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# Evaluation of elastic–viscoplastic self-consistent polycrystal plasticity models for zirconium alloys

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ABSTRACT

Our elastic viscoplastic self-consistent (EVPSC) model is improved by including thermal strain to allow study of the behavior of a Zircaloy-2 slab under moderately large strains. The approach of introducing thermal strain effect is similar to the one developed by Turner et al. (1995) and used by Xu et al. (2008a). Various self-consistent schemes (SCSs) of the EVPSC model are then evaluated in terms of the deformation behavior of the material under different uniaxial strain paths. The material parameters for the various models are determined by fitting experimental data from uniaxial tension and compression tests along the normal direction (ND) and from uniaxial tension tests along the rolling direction (RD). The quality of the various SCS predictions is assessed based on comparisons of macroscopic deformation behavior (stress–strain curves and R-values) and microscopic mechanical response (the evolution of lattice strains and texture coefficients) between the predicted and experimental data. It is revealed that the Affine and Meff = 0.1 self-consistent models give much better performance than the Secant and Tangent models.



## 1. Introduction

Due to the variety of slip and twinning systems typically active in Hexagonal-Close-Packed (HCP) crystals, aggregates of HCP crystals often show strong anisotropic mechanical behavior. As a result, the predicted overall mechanical response of a polycrystal depends strongly on how the various slip and twinning systems are activated and evolve with deformation in different grain orientations, and is thus very sensitive to the homogenization method used in the model. The wide variation in grain response in HCP metals such as zirconium and its alloys provides an excellent opportunity to evaluate various homogenization methods used in models of polycrystal plasticity.

Different homogenization schemes have been employed to model polycrystal plasticity. The self-consistent approach (Kroner, 1958; Hill, 1965; Hutchinson, 1976) has proven to be more suitable than the classic Taylor model (Taylor, 1938) for modeling mechanical behavior of HCP polycrystals (see e.g. MacEwen et al., 1983; Wang et al., 2010a). In self-consistent models, all grains with the same orientation are treated as a single inclusion embedded in a Homogenous Effective Medium (HEM), which is the aggregate of all inclusions. Grain interaction is captured indirectly through the interactions of the inclusions with the HEM using the Eshelby inclusion formalism (Eshelby, 1957). The macroscopically imposed stress and strain coincide with the corresponding averages for the aggregate without imposing equal strains (or stresses) for all the grains. Among the self-consistent plasticity models, the Elasto Plastic Self-Consistent (EPSC) model (Turner and Tomé, 1994), the Visco-Plastic Self-Consistent (VPSC) model (Molinari et al., 1987; Lebensohn and Tomé, 1993) and the Elastic–Viscoplastic Self-Consistent (EVPSC) model (Wang et al., 2010b) have been successfully employed to simulate the deformation behavior of HCP polycrystals (Agnew and Duygulu, 2005; Clausen et al., 2008; Hutchinson et al., 2012; Muránsky et al., 2008, 2009; Neil and Agnew, 2009; Oppedal et al., 2013; Xu et al., 2008a, 2009; Turner et al., 1995; Wang et al., 2010c,d, 2011, 2012a,b, 2013b,c; Wu et al., 2012; Guo et al., 2013; Qiao et al., 2015). It is now generally accepted that the numerical results are very sensitive to the stiffness of the grain-matrix interaction associated with different self-consistent schemes (SCSs). Various SCSs have been evaluated by Wang et al. (2010a) through the study of the deformation behavior of a magnesium alloy AZ31B sheet under different uniaxial strain paths. It was found that the Affine self-consistent scheme gave the best overall performance among the SCSs examined.

In the nuclear industry, zirconium alloys (for example Zircaloy-2, Zircaloy-4 and Zr-2.5Nb) are used for pressure tubes

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and for thin-walled fuel cladding (Murty and Charit, 2006). Single phase zirconium alloys have an HCP crystal structure over a wide temperature range (alpha phase) and exhibit strong anisotropy in thermal, elastic and plastic properties. The thermal expansion coefficient along the *c*-axis is nearly twice that along the *a*-axis, resulting in strong thermal intergranular residual stresses after cooling from an elevated temperature. The elastic properties of alpha-zirconium are also anisotropic. The most readily activated slip mode in alpha-zirconium and its alloys over a wide temperature range is prismatic $\langle a\rangle$ slip $\{10\bar{1}0\}\langle 11\bar{2}0\rangle$. Zirconium alloys have been extensively studied experimentally in terms of stress–strain behavior, evolution of texture, and evolution of internal elastic strain (Francillette et al., 1998; Castelnau et al., 2001; Tomé et al., 2001; Proust et al., 2007; Xu et al., 2008a,b, 2009).

For Zr alloys, the EPSC model is usually used to study lattice strain evolution at relatively small strains, while the VPSC model has been most frequently applied to study the stress–strain response, texture evolution and R-value. However, the EPSC model works only for small deformation and earlier EPSC models did not include texture evolution associated with slip or twinning reorientation. Clausen et al. (2008) extended the EPSC model by including texture development and stress relaxation due to twinning, while Neil et al. (2010) developed a large strain EPSC model to approximately account for the kinematics of large strain, rigid body rotations, texture evolution and grain shape evolution. However, the rate-insensitive character of the constitutive law upon which the EPSC model is based prevents us from addressing strain rate-sensitivity in general, and the experimentally observed stress relaxation and creep associated with finite hold times for acquisition of lattice-strain data. Such macroscopic relaxation and creep can only be accounted for using a rate-sensitive elastic–plastic model.

