A strain-rate and temperature dependent constitutive model for BCC metals incorporating non-Schmid effects: Application to tantalum-tungsten alloys

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Abstract

In this work, we present a multiscale physically based constitutive law for predicting the mechanical response and texture evolution of body-centered cubic (BCC) metals as a function of strain-rate and temperature. In the model, deformation of individual single crystals results not only from the resolved shear stress along the direction of slip (Schmid law) but also from shear stresses resolved along directions orthogonal to the slip direction as well as the three normal stress components (non-Schmid effects). We account for coupled Schmid and non-Schmid effects through the modification of the resolved shear stress for both $1/2\langle 1\bar{1}1 \rangle\{110\}$ and $1/2\langle 11\bar{1} \rangle\{112\}$ slip systems and the modification of the slip resistance for $1/2\langle 11\bar{1} \rangle\{112\}$ slip systems. The single crystal model is implemented into a self-consistent homogenization scheme containing a hardening law for crystallographic slip. The hardening law is based on the evolution of dislocation densities that incorporates strain-rate and temperature effects through the Peierls stress, thermally activated recovery, dislocation substructure formation and dislocation interactions. The polycrystal model is calibrated and validated using a set of mechanical and texture data collected on a tantalum-tungsten alloy, Ta-10W, at temperatures ranging from 298 K to 673 K and strain-rates from 10^{-3} to 2400 s^{-1} . We show the model effectively captures the anisotropic hardening rate and texture evolution for all data using a single set of single-crystal hardening parameters. Comparisons between predictions and measured data allow us to discuss the role of slip on $\{110\}$ and $\{112\}$ in determining plasticity and texture evolution in Ta-10W.

Keywords: Tantalum-tungsten; EBSD; Texture; Constitutive modeling; Non-Schmid effects

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1.0 Introduction

Tantalum (Ta) and its alloys exhibit a range of desirable properties such as high melting temperature, ductility, strength, fracture toughness, and conductivity. As such, they are excellent candidates for components that operate under mechanical and thermal extremes. Examples of applications include aircraft engine and rocket motor parts, anti-armor systems, missile parts and bone replacement implants (2013; Matsuno et al., 2001). The deformation behavior of Ta, like other body-centered cubic (BCC) metals, is markedly influenced by alloying additions and crystallographic texture and is sensitive to temperature and strain-rate (Arsenault and Lawley, 1967; Chen and Gray, 1996; Clark Jr et al., 1991; Gray and Vecchio, 1995; Gray III, 2012). The controlling mechanisms giving rise to these sensitivities in deformation behavior have been related to (1) Peierls stresses, (2) dislocation substructure formation due to a low degree of thermally-activated dynamic recovery of screw dislocations, and (3) dislocation interactions (Arsenault and Lawley, 1967; Christian, 1983; Foxall and Statham, 1970; Mitchell and Spitzig, 1965; Yang et al., 2001).

Studies have shown that modeling plasticity of BCC refractory metal single crystals requires incorporation of non-glide stress effects on yielding (Gröger et al., 2008a; Gröger et al., 2008b; Lim et al., 2013; Qin and Bassani, 1992b; Vitek et al., 2004; Wang and Beyerlein, 2011). While twinning/detwinning is the main cause of tension/compression asymmetry in low-symmetry metals (Fast et al., 2008; Fromm et al., 2009; Knezevic et al., 2013a; Knezevic et al., 2012; Knezevic et al., 2013c; Knezevic et al., 2010; Proust et al., 2010), these non-Schmid effects are the main cause of asymmetry in BCC metals. The applied stress components that do not lay in the slip planes alter the core structure of screw dislocations, which influences the Peierls stress required to move the dislocation. Screw dislocations, as dominant defects in BCC metals, exhibit distorted and/or non-planar core structures (Duesbery et al., 1973). Distortion of the dislocation core relative to the loading direction causes asymmetry in the stress required to move the dislocation (Duesbery et al., 1973). In addition, intrinsic to BCC structure, slip occurs in the $\langle 111 \rangle$ directions and the Peierls stress is symmetric on $\{110\}$ and asymmetric on $\{112\}$ planes (Byron, 1968; Byron and Hull, 1967; Duesbery et al., 1973; Duesbery and Vitek, 1998). It has also been argued that the non-Schmid effects destabilize plastic flow, which becomes non-associative, and therefore increase the tendency for localization in single crystals (Qin and Bassani, 1992a; Steinmann et al., 1998). Atomistic simulations have shown that the yield

