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Quantifying dislocation microstructure evolution and cyclic hardening in fatigued face-centered cubic single crystals

Ahmed M. Hussein *, Jaafar A. El-Awady

Department of Mechanical Engineering, Whiting School of Engineering, Johns Hopkins University, 3400 North Charles St., Latrobe Building, Baltimore, MD 21218, USA

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ABSTRACT

Discrete dislocation dynamics simulations were performed to investigate the dislocation microstructure evolution and cyclic hardening during the early stages of fatigue loading in nickel single crystals. The effects of the crystal size and initial dislocation densities on both the mechanical response and the evolution of dislocation microstructure were quantified. Crystals having an initial dislocation density of 10^{12} m^{-2} and diameter less than 2.0 μm do not show any dislocation density multiplication or cyclic hardening. In contrast, crystals having the same initial dislocation density and diameters larger than 2.0 μm show a significant dislocation density accumulation in the form of dislocation cell-like structures, even after only a few number of loading cycles. This dislocation density accumulation was also accompanied by considerable cyclic hardening. The dislocation cell size and its wall thickness increase with increasing crystal size. With increasing dislocation density the critical crystal size, at which dislocation cell-structures form, decreases. The information theoretic entropy is utilized as a metric to quantify the extent of dislocation patterning and the formation and evolution of dislocation cell structures over time. Cross-slip was found to play a dominant role in the dislocation cell-structure formation. Further insights on the mechanisms contributing to the observed behavior are presented and discussed.

1. Introduction

The need to develop and formulate reliable fatigue damage life prediction methods for metals in aerospace applications is ever-growing. Fatigue failure is considered to be one of the main causes leading to structural and mechanical systems failure (Stephens et al., 2000; Schijve, 2009). It has been estimated that the cost of failed mechanical components due to fatigue is around 4% of the U.S. gross national product (Stephens et al., 2000). While fatigue failure has been one of the earliest failure mechanisms to be studied, a complete understanding of mechanical fatigue still does not exist (Mughrabi, 2010; Suresh, 1998). The evolution of the material microstructure under cyclic loading is sensitive to the loading conditions, environmental effects, strain rate, and the material crystal structure, among other factors. This partially explains the complexity of fatigue related failures. In addition, the recent growing interest in nanocrystalline metals for MEMS applications has lead to new questions regarding the cyclic response of these materials that are yet to be answered (Mughrabi and Hoppel, 2010). Thus, an in depth effort to provide physical

* Corresponding author. Tel.: +14434493395.
E-mail addresses: ahussei4@jhu.edu (A.M. Hussein), jelawady@jhu.edu (J.A. El-Awady).

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insights regarding the important deformation mechanisms active during cyclic loading is needed to develop more robust fatigue failure predictions.

The evolution of the dislocation microstructure during cyclic loading is a complicated process, where several deformation mechanisms that span multiple length and time scales are strongly interacting. Both in situ and post-mortem experiments can only provide limited information on how the dislocation microstructure evolves under highly controlled and usually idealized loading environments. Furthermore, theories that attempt to explain the microscopic behavior, especially dislocation patterning, are usually based on simplified models in which the stress triaxiality and the dislocations interactions are either neglected or modeled using ad hoc assumptions (Bako and Groma, 1999; Groma and Bako, 2000; Koslowski et al., 2006). However, a full consideration of the evolution of dislocations structures is essential in an effort to partially unravel the complexity of the problem.

High fidelity computer simulations at the appropriate length scales can provide better insights on details of the dislocation microstructure evolution. Discrete Dislocation Dynamics (DDD) simulations (Kubin et al., 1992; Ghoniem et al., 2000; Zbib et al., 2002; Weygand et al., 2002), where the physics-based evolution of dislocation microstructures is captured, can provide such needed understanding. DDD has been extensively utilized in the past to study the effects of crystal size on its mechanical response (e.g. Motz et al., 2009; El-Awady, 2015), the behavior of thin films (e.g. Pant et al., 2003), nanoindentation (e.g. Fivel et al., 1998), and irradiation hardening (e.g. Khraishi et al., 2001). In DDD, most physical mechanisms required to accurately replicate the evolution of dislocations are accounted for with minimal constitutive rules or empirical laws incorporated. This makes DDD a suitable choice for explicitly modeling the collective behavior of dislocations with minimum ad hoc assumptions if any.

