the model predicts the expected linear relationship between log(plastic strain amplitude) and log(cycles to failure).

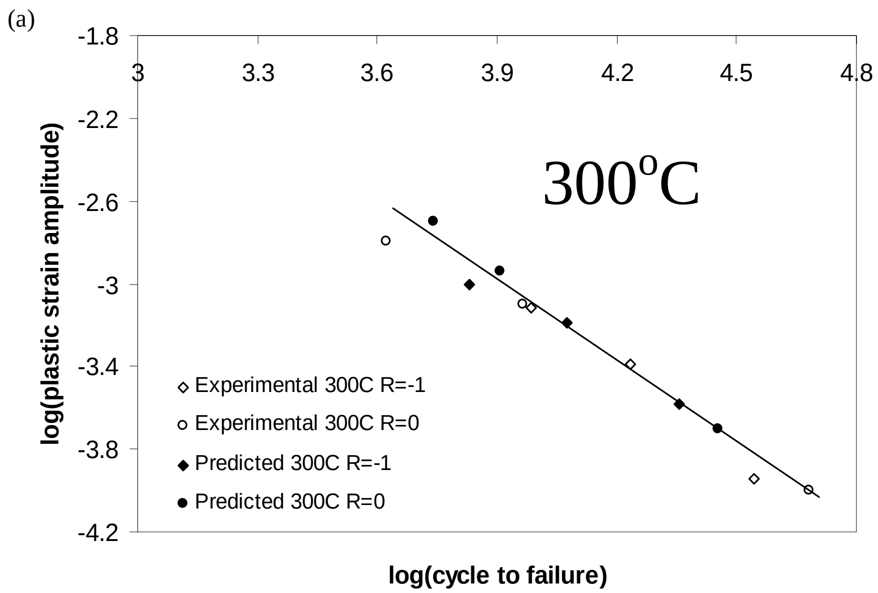

Figure 4

3. Experimental Studies

Figure 5 shows the grain morphology and crystallographic orientation (indicated by colour) of a region of the ‘two-dimensional’ material subjected to low cycle fatigue testing. The average grain size is about 0.6 mm. The region was located on the test specimen by means of micro-hardness indentation points which can be seen in the figure.

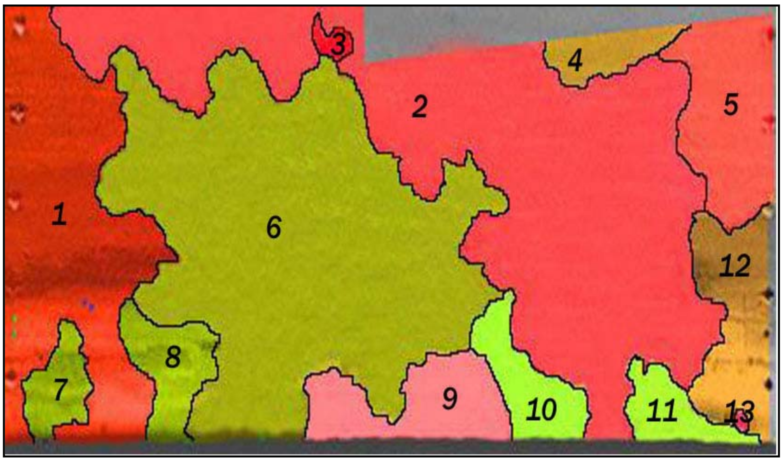

Figure 5

During testing, the specimen was repeatedly removed from the test rig to enable frequent examination, using optical microscopy, of the initiation and development of micro-cracking. Figure 6 shows the development of a macro-crack which initiated at the boundary between grains 11 and 12, propagated transgranularly through grain 12 until it reached a triple point at grains 2, 5 and 12. The crack then bifurcates with the more dominant part growing in to grain 5 transgranularly and through to an area outside of that examined using EBSD shown in figure 6(a). The other part of the crack, shown in figure 6(b) follows the grain boundary (*I*) between grains 2 and 5, then follows a zig-zag path following the macroscopic slip directions (*II*) close to the grain boundary (*III*). Micro-cracks initiated almost always at grain boundaries and if growing transgranularly, almost always followed a direction perpendicular to the principal tensile stress. To do so, small amounts of growth took place along slip directions with regular changes from one slip system to another generating the zig-zag effect.

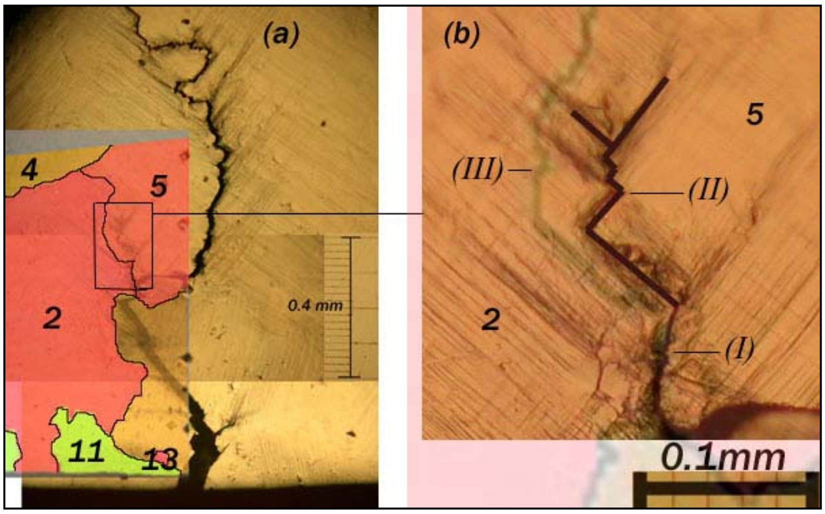

Figure 6

4. Conclusion

Polycrystal plasticity finite element models have been developed for 'two-dimensional' nickel alloy which, with a simple crack initiation criterion, have been used to predict initiation life under conditions of low and high cycle fatigue. Tests carried out on the two-dimensional nickel showed cracks initiating in locations with the highest tensile stress but almost always at grain boundaries. Transgranular growth occurred by repeated switches from one slip system to another to facilitate a propagation direction perpendicular to the maximum principal stress. Polycrystal plasticity simulations are being used to provide explanation and insight in to the initiation and growth processes.

5. References

1. Anand, L. and M. Kothari (1996), 'A computational procedure for rate-independent crystal plasticity', J. Mech. Phys. Solids, 44, 525-558.

2. Manonukul, A., Dunne, F.P.E. (2004), 'High and low cycle fatigue crack initiation using polycrystal plasticity', Proc. R. Soc. Lond, A460.