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Crack initiation in fatigue: experiments and three-dimensional dislocation simulations

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Abstract

In an attempt to better understand damage accumulation mechanisms in high cycle fatigue, a three-dimensional discrete dislocation simulation has been used both to simulate the dynamic evolution of the dislocation microstructure and the topography of the free surface where the plastic deformation is localised. The numerical tool is validated by comparing the dislocation structure obtained in double slip configuration to transmission electronic microscopy observation performed in 316L austenitic stainless steel. In the case of single slip loading conditions, the stress level obtained by the dislocation simulations are found to be consistent with results from the literature. After this validation stage, results of the dislocation simulations are analysed and a mechanism for the formation of intense slip bands is deduced. Finally, the computation of the relief of the free surface shows that extrusions and intrusions develop inside the bands, which demonstrates that plastic shear alone can give raise to crack initiation.

Keywords: Fatigue; 316L steel; Crack nucleation; Discrete dislocation dynamics; FEM; TEM

1. Introduction

In fcc single crystals, high cycle fatigue, that is to say, low strain amplitude fatigue solicitation give rise to strain localisation in persistent slip bands. In the case of a grain close to the free surface of the material specimen, elimination of the dislocations at the free surface results in plastic steps. Some of these plastic steps are permanent while others are cyclically removed. The irreversibility of these step formations is the origin of the crack nucleation which is experimentally observed to begin at the free surface [1–3] independently of the surface finish [4].

Several models have been proposed to justify the crack initiation. They can be classified into two categories: (i) the nucleation of an intrusion of a critical size generated by the plastic shear accumulated inside the slip band that may be assisted by diffusion mechanisms, (ii) the local decohesion of the crystal due to surface contamination at the plastic steps left at the free surface.

Since the fatigue crack initiation is a complex mechanism involving all these phenomena, it is very difficult to analyse separately the contribution of each effect. Numerical models, however, can give this kind of information. As an example, discrete dislocation dynamics (DDD) simulations give access to the single contribution of the plastic deformation to the damage accumulation. Hence the aim of this paper is to investigate the fatigue behaviour of fcc single crystals using DDD simulations. The material chosen both for the numerical modelling and the experimental validation is chosen to be 316L austenitic stainless steels.

2. Validation of the numerical modelling

The DDD code used in this study is the simple edge-screw model as detailed in [5]. The parameters corresponding to 316L stainless steel are those proposed in [6]. The simulation box is taken as a cylinder or half a dodecahedron admitting a diameter comprised between 10 and 22 μm. In both cases, one of the surfaces is traction free whereas all the others are considered as impenetrable facets mimicking strong grain boundaries. The initial configuration consists

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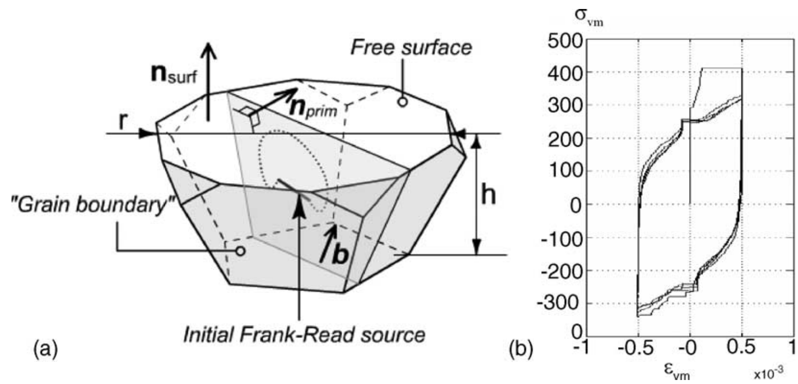

Fig. 1. Initial configuration for the DDD simulations and mechanical response in Von Mises equivalent components.

of Frank–Read sources represented by dislocation segments artificially pinned at both ends. Simulations have been performed with 12 Frank–Read sources randomly spread inside the simulation box on all the 12 glide systems. It appeared that only two glide systems accumulate dislocation density. These systems are selected among the activated systems and correspond to the couple of systems sharing a common Burgers vector and close to a double slip configuration. The dislocation density on all the other systems vanishes cyclically which denotes a reversible behaviour. Thus, for all the simulations presented in this study, the starting configuration will always consist of a single pinned segment put in the 'primary system' and located at the middle of the simulation box as shown in Fig. 1a. Dislocations in the deviate system, later referred as the deviate system, will automatically be generated by cross slip.

