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Incorporation of twinning into a crystal plasticity finite element model: Evolution of lattice strains and texture in Zircaloy-2

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ABSTRACT

A crystal plasticity finite element code is developed to model lattice strains and texture evolution of HCP crystals. The code is implemented to model elastic and plastic deformation considering slip and twinning based plastic deformation. The model accounts for twinning reorientation and growth. Twinning, as well as slip, is considered to follow a rate dependent formulation. The results of the simulations are compared to previously published *in situ* neutron diffraction data. Experimental results of the evolution of the texture and lattice strains under uniaxial tension/compression loading along the rolling, transverse, and normal direction of a piece of rolled Zircaloy-2 are compared with model predictions. The rate dependent formulation introduced is capable of correctly capturing the influence of slip and twinning deformation on lattice strains as well as texture evolution.

1. Introduction

Polycrystalline materials can have grains with a non-random distribution of crystal orientations or texture. The overall deformation of polycrystal materials is influenced by the properties and morphology of each single crystal and how these combine at different length scales. The crystal plasticity class of constitutive models can be used to model deformation and texture evolution of polycrystals, taking into account the effects and interactions of each grain or families of grains. The constitutive model is based on decomposing the deformation into an elastic stretching of the crystal lattice and permanent deformation due to twinning and slip, i.e. motion of dislocations through the lattice. The concept of crystal plasticity was shaped by contributions of Taylor, Schmid and their coworkers (Taylor and Elam, 1923; Schmid and Boas, 1935) after early qualitative observations of slip in aluminum. Quantitative analysis of slip based plastic deformation is feasible by a number of constitutive models, e.g., that established by Asaro and Needleman (1985). The nature of this formulation is such that a wide variety of modeling can be performed to inspect both local and global behavior of materials. Slip based crystal plasticity has shown noticeable success in, e.g., modeling grain boundary mechanics (Mika and Dawson, 1999; Kanjarla et al., 2010; Diard et al., 2005), texture evolution (Li et al., 2004), yield surfaces of single crystals (Zamiri et al., 2007; Zamiri and Pourboghrat, 2010), and surface roughening (Hamelin et al., 2011).

The complexity of modeling deformation in hexagonal close packed (HCP) materials originates from the anisotropic single crystal properties and highly textured structure found in most practical HCP materials. In these types of metals, the low number of easy slip systems, their asymmetric distribution, and the strict crystallographic orientation relationships for twinning result in the formation of a strong deformation textures (e.g. Tenckhoff, 2005). A low number of easy slip systems also tends to promote deformation by twinning. In the current study, a dilute zirconium alloy with HCP crystal structure and moderately high tendency to twin is considered as a case study. Zirconium and its alloys are extensively used in various

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