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Irreversibility of dislocation motion under cyclic loading due to strain gradients

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ABSTRACT

Mechanisms that make dislocation motion irreversible are associated with the formation of dislocation junctions and cross-slip, leaving dislocations trapped inside the specimen. Using Discrete Dislocation Dynamics simulations, we identify another mechanism that produces irreversible plastic deformation and leaves no or only very few dislocations inside the sample: Under cyclic loading, dislocations which pass the neutral plane during loading (pile-up formation), generate a slip step upon unloading. The explanation is an intrinsic asymmetry between the backward and forward motion. An additional bias may be introduced by the geometry of the specimen due to the shortening of the line length of dislocations.

Irreversible plasticity is associated with the glide and storage of dislocations through multiplication under load by dislocation junction formation [1–3] or absorption of dislocations in grain boundaries [4]. For bulk-like fcc materials under fatigue conditions, complex dislocation microstructures develop consisting of veins and almost dislocation free channels [5]. These dislocation microstructures lead to the surface roughness and finally to failure due to crack growth [6–8]. On the other hand, specimens with a thickness less than a few micrometers, e.g. thin metallic films, have a higher fatigue resistance, as the formation of extrusions and intrusions is reduced by the confinement of the dislocation glide within the much smaller structure [9].

Recent investigations of the fatigue behavior of single crystalline microbeams with thicknesses of ≈2 and ≈10μm under cyclic bending show the development of slip traces on the surface, generated by dislocations leaving the specimen [10]. The normalized stress versus displacement plot shows a clear Bauschinger effect, which is also observed in the complementary Discrete Dislocation Dynamics (DDD) simulations [10]. The origin of the Bauschinger effect in this case is the specific dislocation arrangement, found to be typical for bending: Dislocations cross the neutral plane and form a symmetric pile-up around the neutral axis [11]. The internal stress gradient stabilizes the dislocation pile-up within the specimen [11–13]. From more recent experimental measurements, by Laue diffraction, the formation of geometrically necessary dislocation (GND) arrangements is reported, compatible with the formation of the pile-ups around the neutral plane [14]. These GNDs disappear upon unloading, but the amount of permanent plastic deformation and the evolution of the pile-up during unloading is less clear. Upon unloading, it is suggested that dislocations move towards both surfaces [10,14], which leads to an irreversible plastic deformation. The Bauschinger effect is in general attributed to the dissolution of pile-ups of dislocations in front of interfaces or dissolution of dislocation cells during reverse loading [15]. Several studies with DDD have addressed the question of reversibility of dislocation motion and its conditions in detail, e.g. [16–18]. The current study does not consider the role of strong fixed obstacles on dislocation glide. The focus is on inhomogeneous loading conditions, e.g. bending or torsion, where the imposed stress gradients inhibit dislocation motion within the volume during loading. These imposed gradients vanish gradually upon unloading. While the formation of pile-ups in bending loading conditions is well documented [10,11,13,14,19], the evolution of the dislocation microstructure upon unloading has not yet been studied in detail especially in the limit of a very low dislocation density, e.g. for individual pile-ups. Neither has a generalization to other gradient-type loading conditions (e.g. torsion) been attempted yet.

Therefore the focus in this study is on the properties of a minimal setup showing irreversible plastic deformation under cyclic

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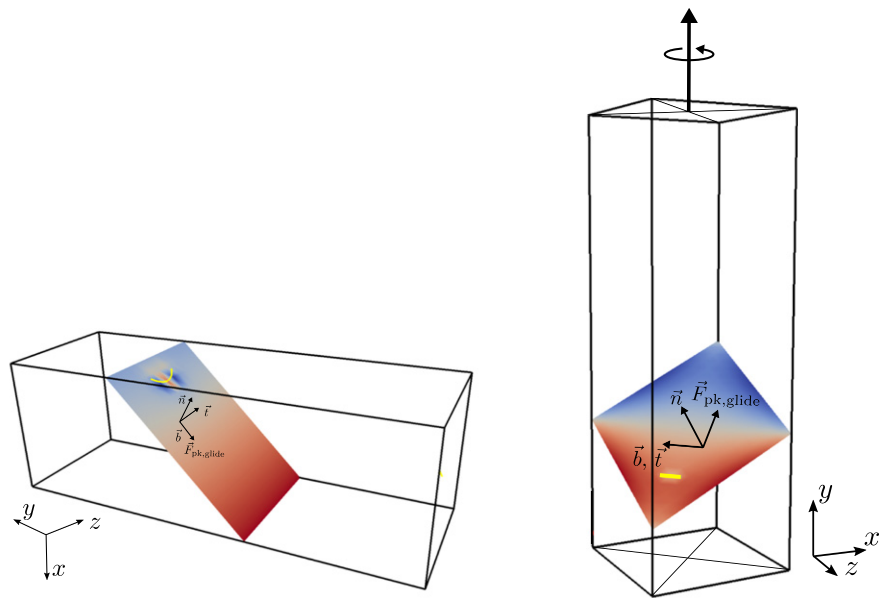

(a) Pure bending case.