As shown in Fig. 1b, the plastic strain amplitude is imposed to be constant for all cycles. Thus, the stress tensor is increased step by step in a quasi static manner until the maximum plastic strain is reached and it is then decreased the same way until the minimum strain is attained. Fig. 1b shows a typical response in the case of a double slip configuration of the loading and for a Von Mises plastic strain amplitude of $\Delta\varepsilon_{VM} = 0.5 \times 10^{-3}$. During the first cycling, the dislocation source has to generate the dislocation density needed to accommodate the plastic strain. This creates a peak in the stress amplitude. After this first cycle, a small amount of softening is observed which corresponds to the classical response of 316L.

In order to validate the numerical procedure, a single slip solicitation has been tested. Indeed, this kind of solicitation is the one commonly used in the literature for fatigue analysis. The stress level computed by the DDD code in this case and for a imposed plastic strain amplitude of $\Delta\varepsilon_{VM} = 0.5 \times 10^{-3}$ is found to be close to 200 MPa which fits well Li and Laird [7] results in a similar configuration.

The dislocation microstructure has also been compared to the experimental observations. Transmission electron microscopy of a 316L specimen solicited in thermal fatigue has been performed and a typical dislocation microstructure for a surface grain is given in Fig. 2a. This dislocation microstructure has to be compared with Fig. 2b which

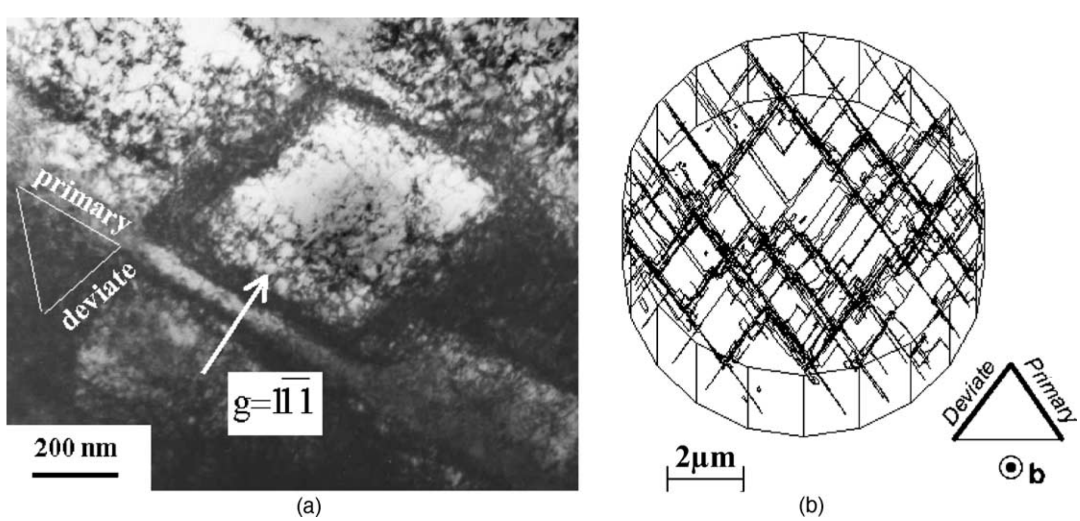

Fig. 2. Dislocation microstructure obtained in double glide configurations both experimentally by thermal fatigue and as computed by the dislocation simulation code.

