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Grain-scale experimental validation of crystal plasticity finite element simulations of tantalum oligocrystals

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ABSTRACT

In this work, the grain-scale elastoplastic deformation behavior of coarse-grained body centered cubic (BCC) tantalum was simulated using a crystal plasticity finite element method (CP-FEM) and compared to experimental measurements of intragranular strain and rotation fields. To mitigate the effects of unknown subsurface microstructure, tantalum tensile specimens with millimeter-sized grains provided nearly constant microstructure through the thickness of the tensile bar. Experimental validation was performed in three ways: (1) electron backscatter diffraction (EBSD) to map intragranular rotation, (2) high-resolution digital image correlation (HR-DIC) to map the surface strain field, and (3) surface profilometry to map the out-of-plane topographic distortion. To ensure a direct apples-to-apples comparison to experiments, the details of the initial microstructure and boundary conditions were carefully replicated in the model. The deformation predictions using this novel BCC CP-FEM model for tantalum agree reasonably well with the experimental measurements. In addition, the model successfully predicted the failure location of a specimen subjected to large plastic strains. Several model parameters were explored that influence the BCC CP-FEM predictions such as the mesh dependence, the choice of active slip planes in BCC metals and the assignment of initial crystal orientations.

1. Introduction

Understanding deformation behavior of polycrystalline metals at the grain scale is challenging due to the complexities of heterogeneous grain morphology, differing crystal orientations of each grain and neighboring effects from other grains. Although relatively simple analysis using Schmid factors or other stress projection factors have been used with some success (Carroll et al., 2013), these factors can only consider a single grain at a time and ignore the effects of adjacent grains. Crystal plasticity models have the capability to employ stress projection factors in a framework that considers geometrical parameters and inter-grain interactions. Classical plasticity models enforce equal strain (Taylor, 1938) or equal stress (Sachs, 1928; Parks and Ahzi, 1990) across the grains to predict texture evolution. Other polycrystalline models such as relaxed constraints models (Honneff and Mecking, 1978) and self-consistent models (Kröner, 1961; Molinari et al., 1987) were proposed to relate individual grains to the polycrystalline behavior. Modern crystal plasticity finite element method (CP-FEM) models (Peirce et al., 1982; Asaro, 1983; Anand and Kalidindi, 1994; Dawson et al., 2003) enforce both inter-grain equilibrium

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and compatibility using a continuum of finite elements. Recent CP-FEM models successfully predicted texture and mechanical behaviors of various single crystals and polycrystals, e.g. FCC (Anand and Kalidindi, 1994; Delaire et al., 2000; Raabe et al., 2001; Zhao et al., 2008; Turner et al., 2013; Sabnis et al., 2013; Aoyagi et al., 2013; Gérard et al., 2013), BCC (Yalcinkaya et al., 2008; Weinberger et al., 2012; Lim et al., 2013b; Alankar et al., 2014; Narayanan et al., 2014) and HCP metals (Mayama et al., 2011; Wang et al., 2013; Abdolvand and Daymond, 2013), as well as non-local size effects (Ohashi et al., 2007; Counts et al., 2008; Lim et al., 2011; Aoyagi et al., 2014).

