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Multi-scale modeling and experimental study of twin inception and propagation in hexagonal close-packed materials using a crystal plasticity finite element approach; part II: Local behavior

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ABSTRACT

In-situ tensile tests are performed on Zircaloy-2 samples with various grain sizes to study twin inception and propagation. Orientation maps of some areas at the surface are measured before and after deformation, using the Electron BackScattered Diffraction (EBSD) technique. Strain fields of the same areas are determined using the digital image correlation technique and are compared with results from Crystal Plasticity Finite Element (CPFE) simulations. Different assumptions are made within the CPFE code to simulate twin propagation. It is observed that the predictions of different models does not really change from one model to another when statistical information on the twins is compared, yet local predictions for each grain, i.e. twin direction, twin variant selection, and twin inception site, do change. Also, it is shown that the twin Schmid factor can vary drastically within grains and that for those grains with a low tendency for twinning this variation may make them susceptible to twinning.

1. Introduction

Characterization of the mechanical response of materials under varied loading conditions can provide insight into the operating micro-deformation mechanisms. Various experimental and numerical methods have been implemented to answer critical questions about deformation mechanisms with the goal of e.g., improvement of in-service life-time of materials. While in-situ deformation studies, such as neutron or synchrotron diffraction are very powerful, and can provide extensive data as to the operating micro-mechanisms (Hutchings et al., 2005) they can be difficult or expensive to perform. Hence laboratory based techniques, such as digital image correlation (DIC), are also an important characterization tool. DIC is a versatile technique that has been used to understand deformation at various length scales from micro to macro. The basic concept behind image correlation is to find features in the images taken from areas of interest at different loading stage and try to find one-to-one correspondence between positions of these features (Lee et al., 1987; Fonseca et al., 2005; Tan et al., 2005; Amy, 2006; Peters and Ranson, 1982). Once the relations between images are resolved, strains can be extracted and deformation evolution can be studied. As the images are usually captured from the surface, strains at the surface can be measured and bulk information, in contrast to penetrating diffraction methods, is not monitored. Crystal plasticity in the finite element framework has been used in parallel with image correlation techniques to answer experimentally-irresolvable questions. Study of materials at this scale usually consist of mapping of grain shapes into a

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finite element solver and investigating the effects of grain–grain interaction on the average and local behavior of materials (Nakamachi et al., 2007; He′ripre′ et al., 2007; Ge′rard et al., 2009; Demir et al., 2010; Merzouki et al., 2010).

Because of their low absorption cross sections towards neutrons, zirconium and its alloys have been extensively used in nuclear reactors. Alpha-zirconium has Hexagonal Close-Packed (HCP) crystal structure with high tendency to twin under tensile loading along the *c*-axis of the crystal. It is known that twins form readily at the stress concentrations of crack tips in zirconium alloys (Kerr et al., 2010). Hence, a precise understanding of the interaction of local neighborhood on twinning has potentially significant practical interest as well as providing insight into the physical mechanism of twinning. In this paper, we report a study of twin formation, including both inception and propagation, in Zircaloy-2 samples.

Deformation twinning at the grain scale in a CPFE framework has been studied to some extent. Texture evolution as well as deformation and activity of twin variants of each grain were studied by Prakash et al. (2009) and Choi et al. (2010). To reduce numerical instability, an implicit-dynamic formulation was implemented by Barton et al. (2009) to model twin formation in a 125 grain polycrystal. A good picture of twin formation is presented in Barton et al.'s work, but the lack of CPFE results being compared with experiment, leaves questions as to the assumptions made. Formation of twins in single crystal zinc has been studied by Forest and Parisot (2000) where twin nucleation was virtually controlled by introducing a geometrical defect and twin growth was the result of the motion of the localization front on one or both sides of the twin, in the spirit of Maugin (1998). In the current study, local twin formation in Zircaloy-2 polycrystal samples is studied experimentally as well as numerically. Grain orientations and geometries at the surface of the samples are measured for different samples before and after uniaxial straining. In-situ tensile tests are carried out in an SEM chamber where grains' strains are measured by the digital image correlation technique. Grain maps are imported into the ABAQUS FE solver to study inception and propagation of twins using different assumptions within a crystal plasticity formulation. The CPFE results are compared against experimental results both locally and statistically.

2. Experimental procedure

Set one of dog bone samples (S1) with 14 mm gauge length, 3 mm width, and 2 mm thickness were prepared from a previously well characterized Zircaloy-2 slab (Xu et al., 2008b, 2009; Mareau and Daymond, 2010). The initial texture of the slab is shown in Fig. 1a. Due to having a relatively small grain size ($\sim$13 μm) and an inability to readily resolve grain boundaries in S1, cubes from the original slab were cold-rolled to 10% (compression along previous rolling direction with 10% thickness reduction) and then heat treated at 720 °C for 48 h. The heat treatment was conducted in an Argon gas environment to prevent oxide layer formation. This resulted in a material with equiaxed grains and average grain size of 50 μm; from which a second set of dog-bone samples (S2) were prepared, with the same dimensions as S1. One side of each sample was mechanically polished down to 1200 grid and then with 6, 3, and 1 μm diamond paste. Subsequent attack polishing of the samples was performed with a solution of 5% H_2O_2, 5% HNO_3, 5% HF, and 85% H_2O for 15 s several times until it resulted in a shiny surface with no visible scratches. A micro-indent was then placed on each sample's surface to define the sample coordinate system for pre- and post-loading EBSD as well as image analysis on the same area. Samples were finally electro-polished for 60 s at 25 V in a -30 °C solution of 10% perchloric acid and 90% methanol. The quality of EBSD indexing process at each point can be characterized by a parameter called Mean Angular Deviation (MAD) that reflects how close the indexed pattern is to the standard values available in the internal library of the indexing program. In our EBSD measurement, points with MAD >0.7 are considered as un-indexed point. Also, for identification of grain boundaries, more that 5° misorientation was not allowed within each grain.

Orientation maps of some selected areas in S2 samples were measured before applying load; three different areas with a total 775 grains were investigated in this set. The initial texture of the S2 set achieved from these areas is shown in Fig. 1b. Similar to S1 set, the normal to basal planes are mostly oriented toward Normal Direction (ND). Hence, tensile load was applied along the ND to activate twinning; the tensile stage was placed in a JEOL-840 SEM chamber where images from the selected areas were captured at different loading steps. The loading process was under load control during elastic deformation and strain control ($\dot{\varepsilon}=5.5\times10^{-5}$ s^{-1}) during plastic deformation. The average flow curves of the S1 and S2 series are shown in Fig. 1c. Orientation maps of the selected areas were measured again after 3% straining. Fig. 1d shows the post-deformation texture of the S2 set.

Due to difficulties in achieving good post-deformation EBSD patterns on the small grain size material, we did not carry out pre-deformation EBSD and image analysis on the S1 set. Instead, post-deformation orientation maps of two different areas were measured from an annealed S1 sample. As the recrystallization temperature of Zircaloy-2 is 450 °C (Lee, 1970), S1 samples were annealed at 300 °C for an hour; this recovered sufficient dislocation density that EBSD mapping could be achieved, while it should not remove twins (Lee, 1970). In order to create a 'starting' microstructure for modeling, the twins were identified by orientation relationship and shape, then removed from the grain map; these modified approximate starting maps were used for the starting point of the CPFE simulations. In total 1016 parent grains were investigated in the S1 set.

3. CPFE simulation

3.1. Input models

The pre-deformation orientation maps of grains, either directly determined (S2) or extrapolated (S1) were used to generate input files for the FE solver. For this purpose, the average orientation of each grain was calculated (Cho et al., 2005;