(b) Torsion case.

Fig. 1. Dislocation source positions for both loading conditions: (a) pure bending and (b) torsion. The glide plane is colored using the resolved shear stress (qualitatively) acting on the dislocation, characterized by its Burgers vector $\vec{b}$, glide plane normal vector $\vec{n}$ and initial line direction $\vec{t}$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

loading involving both macroscopic strain gradients – as a consequence of boundary conditions – and the shape of the specimen. The setup mimics the situation in small micrometer-sized samples with a low number of activated dislocations sources. Cross-slip of screw dislocations as a possible additional source of irreversibility is not allowed. The DDD code described in [20–22] is used for this study. Dislocations are represented by nodal points, connected by straight segments. Nodal forces are calculated from the resolved Peach-Koehler force acting along the segments. Boundary conditions, finiteness of the specimen and image forces are included following the superposition scheme [23]. As a model system, material parameters for aluminum are used assuming isotropic elasticity (lattice parameter $a = 0.404$ nm, shear modulus $G = 27$ GPa, Poisson's ratio $\nu = 0.347$, fcc glide systems). The single crystalline specimen has a quadratic cross section (x-z plane) with a side length (thickness) of 1.5μm and an aspect ratio of 3. The long axis is along the y-direction. Cross-slip is not activated in this study.

Fig. 1 shows the dislocation source positions for both setups. In case of bending, the source is of edge type; the torsion setup has a screw type source. If not specified otherwise, the boundary conditions are as follows:

- Pure bending: Load is applied by prescribing a moment around the z-axis, prescribing displacements at $y_{\min}$ and $y_{\max}$ [11]. The tensile stress component in y-direction is balanced to be zero by adapting the displacement in y-direction of the beam at the neutral plane at the face $y_{\max}$. All other faces have traction free boundary conditions.

  One load cycle consists of a linear load increase to a maximum normalized displacement (normalized by beam thickness $t = 1.5$μm) $u_{\text{norm}} = 0.6\%$, and subsequent unloading to $u_{\text{norm}} = 0\%$.
- Torsion: Loading is applied by fixing all displacement components of the lower face to zero ($u_x = u_y = u_z = 0$) and rotating the upper face in clockwise direction around the torsion axis (parallel to the y-direction) using a torsion rate of $\dot{\varphi} = 3^{\circ}\mu s^{-1}$ during loading as described in [24]. Traction free boundary conditions are assumed for all other degrees of freedom on the surface. One load cycle consists of a linear loading up to a maximum torsion angle of $\varphi = 1.7^{\circ}$ and a linear unloading part back to $\varphi = 0^{\circ}$ with the same rate.

The shear stresses acting on the used glide systems of the two setups are shown in Fig. 1. Both show a change in sign of the resolved shear stress (indicated by a change from blue to red). The zero-stress plane (neutral plane) spans through the whole specimen and only the cut with the glide plane is visible. In case of bending the neutral plane has a normal vector parallel the x-direction. For torsion, the neutral plane has a normal parallel to the sample cross-section diagonal $(10\bar{1})$.

Fig. 2 gives a two dimensional representation of the bending beam of Fig. 1 (a). In this gradient setting, the dislocations take stable positions according to an equilibrium between the stress induced by the bending boundary condition and the growing back stress of the dislocation pile-up [11,13]. The dashed grey line indicates the neutral plane. Dislocation positions before, during and after the maximum applied bending moment $M_{\text{B,max}}$ of one load-unload cycle are shown: the positions before the maximum moment are colored in red. An increase in load to $M_{\text{B,max}}$ pushes the dislocations further into the center of the beam (black positions). Upon unloading (blue positions and arrows indicating motion), the dislocations, which have crossed the neutral plane, move to the opposite side of the source and leave the specimen. The ones, which did not cross, leave on the source side, if they succeed to cross the source location.

This process is repeatable. In the next load cycle, further dislocations are emitted from the source and upon unloading, the ones, which crossed the neutral plane, leave the specimen on the side opposite to the source, creating a slip trace of increasing height on the surface with increasing number of cycles.

For the torsion specimen, the torsion angle is increased until one dislocation passes the neutral plane (Fig. 3 (a), indicated by arrows). Dislocations leave the volume almost orthogonal to the surface, due