FINITE ELEMENT AND POLYCHROMATIC MICRODIFFRACTION ANALYSIS OF PLASTIC DEFORMATION MICROMECHANICS NEAR A GRAIN BOUNDARY

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ABSTRACT In this study we report inhomogeneous of plastic deformation in a natural Ni bicrystal after uniaxial loading. Focused, polychromatic synchrotron X-ray microbeam together with orientation imaging microscopy, scanning electron microscopy, and finite element simulations were used to characterize the physics of geometrically necessary dislocation formation and collective behavior during plastic deformation. The local crystallographic orientations in the grain determine its submicron-resolved plastic response during deformation. Finite element simulations were used to understand the influence of grain orientation and initial structural inhomogeneities on the geometrically necessary dislocation arrangement and distribution. Strain in both grains increases in the vicinity of the coherent boundary.

INTRODUCTION: Development of heterogeneous dislocation substructure even in single crystals was observed by a number of authors [Aifantis *et al.*2006; Arsenlis and Parks, 1999]. Inhomogeneity in dislocation arrangements increases as straining proceeds (even when slip is mainly homogeneous). Plastic strain gradients appear either because of the geometry of loading or because the material is plastically inhomogeneous. The density of geometrically necessary (GN) dislocation population, n^+, may be related to the effective strain gradient, η [Arsenlis and Parks, 1999; Ohashi, 1997; Ohashi, 2005].
Grain boundaries and triple junctions are special sites for inhomogeneous deformation because of strain compatibility necessary to accommodate shape and orientation changes in neighboring grains at their mutual boundary; boundaries create additional constraints for the plastic response of materials and alter the distribution of both GN and Statistically Stored (SS) dislocation arrangement [Ohashi, 1997; Ohashi, 2005]. This paper presents the analysis of GN and SS dislocation population distributions and lattice curvature in a natural Ni bicrystal during *in situ* tensile loading as a function of the grain orientation, distance from the boundary and as a function of depth. Experimental characteristization is with polychromatic microdiffraction and theoretical model is with finite element (FE) simulations.

PROCEDURES, RESULTS, AND DISCUSSIONS: The general view of the sample and orientation of crystallographic axes relative to the tensile loading direction is shown in Fig.1. Data collection has been carried out using polychromatic X-ray microbeam (PXM) Laue diffraction on beamline ID-34E at the APS. In this experiment, lattice rotations in a Ni bicrystal tensile sample were determined with PXM during *in situ* uniaxial pulling at 0, 12 and 16% mesoscopic plastic strain. The laboratory Cartesian reference frame is set such that the loading direction is aligned along the X axis (Fig. 1a). The beam is parallel to the Y axis and the sample surface is inclined at 45° to the beam. Dimensions of the beam were 0.46 by 0.55 μm with a penetration depth of ~ 50 μm for Ni sample. Lattice rotation at depth can be resolved to a resolution of ~1 μm by differential aperture microscopy [Larson and Lengeler, 2004; Ice *et al.*, 2005; Ice and Barabash, 2007]. SEM and OIM images, based on electron backscattering, were collected using a Philips XL30 field-emission scanning electron microscope equipped with a DigiView camera.

PXM patterns were recorded along several lines parallel to the sample X-axis at different points with a varying spacing: 2 μm in the vicinity of the boundary and increasing spacing in the regions further (up to 400 μm) from the boundary. In grain A the orientation of the surface normal before deformation was almost parallel to $[233]$ with the loading direction approximately in a $[1\bar{1}0]$ direction. In grain B the X axis is close to the $[\bar{1}25]$ direction with its surface normal close to $[03\bar{1}]$. Bending of slip bands parallel to the boundary is observed in SEM image of the grain B at the distance of several micrometers from the boundary (Fig. 1b). Typical Laue patterns from the deformed A and B grains and the boundary region are shown at Fig. 2. Regions with large strain gradients and high density of geometrically necessary (GN) dislocations manifest themselves by streaking of the Laue spots [Ice *et al.*, 2005; Ice and Barabash, 2007] as observed in Fig.2 b. The plastic response of the material in both A and B grains of the bicrystal can be described by formation of GN and SS dislocation population in the material to relax the stress field induced during pulling. In FCC crystals, typical edge dislocation lines are parallel to the directions of <112> with Burgers vectors being parallel to the directions <110> and corresponding glide planes {111}.

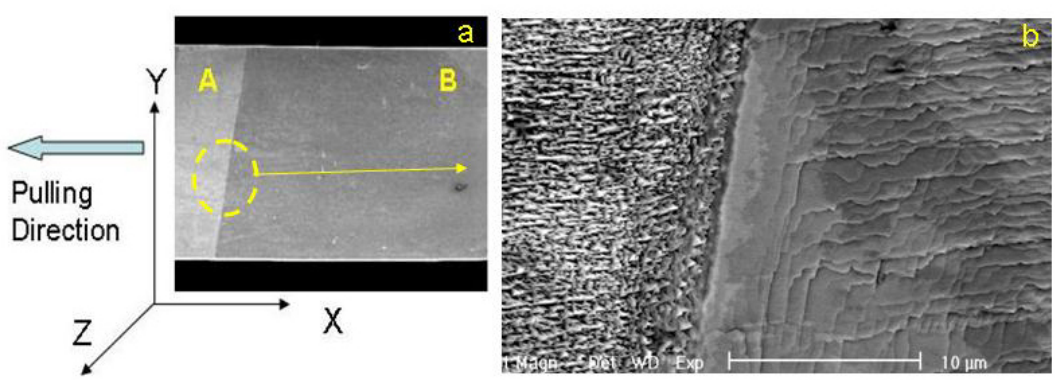

Figure 1. (a) SEM images of the sample showing orientation of the boundary relative to pulling direction; (b) blown up a near boundary region marked with dashed circle at large magnification showing the dislocation lines curving near the boundary.

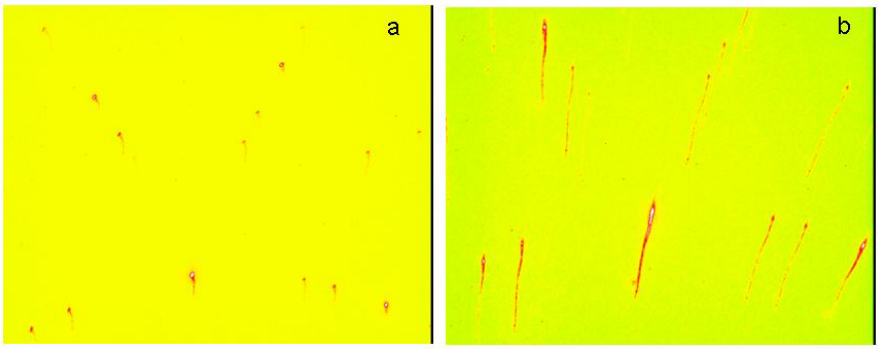

Fig. 2. Typical Laue patterns from the regions with low (a) and large (b) strain gradients.

Finite element simulations were performed using the method developed by Ohashi [Ohashi, 1997; Ohashi, 2005]. For numerical simulations the dimension of the specimen was same that used in experiment. The specimen was meshed in non-uniform manner in x and y direction which enabled one to follow a possible sharp change of physical quantities in the vicinity of the grain boundary and specimen surface. Crystal plasticity analysis together Finite Element simulation confirms experimentally observed dependence of plastic response of both grains on their orientation and initial structural conditions.

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