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A dislocation-based constitutive law for pure Zr including temperature effects

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Abstract

In this work, a single crystal constitutive law for multiple slip and twinning modes in single phase hcp materials is developed. For each slip mode, a dislocation population is evolved explicitly as a function of temperature and strain rate through thermally-activated recovery and debris formation and the associated hardening includes stage IV. A stress-based hardening law for twin activation accounts for temperature effects through its interaction with slip dislocations. For model validation against macroscopic measurement, this single crystal law is implemented into a visco-plastic-self-consistent (VPSC) polycrystal model which accounts for texture evolution and contains a subgrain micromechanical model for twin reorientation and morphology. Slip and twinning dislocations interact with the twin boundaries through a directional Hall–Petch mechanism. The model is adjusted to predict the plastic anisotropy of clock-rolled pure Zr for three different deformation paths and at four temperatures ranging from 76 K to 450 K (at a quasi-static rate of 10^{-3} 1/s). The model captures the transition from slip-dominated to twinning-dominated deformation as temperature decreases, and identifies microstructural mechanisms, such as twin nucleation and twin–slip interactions, where future characterization is needed.
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1. Introduction

This work is part of a comprehensive study focused on the deformation mechanisms in hcp materials and incorporating them into constitutive laws for the plastic deformation of hcp materials. Our previous work clearly establishes the necessity of applying a crystallographic approach for this pursuit (as opposed to continuum type hardening laws), in order to account for the variety of slip and twinning modes present in the grain, their relative strengths, and their relative activity depending on their orientation with respect to the loading direction. In addition, crystallographic texture and twin evolution strongly influence macroscopic hardening and anisotropy of the mechanical response and therefore, need to be incorporated into constitutive models.

In the past we used Voce-type hardening for the critical resolved shear stress of slip and twinning, and implemented it into a visco-plastic self-consistent (VPSC) polycrystal model (Lebensohn and Tomé, 1993; Tomé and Lebensohn, 2004). Using this approach, constitutive descriptions for Zr applicable to fixed temperatures (76 K or 300 K) (Tomé et al., 2001) and strain path changes (Yapici et al., in press) have been developed. This formulation was later applied to predict the flow response of Zr when the temperature changes from 76 K to 300 K while keeping the test direction fixed (Kaschner et al., 2006). In these applications the treatment of twinning was greatly simplified. Twin reorientation was modeled according to a Predominant Twin Reorientation scheme (Tomé et al., 2001), in which the original grain orientation is replaced by the orientation of its most active twin. Twin–twin or twin–slip interactions were modeled via empirical latent hardening factors, which were assumed to be temperature independent. This twin model proved to be too simplistic for modeling strain path changes, where twins introduced in the pre-load stage act as directional barriers to newly activated systems in the reload stage. As a consequence, we improved the treatment for twinning by representing each twinned grain as a Composite Grain (CG) consisting of layers of twin and matrix (see Fig. 1). This approach allows us to account for the directional barriers that a specific twin poses to specific dislocations via a Hall–Petch effect. With this CG approach, VPSC effectively predicted the texture and hardening evolution when clock-rolled Zr is deformed in compression along the in-plane direction followed by compression along the through-thickness direction (and vice versa) (Proust et al., 2007).

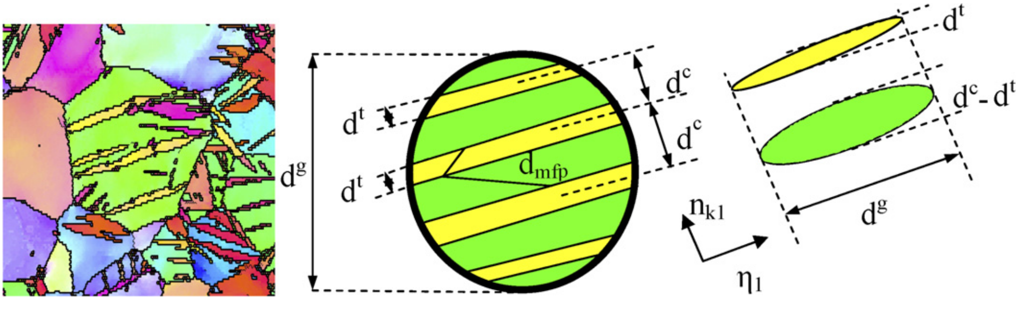

Fig. 1. EBSD image of Zr deformed 5% at 76 K. Schematic of Composite Grain model implemented in VPSC, showing morphology and orientation of twins and matrix, and indicating the parameters of the Composite Grain model.