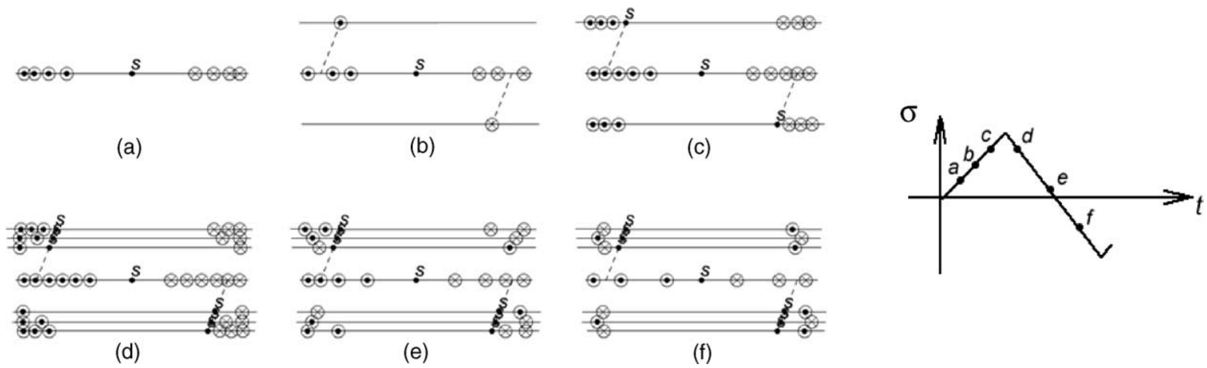

Fig. 3. Schematic representation of the dipole formation during cyclic loading.

corresponds to the results of DDD code in the case of a double glide configuration for which the mechanical response is given in Fig. 1b.

One can verify that high dislocation densities are localised in intense slip bands in the two glide systems. Complementary simulations have been performed using several box sizes. We found that the size of the bands increases linearly with the diameter of the simulated box whereas the thickness of the bands increases as the square of the diameter.

These two comparisons, the first one based on the stresses obtained in single slip configuration and the second one based on the microstructure obtained in double slip configurations validate the numerical procedure. The DDD results can now be used as a predictive tool to study the localisation process and the crack initiation.

3. Analysis of the DDD results

3.1. Formation of the dislocation microstructure

A detailed analysis of snapshots of the DDD simulations shows how the dislocation microstructure quickly localises into intense slip bands. The process is directly related to cross slip events occurring at pile-ups on the grain boundaries: dislocations emitted from the source are piling up on the impenetrable facets of the simulation box (see Fig. 3a). As soon as a certain number of dislocations is stored in the pile-up, the resolved shear stress in the deviate plane becomes high enough to induce cross slip on the screw part of the dislocation loops (Fig. 3b). Then, some dislocations cross slip and glide in this deviate plane until the forces generated by the pile-up are no more important and the applied loading is predominant. Then, the dislocations cross slip back on the primary plane (Fig. 3c) creating new sources pinned at the intersections between primary and deviate slip planes.

These new sources cause new pile-ups that once again will cross slip and propagate the slip in parallel planes (Fig. 3d). When the applied stress level is below a critical value (Fig. 3e), the stress coming from the dislocation pile-up is predominant and can activate sources in the opposite direction, emitting dislocations of opposite signs (Fig. 3f). This explains how dipoles form in the dislocation microstructure. If the dipoles are stable enough to persist throughout a complete cycle, they can be crossed by the

