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Tensile twin nucleation events coupled to neighboring slip observed in three dimensions

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Abstract

Low-symmetry crystals and polycrystals have anisotropic mechanical properties which, given better understanding of their deformation modes, could lead to development of next generation materials. Understanding how grains in a bulk polycrystal interact will guide and improve material modeling. Here, we show that tensile twins, in hexagonal close-packed metals, form where the macroscopic stress does not generate appropriate shear stress and vice versa. We use non-destructive high-energy X-ray diffraction microscopy to map local crystal orientations in three dimensions in a series of tensile strain states in a zirconium polycrystal. Twins and intragranular orientation variations are observed and it is found that deformation-induced rotations in neighboring grains are spatially correlated with many twins. We conclude that deformation twinning involves complex multigrain interactions which must be included in polycrystal plasticity models.
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1. Introduction

Twinning is a plastic deformation mechanism that produces a fixed amount of lattice shear in a given volume. It occurs frequently in materials with crystal symmetry less than cubic and in hexagonal metals such as Zr in particular. Twinning occurs during plastic deformation because of a lack of slip systems (dislocation glide) that operate at sufficiently low resolved stresses. Twinned volumes generally appear as thin plates whose surfaces correspond to the twinning plane; this morphology minimizes the accommodation required in the surrounding material. Twinning is distinct from slip in that it produces a discrete jump in orientation, as opposed to the gradual lattice rotation associated with slip. Thus distinctive signatures of mechanical twinning are that new orientations appear in a material and subdivision of grains occurs. These responses enhance work hardening and are therefore an important component of the plastic response.

Twins have a specific orientation relationship with the parent crystal (or grain), which is determined by the twin plane, twinning direction and magnitude of the shear [1]. In the tensile test performed here, the relevant twin plane is the $\{10\bar{1}2\}$ with shear displacement in the $\langle\bar{1}011\rangle$ direction. This is called a tensile twin because its operation

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results in extension of the grain along the c-axis (of the parent grain) and compression in the transverse plane, thus accommodating the imposed macroscopic strain. The geometry of the twin is such that the orientation relationship is equivalent to a rotation of $2\tan^{-1}\left(\frac{1}{\sqrt{3}}\frac{c}{a}\right)$, or, in Zr, $\sim 85.2^\circ$ about $< 10\bar{1}0 >$ with a shear strain of 0.167. This corresponds to a $\Sigma 11b$ coincident site lattice relationship; as in all such relationships it is useful to keep in mind that crystal symmetry provides for a large number (i.e. 288) of crystallographically equivalent descriptions of any grain boundary, including 180° about the twin plane normal [2,3].

The tendency for a specific grain in a polycrystalline aggregate to twin or slip depends on both its own orientation and those of neighboring grains. One standard metric to quantify the orientation dependence for a particular slip or twin mode to become active is the geometrical Schmid factor [4]:

$$m = \cos\phi\cos\lambda, \tag{1}$$

which resolves the applied force onto the slip plane in the slip direction, ϕ being the angle between the slip plane normal and the applied force and λ that between the force and slip direction. The Schmid factor accurately predicts twinning and twin variant selection in textured materials preferentially oriented for twinning (i.e. those with large Schmid factor) [5]. However, for a given orientation in a polycrystal, one grain can show twin activation while another does not [6]. Thus, orientation alone cannot be the sole determinant [7]. Recent work has shown that local stress states experienced by individual grains can vary significantly from grain-to-grain and that stress tensors have principle components that are rotated relative to the external load [8]. These local stress states should be improved predictors of twinning transitions relative to Schmid factors based on external loading parameters but are much more difficult to calculate or to measure. For example, the effect of neighboring grains has been hypothesized to be associated with the extent to which slip directions are compatible with the shear displacement due to twinning so that “hard” neighbors will impede the transformation while “soft” ones will make it more likely [9].

There exists little empirical evidence with which to quantify neighborhood effects because no measurement has characterized a complete neighborhood and then watched twin formation occur. Bulk texture measurements [10] observe macroscopic changes in c-axis orientation distributions associated with twinning but cannot identify specific grains or environments. Numerous surface studies using electron backscatter diffraction (EBSD) to map local crystal orientations have been performed but these lack neighborhood information below the surface, and the influence of the free surface on the transformation is unclear. Dynamic experiments have been performed which allow the microstructure to evolve, but again EBSD can only capture the surface dynamics which could be very different to the bulk response [11]. A recent hard X-ray measurement observed a twinning event that occurred inside of a bulk Mg sample, but did not resolve the microstructural neighborhood of the grain which is required in order to be able to calculate the stress state [12].

2. Experimental methods

Over the past five years, near-field high-energy X-ray diffraction microscopy (nf-HEDM) [13,14], performed primarily at the Advanced Photon Source at Argonne National Laboratory and combined with the forward modeling method (FMM) of orientation reconstruction [15], has been demonstrated to yield spatially resolved 3-D maps of local crystal orientations across varying levels of plastic deformation [16,17]. Using FMM, 3-D digital representations of microstructures are produced by simulating the measurement and sample using ∼100 Bragg peaks (which are grain projections) for each spatially resolved element of the orientation field [15,16]. With current apparatus and procedures, this method has been shown to exhibit spatial resolution of roughly ∼1 μm and sensitivity to orientation differences of 0.1° [13,16–19].

In the Zr tensile deformation measurements presented here, we use 64.3 keV photons focused to a 1.3 mm × 4 μm beam at the sample position. The optically coupled CCD-based imaging system has a 1.48 × 1.48 μm effective pixel size and 2048 × 2048 pixels. For most of the layer sections probed, diffraction images are collected at rotation axis-to-detector distances of $L = 5.20$ and 7.20 mm. Each image is collected over a sample rotation range $\delta\omega = 1^\circ$ and such images are collected over a 180° contiguous range at each successive L-distance. The counting time depends on the state of deformation and ranges from 2.0 s per image in the well-ordered, $S0$, state to 2.8 s in the final, $S3$ state. The data collection methodology and orientation field reconstruction approach are summarized in Refs. [13,15]. Recent algorithmic developments are presented in Ref. [16] and results on deformed microstructures are illustrated in Ref. [17]. The beamline hardware and data collection parameters used here are similar to those described for near-field measurements in Refs. [13,20].

A voxelized orientation field is determined (without reference to or definition of extended grains) by optimizing, for each voxel, overlap of simulated and experimental intensities corresponding to ∼100 Bragg peaks observed in the experimental space for each orientation. Each voxel has an associated confidence parameter, $\mathcal{C}$, which is defined as the fraction of simulated pixels that overlap experimentally observed signals. The reconstructions exhibit sensitivity to intra- and intergranular orientation variations at the 0.1° level in ordered materials [18,19] with gradual degradation with increased deformation [16,17].

3. Experimental procedure

A tensile load frame was specifically designed to perform this experiment. The main geometrical constraint imposed