# Surface roughness evolution during early stages of mechanical cyclic loading

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ABSTRACT

The effect of crystal size and initial dislocation density on surface roughness evolution in FCC single crystals during the early number of cycles of mechanical cyclic loading is investigated using three dimensional discrete dislocation dynamics simulations. Crystals having size less than 2 µm show early development of surface slip localization, while larger ones show a more uniform distribution of surface steps. The surface roughness is found to increase with increasing number of loading cycles with larger crystals showing a high roughening rate compared to smaller crystals. Double cross-slip is observed to be the main mechanism that derives the development, growth and thickening of surface slip bands. The maximum surface height, which is an indicator of the surface stress concentration is observed to increase linearly with the number of loading cycles and quadratically with the crystal size for the simulated number of cycles. Finally, the results are shown to be in agreement with experimental results and provide further physics based understanding on the mechanisms controlling the evolution of the surface roughness.

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## 1. Introduction

Fatigue under cyclic loading is one of the leading causes of failure in mechanical and structural components [1,2]. While fatigue failure has been subject to intensive studies for almost 150 years [3,4], a complete understanding of the complex mechanisms that lead to fatigue failure is still elusive [3]. The complexity of the fatigue failure process stems from its sensitivity to many factors, including the loading type, microstructure, material heterogeneity, and environmental conditions among other factors [5]. Furthermore, the mechanisms responsible for fatigue crack initiation and propagation take place over multiple length and time scales [6].

The fatigue failure process can be divided into two stages, fatigue crack initiation (nucleation), and fatigue crack propagation [4,5]. The crack nucleation stage is the least understood of the two and understanding the mechanisms that control it is the first step in the process of extending the lifespan of materials through appropriate microstructure design. Cracks can nucleate at grain/twin boundaries [7], at an inclusion interface [8], or at the crystal free surface [5,6,9], with the latter being more prominent at room temperature [5,9]. One of the earliest experimental observations of

what was understood later as a precursor to fatigue crack nucleation at a free surface was made by Ewing and Humfrey [10], where the surface was observed to roughen in the form of sharp surface slip bands on the surface of polycrystalline iron specimens. These surface slip bands are in the form of extrusions/intrusions that render an initially smooth crystal surface into a rough one, and the heights/depths of these extrusions/intrusions were shown to increase with increasing number of cycles [4,11,12]. The edges of these extrusions/intrusions usually make sharp angles with the crystal surface leading to high local stress concentrations. When these local stresses are high enough, atomic bonds break leading to surface crack nucleation [13,14]. This view was further confirmed by a number of experimental studies [6,15–20].

With the growing interest in micro/nanoelectronics and microelectrical–mechanical systems, significant interest has been directed towards developing an understanding of the mechanical properties of metals at small scales. While numerous experimental and computational studies have focused on size-scale effects on the mechanical properties of metals during monotonic loading (c.f. [21,22]), far less attention has been directed towards understanding the effect of the crystal size on the cyclic response of microcrystals. It should be noted that experimental studies of the cyclic deformation of microcrystals is technologically more challenging than bulk crystal studies. Nevertheless, a number of recent experimental studies have focused on the response of cantilever

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microbeams under cyclic bending [23,24] as well as microwires under cyclic torsion [25,26] loadings. However, none of these studies have focused on the effect of crystal size or initial dislocation density on the surface roughness evolution in microcrystals, which is important to understand as a precursor to crack initiation.

Over the past two decades, discrete dislocation dynamics (DDD) simulations have been extensively used to study many phenomena in the plastic deformation of metals [27]. However, only few DDD studies focused on simulations of cyclic loading. Of these, two-dimensional (2D) DDD simulations of dislocation interactions with pre-existing cracks during monotonic and cyclic loading suggested that the dislocation density multiplication and plastic-zone size near the crack-tip are weakly influenced by the crack size [28]. Moreover, three-dimensional (3D) DDD simulations of a single surface grain during early stages of mechanical cyclic loading showed that the height of surface steps that form by dislocation escape from the free surface increases with increasing number of loading cycles and imposed plastic strain amplitude [29,30]. However, those 3D DDD simulations were performed starting with a single Frank-Read source in the simulation cell, which corresponds to an unrealistically low initial dislocation density. In addition, 3D DDD simulations were also conducted to study the effect of long range stresses on the dynamics of screw dislocations in a PSB channel and the PSB flow strength [31]. Finally, the current authors performed a large set of 3D DDD simulations to quantify the dislocation microstructure evolution and cyclic hardening in free standing single crystals [32]. These simulations showed that the crystal size plays the dominant role in controlling dislocation multiplication, formation of dislocation cell-like structures, and cyclic hardening.