Although CP-FEM models have had some success in predicting grain scale deformation behavior, accurate comparisons with experimental results at the grain-scale are still lacking. This limitation can primarily be attributed to a lack of experimental information about subsurface microstructures in polycrystalline materials (Zeghadi et al., 2007b,a; Carroll et al., 2013) and different length scales between simulations and experimental measurements, e.g. the size of the finite element compared to the step size in electron backscatter diffraction (EBSD) or digital image correlation (DIC) measurements. Thus, the most effective and direct comparisons of CP-FEM and experiments are conducted with a specimen with a simple microstructure, i.e. single crystals or coarse columnar-grain structured specimens. These multi-crystal specimens, usually in sheet form, are referred to as 'oligocrystals' and have a small numbers of grains, typically 3–20, that extend through the thickness of the gage section. Oligocrystal specimens are used to compare and validate CP-FEM models with experiments; e.g. predictions of hardening behavior (Cheong and Busso, 2006; Lim et al., 2011), texture evolution (Delaire et al., 2000, 2003; Cheong and Busso, 2006; Zhao et al., 2008; Klusemann et al., 2012, 2013), inter- and intra-grain strain fields (Ziegenbein et al., 1998; Raabe et al., 2001; Sachtleber et al., 2002; Hoc et al., 2003; Héripré et al., 2007; Zhao et al., 2008; Badulescu et al., 2011; Klusemann et al., 2012, 2013; Turner et al., 2013), deformed specimen shapes (Klusemann et al., 2012, 2013) and activated slips (Havliček et al., 1990; Yao and Wagoner, 1993; Ziegenbein et al., 1998; Delaire et al., 2000). However, most previous studies focus on FCC metals and many lack direct and quantitative comparisons between model predictions and experimental measurements.

In this work, a technique combining EBSD, profilometry and high resolution DIC (HR-DIC) measurements Carroll et al. (2010, 2013) was used to measure intragranular deformation of coarse-grained tantalum subjected to considerable plastic deformation under uniaxial tensile loading. The BCC CP-FEM model, parameterized by single crystal experimental data based on dislocation kink-pair theory (Lim et al., submitted for publication), was then used to simulate the deformation of the whole gage section of two different tantalum oligocrystal specimens subjected to uniaxial loading. Simulated strain and texture evolution were quantitatively compared with experimental measurements. Furthermore, various constitutive effects in the model including the choice of active slip planes, the assignment of initial crystal orientations, mesh size dependence and 2D versus 3D modeling of the 2D structured specimen, were explored.

2. Experimental procedure

Flat tensile specimens were machined from a 1 mm thick rolled sheet of 99.9% pure tantalum (Goodfellow Corporation), using electro-discharge machining (EDM). The gage section had a slight hourglass radius of curvature of 51 mm with nominal specimen dimensions shown in Fig. 1. Heat treating specimens at 2000 °C for 10 h and 10^{-6} Torr in a vacuum furnace created specimens with millimeter-sized grains in pseudo-two-dimensional grain structures (Carroll et al., 2013). Specimens were then polished to a surface finish suitable for EBSD measurements (Boyce et al., in press). A region of interest was

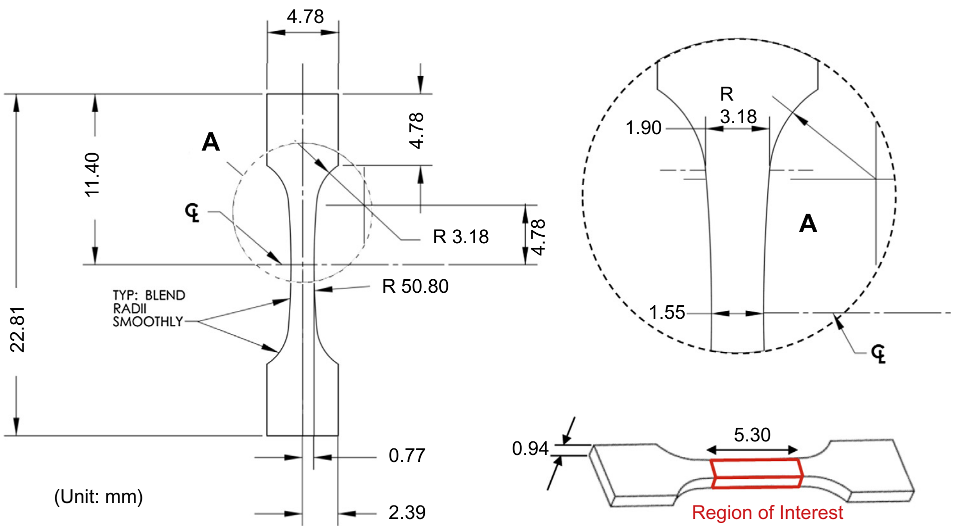

Fig. 1. Nominal dimensions of the tantalum tensile specimens (units: mm).