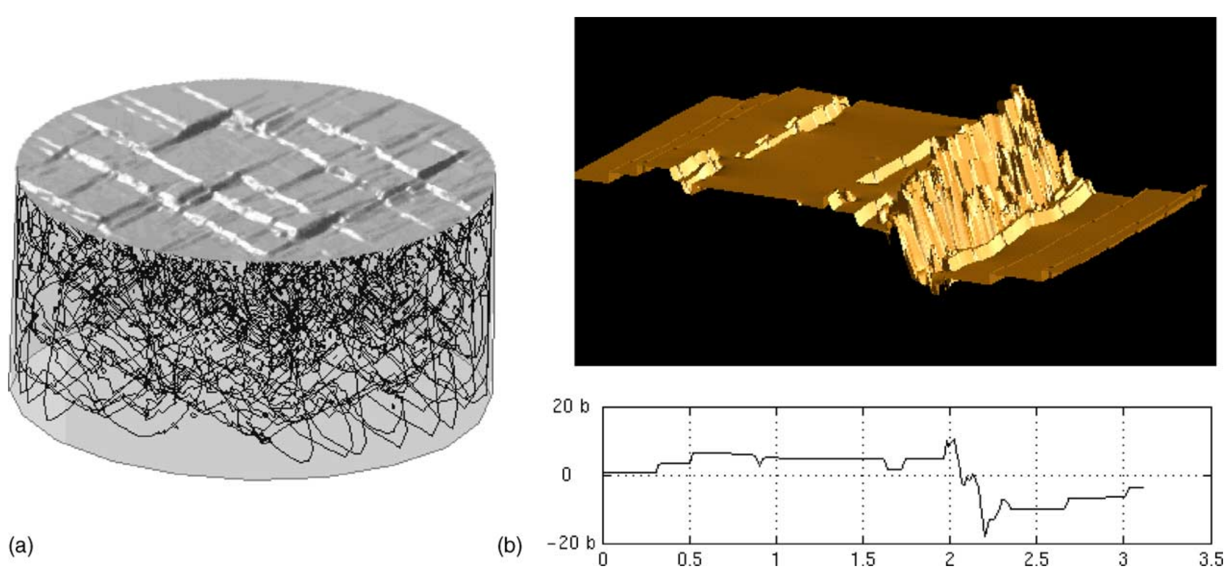

Fig. 4. Surface topography associated to dislocation microstructure and extrusion/intrusion at the strain localisation.

dislocations emitted from the sources at the next cycle. Then, since both dislocation systems share the same Burgers vector, the dislocations arms of the dipole and the incoming sources are reconnected leading to helical dislocations or prismatic loops. This second mechanism observed as a result of DDD simulations was already proposed by Li and Laird [7]. The resulting structure is at the origin of the ladder-like dislocation microstructure observed in the slip bands.

3.2. Formation of extrusion–intrusion relief

During the cycling loading, the plastic steps left by the dislocations escaping the grain through the free surface are computed and the evolution of the surface topography can be visualized. A typical example showing both the dislocation structure and the relief of the free surface is shown in Fig. 4a. It appears that the plastic steps are mainly reversible. Only a low fraction, about 10%, remains stable from one cycle to another.

Interestingly, extrusions and intrusions are observed inside the bands. These extrusions are created by the prismatic loops gliding in the slip bands and emerging at the free surface. An example of such a topography is shown in Fig. 4b. This demonstrates that extrusions and intrusions can form without the assistance of a diffusion process.

Complementary studies of the elastic energies stored in the crystal show that the critical zone where a crack may nucleate is initially located close to the grain boundary but quickly move towards the free surface. This means that the crack will certainly initiate at the intrusion, after a critical number of cycles.

4. Conclusion

DDD simulations have shown that a cyclically solicited dislocation source can generate heterogeneous dislocation microstructures similar to those observed in TEM with a mechanical response in good agreement with literature. A mechanism describing the microstructure formation has been observed and analysed. It appears that cross slip is a crucial phenomenon for the dipole formation at the origin of the irreversibility of the plastic strain localisation. Computations of the surface topography associated to the dislocations crossing the free surface have shown extrusions and intrusions which remain stable during the cycling. This study shows that plastic shear alone can produce cracks and that these cracks will initiate at the free surface and quickly propagate to the grain boundary.

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