While such DDD studies have shed light on some aspects of cyclic loading, many important open questions remain to be addressed, including the role of crystal size and initial dislocation density on the surface roughness evolution and surface slip localization. To this end, the current work is an attempt in that direction. The paper is organized as follows. In Section 2, the computational methods are discussed, while the details of the numerical simulations are given in Section 3. In Section 4, the simulations results are presented and discussed in terms of the active dislocation mechanisms in an attempt to correlate the surface roughness evolution and the dislocation microstructure evolution. Finally, in Section 5 a summary and conclusions are presented.

## 2. Computational methods

All simulations results presented here are performed using a version of the open source 3D DDD code ParaDiS [33] that has been extensively modified by the authors at Johns Hopkins University. The original ParaDis structure was retained, however, the dislocation mobility routine for face-centered-cubic (FCC) crystals was altered to enforce the dislocation glide on the proper {1 1 1} slip planes, eliminating any possibility for artificial or unphysical dislocation climb. In addition, the algorithms handling short range interactions (e.g. dislocation collisions and topological operations) were redesigned to prevent the erroneous reorientation of dislocation segments out of their slip planes. Furthermore, a new atomistically-based cross-slip model has been implemented in the code [34]. This model accounts for the three recently characterized cross-slip mechanisms known as bulk, intersection, and surface cross-slip [35–39].

New rules for tracking dislocation interactions with free surfaces were implemented to compute the surface displacement fields and model surface roughness evolution. When a dislocation segment escapes from the crystal free surface it is removed from the pool of active dislocations, and the time, location, and slip

plane of the escape event are stored. In large simulations having large dislocation densities, the continuous storage of the records of escaping dislocation segments can lead to memory issues, as well as significant slow down in the displacement field calculations. Thus, a reduction algorithm was implemented to compress the escaped segment records when possible. The reduction is a lossless compression algorithm, in which the surface displacements due to the original dislocation-surface interaction information can be fully recovered from the compressed data. In the following two subsections, the displacement field calculations and the quantification of the surface roughness are discussed in details.

### 2.1. Displacement field calculation

The closed form solution for the displacement field of a single dislocation loop in an isotropic medium can be expressed as a line integral as follows [40]:

$$u_i = -\frac{b_i \Omega}{4\pi} + \frac{1}{8\pi} \oint_C \left( \epsilon_{ikl} b_l r_{,pp} + \frac{1}{1-\nu} \epsilon_{kmn} b_n r_{,mi} \right) dl_k \qquad (1)$$

where $u_i$ ($i = 1, 2$, and 3) are the three displacement components of the displacement vector, $\Omega$ is the solid angle subtended by the dislocation loop at the field point at which the displacement is calculated, $b_i$ are the components of the dislocation's Burger's vector, $C$ is the dislocation loop curve, $\epsilon_{ijk}$ are the components of the permutation tensor, $\nu$ is the material's Poisson's ratio, and $r$ is the magnitude of the position vector between a point on the dislocation curve and the field point.

The continuous evaluation of the displacement field as defined by Eq. (1) necessitates the tracking of each dislocation loop throughout the simulation. To alleviate the significant computational burden associated with this continuous tracking of all evolving dislocation loops during the simulation, especially in the case of non-planar loops that continuously evolve on new slip planes due to cross-slip, a more efficient algorithm is developed here. In this algorithm, a virtual dislocation loop is created for each dislocation segment under consideration. As shown schematically in Fig. 1, for any dislocation segment (*AB*) that escapes the free surface, an equivalent 5-segment closed-loop (*OACDBO*) is created during the displacement calculation step. This equivalent loop is constructed by first choosing an arbitrary anchor point, *O* inside the simulation volume. In the current simulations this point is chosen to be the point of intersection of the segment's slip plane with the *z*-axis. A copy (*CD*) of the dislocation segment (*AB*) is then
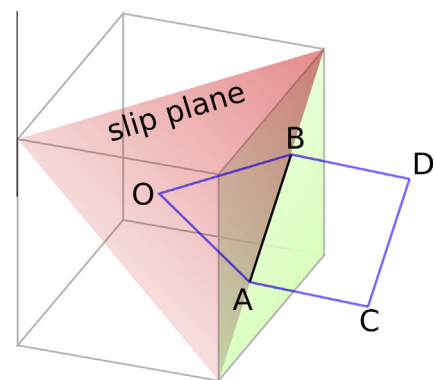


**Fig. 1.** A schematic showing a dislocation (*AB*) that escaped the free surface in black and the equivalent dislocation loop anchored at point O in blue. The dislocation slip plane is shown in green and the crystal surface is shown in red. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)