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Multiple slip dislocation patterning in a dislocation-based crystal plasticity finite element method

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ABSTRACT

Dislocation structures forming during cyclic loading of fcc metals are fatigue damage precursors. Their specific structures are caused by the motion and interactions of dislocations. Depending on the load conditions, the grain orientation, the stacking fault energy, a variety of different dislocation structures appear in the material such as labyrinths, cells, veins and persistent slip bands. We present a continuum dislocation-based model for cyclic fatigue and incorporate it into a crystal plasticity finite element solver. A method for the simulation of dislocation junction formation is introduced, which reproduces the behaviour of discrete objects, such as dislocations, in a continuum framework. The formation of dislocation walls after 50 and 100 deformation cycles at 0.95% and 0.65% strain amplitude starting from an initial random dislocation distribution is predicted for ⟨001⟩ and ⟨1$\bar{1}$0⟩ oriented crystals. Simulations and cyclic tension-compression experiments of polycrystalline 316L stainless steel are performed to compare our model with another model based on edge and screw dislocation densities. The simulated dislocation structures and experimental results, obtained with the electron channeling contrast imaging technique, are compared using a 2D orientation distribution function of the dislocation structures. The dominant orientation of dislocation walls is predicted by the new model; it turns out to be perpendicular to the intersection line between the two slip planes involved in their formation and at an angle of around 45^o from the loading axis. This agrees well with the experimental observations and represents a step forward for understanding the formation mechanism of these dislocation structures.

1. Introduction

Cyclic fatigue in fcc metals is characterised by the formation of dislocation structures, which are localized regions where the dislocation density becomes higher than in pristine materials (Li et al., 2011). Dislocation structures are constituted of dislocation walls separating low dislocation density regions known as channels. The appearance of these dislocation structures is associated with hardening of metals and precedes crack formation (Pham and Holdsworth, 2012). Phenomenological models are often used to describe damage during the first stage of fatigue (Pirondi et al., 2006); however, dislocation-based

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models at the sub-micrometer length scale contain information related to physical parameters and the microstructure, hence, they are helpful in enlightening the underlying mechanisms (Korsunsky et al., 2012).

Current research on models for dislocation structures formation is mostly focused on monotonic loads Sandfeld and Zaiser, (2015), for which the dislocation cell structure has been found (Xia and El-Azab, 2015). Cyclic simulations of single crystals oriented for single slip, for which vein-channel structures and persistent slip bands (PSBs) are observed Li et al. (2011), have been carried out using both continuum Pontes et al. (2006) and discrete Déprés et al. (2008); Fivel (2008) computational approaches starting from random initial dislocation distributions. The use of discrete dislocation dynamics simulations for fatigue is limited by the computational resources needed to reach few cycles, and is restricted to simplified boundary conditions (Kubin, 1002). Details about the positions of single dislocations are not a necessary condition to study the micrometer-scale features of dislocation structure formation, therefore continuum models, based on dislocation densities, are a suitable alternative. A finite element method based approach is capable to take into account displacement controlled boundary conditions and the internal stresses caused by plastic deformation. For this reason, we use the crystal plasticity finite element (CPFE) method Roters et al. (2012), a computational method frequently used to simulate polycrystals, mostly considering monotonic loads only (Leung et al., 2015). The CPFE method needs to be complemented by constitutive equations to calculate the plastic strain rate of every slip system. These equations can be based on a phenomenological (Manonukul and Dunne, 2004) or, as in the present work, on a dislocation dynamics model.

