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Modeling mechanical response and texture evolution of α-uranium as a function of strain rate and temperature using polycrystal plasticity

Marko Knezevic *, Rodney J. McCabe, Carlos N. Tomé, Ricardo A. Lebensohn, Shuh Rong Chen, Carl M. Cady, George T. Gray III, Bogdan Mihaila

Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

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ABSTRACT

We present a polycrystal plasticity model based on a self-consistent homogenization capable of predicting the macroscopic mechanical response and texture evolution of α-uranium over a wide range of temperatures and strain rates. The hardening of individual crystals is based on the evolution of dislocation densities and includes effects of strain rate and temperature through thermally-activated recovery, dislocation substructure formation, and slip-twin interactions. The model is validated on a comprehensive set of compression tests performed on a clock-rolled α-uranium plate at temperatures ranging from 198 to 573 K and strain rates ranging from 10^{-3} to 3600 s^{-1}. The model is able to reproduce the stress–strain response and texture for all tests with a unique set of single-crystal hardening parameters. We elucidate the role played by the slip and twinning mechanisms and their interactions in large plastic deformation of α-uranium as a function of strain rate and temperature.

1. Introduction

Uranium and uranium alloys are nuclear material systems important for defense-related and energy applications including metallic nuclear fuels. These materials usually have low-symmetry crystal structures and exhibit complex deformation behavior. During manufacturing and in service, these materials may be subject to high temperature and/or high strain rate conditions. Predicting the material behavior and microstructure evolution during processing and service requires material models that account for temperature and strain rate effects. The accuracy of such models is particularly important for nuclear materials where operating conditions and material hazards may limit the ability to perform experiments to evaluate the material behavior.

The room-temperature allotrope of uranium metal, α-uranium (α-U), is stable up to 940 K and has an orthorhombic crystal structure. Due to its low-symmetry crystal structure, the deformation behavior of α-U single crystal exhibits strong anisotropy. Polycrystalline aggregates of α-U are also highly anisotropic due to pronounced texture (non-random distribution of crystallographic orientations) introduced by thermo-mechanical processing. α-U deforms by a wide variety of plastic deformation mechanisms with considerably different activation stresses, and these activation stresses evolve differently with deformation making the evolution of macroscopic hardening also highly anisotropic. Studies of the deformation mechanisms of single-crystal α-U and the mechanical response of α-U aggregates date back over 50 years (Anderson and Bishop, 1962; Cahn, 1951, 1953; Daniel et al., 1971; Fisher and McSkimin, 1958). The dislocation glide and deformation twinning modes accommodating plastic strains were identified and their relative strengths were measured for single crystals. It

* Corresponding author. Tel.: +1 505 665 7587; fax: +1 505 667 8021.
E-mail address: knezevic@lanl.gov (M. Knezevic).

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was established that the easiest slip mode in α-uranium is (010)[100] (Daniel et al., 1971; Yoo, 1968). The (001)[100] slip mode was found to become the predominant slip mode at elevated temperatures (Daniel et al., 1971; Yoo, 1968). It is important to note that both slip modes contain only one independent slip system. The $1/2\{110\}\langle 1\bar{1}0\rangle$ slip mode also operates, but requires a higher driving force than the primary $(010)[100]$ slip mode (Daniel et al., 1971). The $1/2\{1\bar{1}2\}\langle 021\rangle$ slip mode offers the additional degree of freedom necessary to accommodate plastic strain in the [001] direction and, thus, to accommodate an arbitrary plastic strain. In addition to slip, these studies reported the occurrence of deformation twinning in α-U. The most prominent deformation twin was found to be the $\{130\}\langle 3\bar{1}0\rangle$ twin mode (Cahn, 1951, 1953; Daniel et al., 1971). The $\{172\}\langle 3\bar{1}2\rangle$ twin mode and its reciprocal twin, $\{112\}\langle 3\bar{7}2\rangle$, were also frequently observed (Cahn, 1951, 1953; Crocker 1965; Daniel et al., 1971). Illustrations of α-U crystal structure and slip and twinning system geometries can be found in McCabe et al. (2010).

