

Evidence for basal $\langle a \rangle$ -slip in Zircaloy-2 at room temperature from polycrystalline modeling

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Abstract

Polycrystalline modeling has been used to interpret the evolution of lattice strain and texture in zirconium based alloys. Challenges in matching model and experimental results have mainly arisen from an insufficient knowledge of intrinsic deformation mechanisms (slip and twinning). Specifically, there is little concrete evidence that basal $\langle a \rangle$ -slip occurs during room-temperature deformation or whether pyramidal $\langle a \rangle$ -slip is an alternate mechanism. Also, the critical resolved shear stresses (CRSSs) for slip and twinning systems relevant to polycrystals are not well established. We have developed an understanding of the contribution of basal $\langle a \rangle$ -slip to deformation by applying an elasto-plastic self-consistent model to an extensive experimental database, obtained by neutron diffraction measurements on textured Zircaloy-2. By considering a variety of slip system combinations, the roles of each slip system in lattice strain development were investigated. Parameters for the model were obtained by best fitting to a large experimental database, including both macroscopic data (flow curves and Lankford coefficients) and microscopic internal strain data. Based on optimized agreement between model and experimental data we conclude that there is evidence that basal slip does occur, while the effects which might be attributed to pyramidal $\langle a \rangle$ -slip can be represented by the influence of other combinations of slip systems. We propose reasonable ranges of initial CRSSs for each slip system, which should benefit the modeling of similar materials (e.g. Zircaloy-4).

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1. Introduction

Zirconium and its alloys are characterized by pronounced mechanical anisotropy, which originates from the anisotropic single crystal *hcp* structure and bulk crystallographic texture. This anisotropy is manifest in the thermal expansion coefficients, elastic moduli, and plastic properties, i.e. different critical resolved shear stresses (CRSS), and hardening behavior for different slip and twinning systems. The plastic deformation mechanisms observed in Zr and its various alloys [1] include slip in $\langle a \rangle$ -direction: $\{10\bar{1}0\}\{11\bar{2}0\}$ prism slip (pr), $\{0001\}\{11\bar{2}0\}$ basal slip (bas) and $\{10\bar{1}1\}\{11\bar{2}0\}$ pyramidal slip (pya); slip in $\langle c + a \rangle$ -direction: $\{10\bar{1}1\}\{11\bar{2}3\}$ first-order pyramidal slip (pyca) and $\{11\bar{2}1\}\{11\bar{2}3\}$ second-order

pyramidal slip; tensile twinning: $\{10\bar{1}2\}\{10\bar{1}1\}$ (tt) and $\{11\bar{2}1\}\{11\bar{2}6\}$; and compressive twinning: $\{11\bar{2}2\}\{11\bar{2}3\}$ and $\{10\bar{1}1\}\{10\bar{1}2\}$. Prism slip is the most easily activated (i.e. has the lowest CRSS) and is always present when a polycrystal is deformed regardless of deformation conditions. Other deformation systems are activated only under specific circumstances, i.e. combinations of temperature and stress sense relative to the bulk texture. For example, tensile twinning is activated only when the $\langle c \rangle$ -axis of a particular crystal is placed under tension.

There is general agreement in the literature that deformation of Zr and its alloys at room temperature is accommodated by prism $\langle a \rangle$ -slip, first-order pyramidal $\langle c + a \rangle$ -slip and $\{10\bar{1}2\}\{10\bar{1}1\}$ tensile twinning. The experimental evidence, derived from single-trace methods [2] or transmission electron microscopy (TEM) observations, has been well documented for the presence of prism slip [3–5] and pyramidal $\langle c + a \rangle$ -slip [6–8], as well as tensile twinning [4,9,10]. Prism slip always activates first with

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increasing applied stress. As a higher stress is applied, the $\langle a \rangle$ dislocations accumulate, forming local stress concentrations where it is possible for cross-slip to operate. Cross-slip of the $\langle a \rangle$ dislocations is a likely mechanism for the initiation of basal slip and/or pyramidal $\langle a \rangle$ -slip. However, there is little conclusive experimental evidence of the presence of these two slip systems to date, principally due to the difficulty in unambiguously identifying the slip plane by TEM observations. Slip markings belonging to (or close to) basal traces have been discovered in (1) single crystal Zr (99.8–99.9 wt%) in regions of stress concentration at room temperature [11], (2) single crystal Zr at elevated temperatures [12], (3) commercial grade Zr near hydride particles [5], (4) irradiated Zircaloy [13] and (5) polycrystal Zr at elevated temperatures during kink formation [14]. In brief, there is no direct evidence for basal slip in polycrystal Zr alloys at room temperature, but there is evidence for basal slip under other circumstances. To the best of our knowledge, there is no published evidence for pyramidal $\langle a \rangle$ -slip under any circumstances (the paper cited in Ref. [15] was not published).

