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Modeling lattice strain evolution during uniaxial deformation of textured Zircaloy-2

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Abstract

An elastoplastic self-consistent model was used to interpret the experimental lattice strain evolution previously reported for testing in three directions of a thick polycrystalline Zircaloy-2 slab. The model was used to infer the underlying deformation mechanisms. The influences of prism $\langle a\rangle$ slip, basal $\langle a\rangle$ slip, pyramidal $\langle c+a\rangle$ slip and tensile twinning were considered. The critical resolved shear stresses and hardening parameters for each mode were obtained by simultaneously fitting the macroscopic flow curves, Lankford coefficients and internal elastic strain development for all diffraction peaks, for the combination of three measurement directions and three loading directions, for compression and tension. The effects of dislocation interactions during deformation and hardening between deformation modes were considered. Tensile twinning inferred from the intensity changes of the diffraction peaks and its activity was qualitatively reproduced by the simulations for compression in the plate rolling and transverse directions and tension in the plate normal direction.

Keywords: Zirconium alloys; Residual stresses; Neutron diffraction; Texture; Plastic deformation

1. Introduction

Zircaloy-2 and the very similar alloy Zircaloy-4 have extensive applications in the nuclear industry. They are predominantly (>98%) zirconium, with a hexagonal close-packed (hcp) structure that exhibits anisotropic thermal, elastic and plastic properties. The elastic and plastic anisotropy are responsible for striking differences in the local stress–strain response of the differently oriented grains in polycrystals. The intergranular stresses that are generated by thermal and mechanical treatment are complex in origin, but can be interpreted with the aid of polycrystalline models [1], leading to an understanding of the relative contributions of different micromechanical deformation modes to the macroscopic strain. The models can be used to optimize processing routes and predict lifetimes of reactor components.

The differences in stress experienced by differently oriented grains in a Zircaloy polycrystal arise from several sources, all due to the combination of an anisotropic single crystal that is constrained within a polycrystal, which itself may be anisotropic if the material is textured. The constraint can be due entirely to thermal anisotropy; as the material cools after a thermal treatment, stresses are induced. During mechanical loading, differences in the elastic properties of the grains lead to distribution of the load between the grains, in a manner analogous to composite load sharing. Subsequent plastic flow will also be anisotropic due to a combination of the differences in Schmidt factor, differences in critical resolved shear stresses (CRSS) for different deformation modes and differences in stresses in the grains (due to elastic anisotropy). This plastic anisotropy causes further redistribution of the applied load between grains of different orientations.

A difficulty in studying material properties of the Zircaloys and many other modern alloys is the near impossibility of growing even moderate-sized single crystals to make direct measurements of the single crystal properties. In

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addition, the intergranular constraints and presence of grain boundaries in Zircaloy polycrystals are likely to produce differences in the single crystal properties of the aggregate from those of unconstrained single crystals. Hence, matching the results of polycrystalline plasticity models with the experimental data is the only practical means to derive the single crystal properties in a textured polycrystal. Broadly, two classes of the polycrystal plasticity models have been popular in recent years: finite element crystal plasticity models and elastoplastic self-consistent models. The latter is used in this paper.

Here, we model the internal strain evolution of samples cut from a moderately textured Zircaloy-2 slab. An extensive set of experimental measurements of internal strain evolution has been made by neutron diffraction and are reported in Ref. [2]. Compression and tension tests were carried out in situ during neutron diffraction in each of the three principal slab directions (i.e. rolling, transverse and normal) to over 10% strain. For each loading case, lattice strains were measured in all three principal directions. Based on the results obtained from an elastoplastic self-consistent model, we interpret the internal strain evolution by exploring the contributions of the different deformation mechanisms. In the modeling process, we take into account prism $\langle a\rangle$ slip, basal $\langle a\rangle$ slip, pyramidal $\langle c+a\rangle$ slip and tensile twinning modes. The CRSSs and hardening parameters for each mode are derived through simultaneous fitting of the macroscopic flow curves, Lankford coefficients and lattice strain development for all diffraction peaks for all 18 combinations of measurement and loading directions.

This is the first attempt to derive such model parameters by fitting to such an extensive data set. Due to the use of the large data set, it was possible to ascertain that the effects of dislocation interactions on hardening between deformation modes play an important role in determining both internal and macroscopic strains; to date little attention has been paid to this subject.

2. Summary of experimental work

Only a brief summary of the experimental method and observations is given here and the model is compared with various subsets of the entire data set. The entire data set is available elsewhere [2].

The Zircaloy-2 slab from which the specimens were machined was warm rolled after preheating to ~700 K, then cooled to room temperature. Transmission electron microscopy showed the material to be fully recrystallized, indicating that it had reached a temperature of at least 900 K during processing [3], likely as a result of adiabatic heating. The grains are equi-axed with an average size of ~20 μm, and the material has a typical rolling and recrystallization texture, i.e. most $\{0002\}$ normals are orientated along the normal direction (ND) with a spread of ±50° towards the transverse direction (TD) and ±30° towards the rolling direction (RD), and most $\{10\bar{1}0\}$ normals are orientated at ±30° from RD in RD–TD plane [4]. In hcp materials the proportion of basal normals in a particular direction in the sample has a major impact on the deformation response and the texture of the slab provides distinctly different proportions of basal plane normals in the principal directions.

The data presented in Ref. [2] were obtained by neutron diffraction measurements with the gauge volume centered at the mid-height (or mid-length) of the specimens where the deformation can be reasonably assumed to be uniform. Lattice strains were calculated by the shift of the peaks, i.e.

$$\varepsilon_{hkil} = \frac{d_{hkil} - d_{\text{ref}}}{d_{\text{ref}}} = \frac{\sin\theta_{\text{ref}}}{\sin\theta_{hkil}} - 1 \tag{1}$$

where ε_{hkill} is the lattice strain of grain family $\{hkil\}$; d_{ref} and d_{hkil} are the plane spacings before and after deformation, respectively; and θ_{ref} and θ_{hkil} are the diffraction angles before and after deformation, respectively.

Plotted lattice strains are calculated with respect to the start of each test, and therefore represent the increment produced by loading only. Note that the lattice strain is the averaged response over all the grain orientations that satisfy the Bragg's law for a particular $\{hkil\}$ in the gauge volume.

The experimental results are briefly summarized as the following:

(1) On the microscopic scale, $\{10\bar{1}0\}$ and $\{11\bar{2}0\}$ grains parallel to the applied load always yield first as the applied load is increased and $\{0002\}$ grains yield last, or in some cases never yield.
(2) In the plastic regime but at low strains (<2.5%), when measurements were taken parallel to the loading direction, the deviation of the basal orientation strains from elastic linear response is always negative irrespective of the sense of applied stress; the deviations of the prism plane strains are positive compared to the elastic response under compressive loading, while they are negative in tension. When measurements were made in the Poisson directions, generally under compressive loading the lattice strains deviate positively from the elastic linear response for prism planes and negatively for basal planes, in perfect opposition to the behavior in tension.
(3) Both the flow curves and the development of lattice strains are asymmetrical, i.e. there is a significant strength differential between tension and compression and there are substantially larger deviations in lattice strain amongst different crystallographic orientations in the test direction for compression than for tension. The reverse is true for the Poisson directions.
(4) Strong evidence was found for tensile twinning in tensile tests in the plate normal direction and also for tests where compressive loading was applied in TD and RD. The texture changes in these specimens were consistent with the occurrence of tensile twinning [5] and the presence of tensile twins was confirmed by transmission electron microscopy and scanning