Early attempts at modeling and characterization of crystallographic texture in α-U sample took place in the 1950s (Calnan and Clews, 1952; Mitchell and Rowland, 1954). More recent attempts to model texture evolution during rolling of α-U were reported in the early 1990s (Lebensohn and Tomé, 1994; Rollett, 1991) using the relative strength of the deformation modes reported in Daniel et al. (1971). The advent of new experimental characterization techniques such as electron backscattered diffraction (EBSD) (Knezevic et al., 2012; McCabe et al., 2010; McCabe and Teter, 2006) and neutron diffraction (Brown et al., 2009; Choi and Staker, 1996), together with the development of new modeling techniques (Knezevic et al., 2012; McCabe et al., 2010), have created new interest in performing detailed studies aimed at understanding the basic behavior of uranium. Recently, we presented a comprehensive quantitative analysis focused on the room temperature quasi-static mechanical response and concomitant texture evolution of α-U with initial clock-rolled, straight rolled, and swaged textures (Knezevic et al., 2012). The insight obtained from these extensive experimental data sets were incorporated in a multi-scale hardening law based on dislocation densities which was implemented in the visco-plastic self-consistent (VPSC) model to predict the anisotropic stress–strain response and texture evolution of α-U (Knezevic et al., 2012; McCabe et al., 2010). Comparison of simulations and experiments allowed for inference of basic information concerning the various slip and twin mechanisms, their interactions, and their role on strain hardening and texture evolution. It was found that the initial texture plays a significant role in determining the level of plastic anisotropy, and deformation twinning plays a major role in anisotropic strain hardening behavior, tension–compression asymmetry and texture evolution in α-U (Knezevic et al., 2012; McCabe et al., 2010). Hence, it was evident that the accurate modeling of this complex material system requires a crystal-plasticity theoretical framework that accounts for microstructure evolution, rather than a continuum approach.

In this paper, we extend the hardening law based on dislocation densities and report the first microstructure-based model which includes strain-rate and temperature effects on deformation behavior of uranium. The enhanced predictive capabilities of this model will allow us to tackle simulations of complex forming operations of α-U. We calibrate and validate our model against new experimental data. Our model takes advantage of previous studies of strain-rate and temperature dependence of low-symmetry metals such as zirconium (Beyerlein and Tomé, 2008; Song and Gray, 1995a), titanium (Gray, 1997), magnesium (Barnett, 2001; Basinski, 1960), and beryllium (Brown et al., 2012). For those materials, twinning also plays a major role in deformation and studies have confirmed that increases in strain rate and decreases in temperature increase activity of deformation twinning through suppression of thermally-activated dislocation glide processes. Prior to the present study, the influence of temperature and strain rate on the mechanical behavior of uranium has received much less attention: a systematic investigation of the influence of temperature on the critical resolved shear stress for all four slip modes on single crystals of α-U was reported in Daniel et al. (1971) and some theoretical calculations of Peierls–Nabarro stress for (010) and (001) edge dislocations as a function of temperature were given in Yoo (1968).

We begin by presenting a large set of mechanical testing data performed on samples machined from an annealed clock-rolled plate of α-U. The mechanical tests were performed at temperatures ranging from 198 to 573 K and under strain rates ranging from 10^{-3} to 3600 s^{-1}. Subsequently, we discuss the hardening law implemented in VPSC, with an emphasis on details necessary for understanding the deformation mechanisms at various deformation conditions. Then, we calibrate and validate the model against the comprehensive set of rate and temperature-sensitive mechanical data. We show that the model is able to reproduce the stress–strain response for all tests with a unique set of single-crystal hardening parameters. These predictions allow us to elucidate the role played by the deformation mechanisms and their interactions in large plastic deformation and texture evolution of α-U as a function of strain rate and temperature. Strong shifts in the relative contribution of active deformation modes are observed when different deformation conditions are applied and these results will be discussed in detail.

2. Material and experiments

The material discussed here is clock-rolled α-U plate. The processing route was described earlier (Knezevic et al., 2012; McCabe et al., 2010). Samples were machined from the plate and annealed at 820 K for 2 h before testing. The microstructure and texture of the material before testing are shown in Fig. 1. The orientation map shows equiaxed twin-free grains with an average grain size of about 15 μm. The processing route of the starting material induced an orthotropic texture, which allows us to show only one quarter of the pole figures. The pole figures reveal that the material has a strong (001) texture component in the through-thickness (TT3) direction, tilted towards the in-plane 2 (IP2) direction. The (010) and (100) components tend to concentrate away from the (TT3) direction with the peak intensity for (010) being in the in-plane 1 (IP1) direction