Mareau and Daymond (2010) proposed an Elasto-Viscoplastic Self-Consistent (EVPSC) model to study the development of lattice strains in a moderately textured Zircaloy-2 slab. However, their EVPSC model is applicable only to small deformations. The large strain EVPSC model developed by Wang et al. (2010b) is a completely general elastic–viscoplastic, fully anisotropic, self-consistent polycrystal plasticity model, applicable to large strains and to any crystal symmetry. The EVPSC model has been used to study lattice strain evolution in magnesium alloys (Wang et al., 2012b) and stainless steels (Wang et al., 2013a). Very recently, Lee et al. (2014) applied the EVPSC model to understand the deformation mechanisms during loading and unloading under uniaxial tension in a solid-solution-strengthened extruded Mg–9 wt.%Al alloy. Wu et al. (2014) employed the real-time in-situ neutron diffraction technique under continuous loading combined with numerical simulations using the EVPSC model to study the twinning and detwinning behavior of a wrought AZ31B Mg alloy.

In the present paper, various self-consistent polycrystal plasticity models for HCP polycrystals are evaluated by studying the strain behavior of a Zircaloy-2 slab under different deformation processes; strains up to 20% are considered, for which grain rotation is significant. In order to take into account the effects of thermal residual strains generated during the cooling process (from 898 K to 298 K) on the subsequent mechanical loading, the EVPSC model developed by Wang et al. (2010b) is extended by including the thermal strain effect. Values of the material parameters for the various models are fitted to experimental uniaxial tension and compression stress–strain curves along the normal direction (ND) and uniaxial tension along the rolling direction (RD). These values are then used to predict uniaxial tension and compression along other directions. An assessment of the predictive capability of the polycrystal plasticity models is made based on comparisons of the predicted and experimental stress responses, *R*-values, lattice strains, and texture coefficients. The experimental data are taken from Xu et al. (2008a,b, 2009).

Though the mechanical behavior of Zr alloys under various deformation processes has been extensively studied, both experimentally and numerically (see e.g. Camposilvan et al., 2014; Gloaguen et al., 2014; Gurao et al., 2014; Kapoor et al., 2014; Keskar et al., 2014; Li et al., 2014; Morrow et al., 2014; Mozzani et al., 2014; Muránsky et al., 2014; Padilla et al., 2012; Sattari et al., 2014; Knezevic et al., 2013; Yapici et al., 2009), the experiments performed on a Zircaloy-2 slab by Xu et al. (2008a,b, 2009) represent the most extensive sets of currently available experimental data for a Zr polycrystal. We believe that the predictive capability of self-consistent plasticity models can be most efficiently assessed using the experimental data of Xu et al. (2008a,b, 2009).

The Crystal Plasticity based Finite Element (CPFE) approach has also been used to study the large strain behavior of polycrystalline materials (see e.g. Abdolvand and Daymond, 2013; Alharbi and Kalidindi, 2015; Choi et al., 2011; Fernandez et al., 2011; Hama et al., 2014; Ghosh and Anahid, 2013; Herrera-Solaz et al., 2014; Lim et al., 2014; Wu et al., 2004; Zhang et al., 2015). In CPFE simulations, an element of the finite element mesh represents either a single crystal or a part of a single crystal, and the constitutive response at an integration point is described by the single crystal constitutive model. This CPFE approach enforces both equilibrium and compatibility throughout the polycrystalline aggregate in the weak finite element sense (Anand and Kalidindi, 1994; Bronkhorst et al., 1992). Furthermore, the CPFE approach allows consideration of grain morphology and the modeling of deformation inhomogeneity within individual grains (Wu and Lloyd, 2004; Wu et al., 2007; Kanjarla et al., 2010). However, CPFEM simulations are computationally much more intensive than the corresponding self-consistent polycrystal calculations.

The paper is organized as follows: In Section 2, we describe the theoretical basis for including thermal strains in the EVPSC model. The results of the simulations are presented, compared with the experimental data, and discussed in Section 3. Conclusions are presented in Section 4.

## 2. The EVPSC model

The total strain in a single crystal is composed of elastic strain, thermal strain and plastic strain. The elastic constitutive equation for a crystal is as follows:

$$\overset{\nabla^*}{\boldsymbol{\sigma}} = \mathscr{L} : \dot{\boldsymbol{\varepsilon}}^e - \boldsymbol{\sigma}\mathrm{tr}(\dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^T) \tag{1}$$

where $\mathscr{L}$ is the fourth order elastic stiffness tensor, $\dot{\boldsymbol{\varepsilon}}^e$ is the elastic strain rate tensor, $\dot{\boldsymbol{\varepsilon}}^T$ is the thermal strain rate tensor and $\overset{\nabla^*}{\boldsymbol{\sigma}}$ is the Jaumann rate of the Cauchy stress $\boldsymbol{\sigma}$ based on the lattice spin tensor $\boldsymbol{w}^e$

The thermal strain rate $\dot{\boldsymbol{\varepsilon}}^T$ relates to the temperature rate $\dot{T}$

$$\dot{\boldsymbol{\varepsilon}}^T = \boldsymbol{\alpha}^T \dot{T} \tag{2}$$

in terms of the thermal dilation tensor $\boldsymbol{\alpha}^T$ defined as

$$\boldsymbol{\alpha}^T = \begin{bmatrix} \alpha_a & 0 & 0 \\ 0 & \alpha_a & 0 \\ 0 & 0 & \alpha_c \end{bmatrix} \tag{3}$$

where $\alpha_a$ and $\alpha_c$ are the single crystal thermal expansion coefficients along the *a*-axis and *c*-axis, respectively.

Due to the large thermal expansion anisotropy of zirconium, inclusion of thermal strains has previously been demonstrated by other authors to be required for the accurate modeling of internal