criterion in BCC metals depends on both the applied shear stress parallel and perpendicular to the Burgers vector direction (Ito and Vitek, 2001). Based on these findings, a yield criterion was developed in (Gröger et al., 2008b) to include three non-Schmid terms: shear stress on the nearest secondary $\{112\}$ slip plane to a given primary $\{110\}$ slip plane in the twinning or the anti-twinning direction, and shear stresses in the primary $\{110\}$ and the secondary $\{112\}$ slip planes perpendicular to their respective slip directions. The criterion was later incorporated in single crystal plasticity models (Alleman et al., 2014; Weinberger et al., 2012). The other yield criterion developed in (Dao and Asaro, 1993; Lim et al., 2013) is more general and includes the applied shear and normal stresses along all three orthogonal axis on a given slip plane. Another non-Schmid effect characteristic of only slip on $\{112\}$ planes is the dependence of the Peierls stress on the stress component normal to the Burgers vector within the glide plane (Ito and Vitek, 2001; Wang and Beyerlein, 2011). These studies, however, did not examine the effect of non-Schmid effects on texture evolution and hardening during large plastic strains of polycrystals.

Models at higher length scales involve homogenization schemes such as mean-field Taylor type (Knezevic et al., 2009; Knezevic et al., 2008; Knezevic and Savage, 2014; Shaffer et al., 2010; Taylor, 1938) or full-field (Kalidindi et al., 1992; Kalidindi et al., 2006; Knezevic et al., 2014b). A Taylor type relaxed constraints model has been successful in predicting texture evolution in polycrystalline Ta (Raabe et al., 1993; Raabe et al., 1994a; Raabe et al., 1994b). In their work, the authors assumed that slip can occur on any of the $\{110\}$, $\{112\}$ and $\{123\}$ slip planes but did not consider the non-Schmid effects. Some existing models assume that slip can occur on the $\{110\}$, $\{112\}$ and $\{123\}$ slip planes (Bronkhorst et al., 2007; Raabe et al., 1993; Raabe et al., 1994a). It has been shown that slip on $\{123\}$ planes can be expressed as a combination of slips on $\{110\}$, and $\{112\}$ planes (Franciosi, 1983; Franciosi, 1985). Therefore, more often models assume slip on the $\{110\}$ and $\{112\}$ slip planes (Alleman et al., 2014; Ardeljan et al., 2014; Ito and Vitek, 2001; Knezevic et al., 2013b; Ma et al., 2007; Wang and Beyerlein, 2011), and sometimes only on the $\{110\}$ slip plane (Gröger et al., 2008b; Lim et al., 2013; Weinberger et al., 2012). The uncertainty in the identification of active slip systems poses a fundamental problem for simulating texture evolution and mechanical response because the difference in relative activities of slip systems results in a difference in texture evolution.

The above descriptions of the underlying physical mechanism involved in plastic deformation of BCC single crystals present a great challenge when attempting to develop a

constitutive model incorporating all of the physics. Multi-scale polycrystalline plasticity modeling is a way towards reliable constitutive modeling of BCC metals. Models that include the individual kinetics of screw and edge dislocations and account for the effects of core spreading of the screw dislocations on the macro-scale mechanical response were recently reported in (Alankar et al., 2014; Ma et al., 2007). Here, we present a model for predicting macro-scale stress-strain response and texture evolution that incorporates the effects through a non-Schmid law for yielding and a thermally-activated dislocation based hardening law.

In this paper a wide range of data on a tantalum-tungsten alloy, Ta-10W, subjected to quasi-static tension at room temperature and high-rate compression at various temperatures is presented. The data is used to initialize and validate a multi-scale model for BCC metals developed here. Initial and deformed microstructures are characterized using electron backscattered diffraction (EBSD). The yield stress and hardening behavior are sensitive to changes in temperature and strain-rate. Our multi-scale model implements the generalized non-Schmid law for yielding at the single crystal level (Lim et al., 2013) and the recently developed hardening law based on dislocation density for BCC (Knezevic et al., 2014c) within a viscoplastic self-consistent (VPSC) polycrystal model (Lebensohn and Tomé, 1993) to predict macroscopic stress-strain response and texture evolution. The model considers $\langle 1\bar{1}1 \rangle$ slip on both $\{110\}$ and $\{112\}$ planes along their positive and negative direction as potential slip systems accommodating the imposed strain. The non-Schmid contributions are implemented through the generalization of the resolved shear stress for both $\{110\}$ and $\{112\}$ slip systems and the modification of the slip resistance for $\{112\}$ slip systems. We show that the model is able to capture anisotropy (directional dependence) and asymmetry (sense dependence) of the stress-strain response and texture evolution of Ta-10W with a unique set of single-crystal hardening parameters.

2.0 Material and experiments

The material used in this study is Ta-10wt%W (Ta-10W), supplied by H.C. Starck with the following composition in weight ppm unless otherwise noted: 5 C, 26 O, 5 N, 1 H, 9.5 wt% W, 5.5 Nb, 1.2 Mo and Ta balance. The material was provided as a 28.6 mm diameter bar manufactured through a series of processes including high temperature extrusion and

intermediate temperature rotary forging with intermediate annealing treatments. Following the final rotary forging operation, the bar was annealed at 1482 °C.