In polycrystalline samples the specific arrangement of grains and their orientation determines the strain and stress states of a material at the micrometer scale, which controls the active slip systems according to Schmid's law (Roters et al., 2010). The CPFE method has been proven suitable for small-scale plasticity simulations, because the plastic deformation of all the slip systems is considered and, therefore, the active ones can be predicted (Maaβ et al., 2009). The interaction of dislocations on different active slip systems determines the orientation of dislocation walls. Monotonic deformation experiments show 3D cell structures at 2% strain amplitude (Jakobsen et al., 2006). The activation of cross slip is associated with the appearance of these structures, which do not emerge if this mechanism is suppressed in 3D discrete dislocation dynamics simulations (Madec et al., 2002). The dislocation walls during monotonic deformation tend to align along the intersection of cross-slip planes (Xia and El-Azab, 2015). Cyclic deformation experiments show a variety of differently oriented dislocation structures in fcc metals, such as copper, nickel and silver (Li et al., 2011): PSBs and vein-channel structures coexist in ⟨011⟩ oriented crystals and walls perpendicular to the Burgers vector of the most active slip system have also been observed (Li et al., 2011). Cell structures, composed mostly of coplanar dislocations, were reported to form in $\langle\bar{1}11\rangle$ oriented crystals Li et al. (2009a), and labyrinth structures in ⟨001⟩ oriented crystals. The wall orientation of labyrinth structures in [001] oriented crystals is typically perpendicular to [001] and [100] axes Li et al. (2011), thus perpendicular to the sum of the Burgers vectors of the primary and the secondary critical slip systems. In ⟨001⟩ oriented crystals, when the conjugate and the critical slip systems are activated, Lomer-Cottrell and Hirth junctions are formed, respectively. The Lomer-Cottrell junction is known to be stronger than the Hirth junctions. This means that, in presence of Lomer-Cottrell junctions, a higher stress is required to activate the subsequent dislocation movement. Therefore, the dislocation motion and multiplication is slowed down in regions where the primary and conjugate slip systems are activated (Jin and Winter 1984a). This is not the case for the Hirth junction, which does not retard the contemporary motion of dislocations belonging to the primary and to the critical slip system (Jin, 1983; Jin and Winter 1984b; Li et al., 2009b). This suggests that the activation of the critical slip system, and consequently the formation of Hirth locks, is important for the labyrinth structure formation (Li et al., 2011). Further experimental investigations have found wall orientations intermediate between {100} and {210} L'Espe'rance et al. (1986), explained with low energy arrangements of dislocation loops (Dickson et al., 1986). The collinear reaction, which is the interaction of a slip system with its cross-slip system, is also important to determine the geometrical configuration of dislocations during loading (Madec et al., 2003). However, active slip systems interacting by the collinear interaction are not commonly observed in copper (Devincre et al., 2005, 2006).

There have been only a few attempts to model dislocation structure formation under multiple slip conditions. Approaches based on reaction-diffusion equations Aoyagi et al. (2013) have been applied to simulate the formation of labyrinth structures Pontes et al. (2006), where mobile and immobile, positive and negative edge dislocations are the state variables. These attempts successfully reproduced two-dimensional dislocation patterning, resulting in dislocation walls perpendicular to the Burgers vectors of the two active slip systems. This is different from experimental observations, where these walls are oriented perpendicular to the sum and difference of both Burgers vectors. This discrepancy is due to the flux terms used to model the motion of edge dislocation segments along the two slip directions. Opposite signed edge dislocations, belonging to the two active slip systems, move away from emerging channels along the Burgers vector direction, interact and form dislocation dipoles. Therefore, dislocation walls do not align with the dislocation junction direction and remain oriented perpendicular to the Burgers vectors. Thus, it appears necessary to introduce dislocation junctions and their specific geometrical configuration in constitutive models, as has been done in discrete dislocation dynamics models Martínez et al. (2008) but not in continuum formulations. Testing these constitutive models on ⟨001⟩ oriented crystals can indicate if the dislocation junction mechanism is sufficient to describe labyrinth structures.

In this paper we apply the crystal plasticity finite element (CPFE) method and dislocation-based constitutive laws, implemented as a DAMASK subroutine Roters et al. (2012), to model dislocation structures in polycrystalline fcc metals. The main novelty introduced is the treatment of dislocation junction formation in a continuum framework, based on the linear combination of edge and screw dislocation densities into a density aligned with dislocation junctions. When applied to the simulation of cyclic plasticity in ⟨001⟩ oriented crystals, the new model is capable to predict the correct orientation of

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