Discrete Dislocation Dynamics simulations have been previously used to study several aspects of cyclic loading in metals. Deshpande et al. (2003) used two-dimensional (2D) DDD to study the interaction of dislocations with pre-existing cracks under both monotonic and cyclic loading, and concluded that dislocation activities tend to be more localized around the crack tip in cyclic loading. Brinckmann and Van der Giessen (2004) used 2D DDD to study the evolution of the dislocation density and stresses in a surface grain subject to cyclic loading and concluded that stress accumulation takes place even after a low number of cycles. Déprés et al. (2004, 2006) performed an extensive three-dimensional (3D) DDD study of early cycle fatigue behavior using the simple edge-screw model (Kubin et al., 1992). These simulations were performed starting with a single Frank–Read source in cylindrical and half-dodecahedral surface grains. It was concluded that multislip loading orientations lead to more damage accumulation than single slip orientations. The interactions of screw dislocations on parallel slip planes in idealized persistent slip band channels were also investigated using 3D DDD, and the dipole passing mechanism was assessed and interpreted in terms of the fatigue saturation stress (El-Awady et al., 2007).

While these studies are informative, there are still many open questions on the role of crystal size and initial dislocation density on the evolution of the dislocation microstructure and mechanical response during the early stages of cyclic loading in Face Centered Cubic (FCC) metals. To address this, atomistically informed 3D DDD simulations that include key deformation mechanisms, such as physics based cross-slip mechanisms developed earlier by the authors (Hussein et al., 2015), are performed and analyzed. The paper is organized as follows. In Section 2, the simulation setup is briefly presented, and a number of new analysis methods are introduced. In Section 3, the results of the DDD simulations are presented for different crystal sizes, initial dislocation densities, and number of loading cycles. Section 4 discusses the results in view of different dislocation mechanisms. Finally, a summary and conclusions are presented in Section 5.

2. Computational methods

For the current simulations, an in-house modified version of the open source 3D DDD simulations code, ParaDiS (Arsenlis et al., 2007), is used. To avoid any artificial off-plane dislocation climb, ParaDis was modified to enforce that dislocations will always glide on their designated slip planes. This also applies to dislocation–dislocation reactions that result from dislocation collisions and might lead to, erroneously, placing a dislocation segment off of its slip plane. Furthermore, dislocation cross-slip is an important deformation mechanism that affects the evolution of the defect microstructure and its overall mechanical response (Gutmanas and Nadgornyi, 1970; Jackson, 1983, 1985; Saada, 1991; Jumonji et al., 1996; Madec et al., 2002; Kubin et al., 2006). Based on recent extensive molecular dynamics studies, three different cross-slip mechanisms have been identified, namely: bulk, surface, and intersection (repulsive and attractive) cross-slip (Rao et al., 2009, 2010, 2011, 2013a, 2013b). These new mechanisms have been incorporated in the in-house version of ParaDiS by implementing an algorithm that would efficiently detect the longest possible screw-oriented dislocation chains, classify them according to the appropriate cross-slip types then identify their probability for cross-slip to occur (Hussein et al., 2015). The activation energies and activation volumes were obtained from atomistic simulations and were reported for nickel (Ni) in Hussein et al. (2015).

The focus of the current simulations is on FCC Ni (Young's modulus $E=210$ GPa, and Poisson's ratio $\nu=0.31$). However, the same approach can be easily extended to study other crystalline materials. While several models of dislocation interactions with grain boundaries and twin boundaries have been recently implemented in DDD (Zhou and Lesar, 2012; Fan et al., 2015), the current simulations are limited to free standing single crystal simulations to reduce the complexities introduced by dislocation grain/twin boundary interactions. Dislocations are allowed to escape from all six surfaces of the simulation cell, mimicking the experimental case of a free standing single crystal axially loaded with soft grips at both ends, to remove any external influence on the dislocation evolution. The loading is strain controlled with fully reversed cyclic