The inclusion of basal slip in the polycrystalline modeling (e.g. elasto-plastic [16] and visco-plastic self-consistent [17] models) has been found to improve the ability to reproduce experimental macroscopic flow curves [18] and bulk texture development [19–21] caused by plastic deformation. However, other researchers [15,22–24] have instead preferred to include pyramidal $\langle a \rangle$ -slip as an alternative to basal slip in order to achieve optimal agreement with their experimental data.

The lack of sufficient knowledge regarding values of CRSSs appropriate for deformation systems also constitutes a difficulty for performing polycrystalline modeling. Practically, CRSSs must be derived indirectly through polycrystalline modeling using an ‘inverse approach’ [25], since the manufacture of single crystals of many alloys to allow measurement of the CRSSs is either very difficult or in some cases impossible. Further, the observed CRSSs required for model fitting in a polycrystal will be different from those found in a single crystal due to the interactions of the dislocations with grain boundaries.

In this paper we aim to provide a better understanding of the influence of basal slip and its contribution to polycrystalline plasticity. Through *in situ* tension and compression tests in neutron spectrometers, we have obtained an extensive experimental data set of both flow curves and internal lattice strain development along the three principal directions of a textured Zircaloy-2 slab. These data are reported in full in Ref. [26]. This data set represents a far more extensive data set than that available elsewhere in the literature, and hence a more exacting test of polycrystal models.

This paper considers a variety of combinations of deformation systems, using a previously published elasto-plastic self-consistent model (EPSC [16]). The model results are compared to the experimental flow curves, the Lankford coefficients (also referred to as R values), and internal lat-

tice strain development. In particular, we illustrate the influence of basal slip. Reasonable ranges of CRSSs for the commonly selected slip systems are also provided, which may be helpful for the modeling of similar materials (e.g. Zircaloy-4).

2. Background

2.1. Neutron diffraction measurements

We performed the *in situ* neutron diffraction measurements at different sites, using the time-of-flight technique for the compression tests at the ISIS neutron source, Rutherford Appleton Laboratory, UK, and using the constant-wavelength technique for the tensile tests at NRU reactor, Chalk River Laboratories, Canada. We have corrected the tensile test data to a strain rate equivalent to that used in the compression tests [26], for the purpose of direct comparisons. The experimental set-up for each of the neutron diffraction techniques is described in Refs. [27,18]. For the time-of-flight measurement, the sample is placed horizontally at 45° to the (horizontal) incident white beam, with two detector banks sitting at scattering angles of $\pm 90^\circ$. This allows a concurrent measurement of lattice spacings in the loading direction and one of the two Poisson directions. Two tests are needed to obtain the lattice strain development in three principal directions. In a constant-wavelength test, only one detector is used. The sample is positioned so that the scattering vector is parallel to either the loading direction or either of the two Poisson directions. Three samples are needed for a three-dimensional lattice strain measurement. In a neutron measurement, an ‘orientation’ comprises a family of grains with a particular plane normals lying within a few degrees off the nominal orientation (roughly $\pm 6.5^\circ$ at ISIS and $\pm 0.5^\circ$ at NRU) corresponding to the crystals contributing to one measurement. Note that the measured lattice strain is the average lattice strain for an ‘orientation’.

2.2. Elasto-plastic self-consistent model

The EPSC model is an Eshelby equivalent inclusion model, which deals with interactions between Eshelby inclusions and an infinite homogeneous effective medium (HEM) that is subjected to an external load. Each inclusion represents a particular grain orientation. The inclusions, the HEM and the interactions between them are both elastically and plastically anisotropic and the properties of the HEM are the weighted average properties of all the inclusions. A solution is obtained by iteration until the response of the HEM correctly represents the overall response of the polycrystal. The polycrystal can be textured, with grain populations being grouped into different families according to their orientations. A more detailed description of the model can be found elsewhere [16].

The model generates the macroscopic flow history, and as well, it produces the lattice strain evolution for each

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