The microstructure of the material before testing is shown in Fig. 1, and the initial texture is presented using pole figures in Fig.2. We find that microstructure varies as a function of distance from the centerline of the bar (radius = 14.3mm). Based on these variations, we classify the bar microstructures into Region 1 and Region 2, with a transition region in between. Region 1 of the bar extends from the centerline to a radius of about 7.8mm. Within Region 1, the grains have an average radius of 25-30 μm and are slightly elongated in the axial direction with an average aspect ratio of 2.2. Region 1 exhibits a $\{110\}$ fiber texture. The transition region spans from a radius of 7.8 mm to about 10.8 mm and has a similar texture to Region 1, but is not fully recrystallized and exhibits larger degree of internal misorientation and larger grain aspect ratios. Region 2 extends from about 10.8 mm to the bar surface at 14.3 mm. Grains in Region 2 have similar grain sizes (26.7 μm average radius), aspect ratios (2.2), and similar levels of internal grain misorientation as grains in Region 1. Unlike Region 1, Region 2 exhibits a strong $\{100\}$ fiber texture in the axial direction.

The mechanical response was measured in compression and tension from samples machined both from Region 1 and Region 2 of the bar in both the axial and transverse directions. Right cylindrical compression samples had a 5 mm diameter and length and dog bone tensile samples had a 3.2 mm square cross-section. Quasi-static, constant velocity compression tests were performed at strain-rates of 0.001 s^{-1} and 1 s^{-1} at temperatures of 298 K, 463 K, and 673 K using a screw-driven Instron. Polished tungsten carbide plates lubricated with molybdenum disulfide grease were used to reduce frictional effects during loading of the compression samples. The raw data were collected in the form of load-displacement curves and were corrected for machine compliance before computing the true stress-true strain curves. Tension tests were performed at 298 K at 0.001 s^{-1} and 1 s^{-1} on a screw-driven Instron. Dynamic compression tests were performed at strain rates around 2000 s^{-1} at 298 K, 463 K, and 673 K using a Split-Hopkinson Pressure Bar (Follansbee, 1985). The inherent oscillations in the dynamic stress-strain curves make the determination of the yield stress very approximate at low strains. Mechanical testing results will be shown and discussed in the results section of the paper.

Figure 1 EBSD orientation maps showing axial and transverse sections of the initial microstructure in the Ta-10W bar from the center to the surface of the bar. The colors in the maps are based on the unit IPF triangle and indicate the crystal direction normal to the section plane. Note a gradient in grain structure and crystal orientations from Region 1 over the transition region to Region 2. The IPF triangle has the crystal reference frame defined as [001] in the center, [101] to the right, and [111] upward.

Figure 2 Initial texture in Region 1 (left) and Region 2 (right) of the Ta-10W bar. Centerline of the bar is in the center of the pole figures. The transverse direction is to the right.

3.0 Multi-scale model

The crystal plasticity code VPSC is used as a platform to implement the multi-scale model and simulate the texture and polycrystalline macroscopic response of Ta-10W. In VPSC, self-consistent iterations are performed to ensure that every grain, represented as an ellipsoidal inclusion, is in equilibrium with a homogenous effective medium, which represents the polycrystalline aggregate. A detailed description of the VPSC model can be found elsewhere (Lebensohn and Tomé, 1993; Lebensohn et al., 2007). Here, in order to predict the rate and temperature dependence of the mechanical response and texture evolution of Ta-10W,

enhancements specific to BCC metals are made at the single crystal level within the VPSC framework. .

In VPSC, for each slip system within each grain, the slip shear rate, $\dot{\gamma}^s$, on a system s is given by the power-law:

$$\dot{\gamma}^s = \dot{\gamma}_o \left| \frac{\tau^s}{\tau_c^s} \right|^{\frac{1}{m}} \text{sign}(\tau^s) \quad (1)$$

where $\dot{\gamma}_o^s$ is a reference shear-strain-rate and m (equal to 0.05 in this work) is the rate-sensitivity parameter. In our model, the rate sensitivity is accounted for explicitly by the functional form of τ_c^s . Numerically, we eliminate the rate sensitivity that is introduced with the exponent m , by setting the reference shear rate, $\dot{\gamma}_o$, equal to the norm of the macroscopic strain rate $\dot{\gamma}_o = \|\bar{\dot{\epsilon}}\|$ (Knezevic et al., 2013e).

The slip resistance per slip system, τ_c^s , is expressed as a sum of the friction stress $\tau_{o,f}^s$, a barrier effect dependent on initial grain size $\tau_{o,HP}^s$, a forest dislocation interaction stress τ_{for}^s (dependent on a spatially random distribution of stored dislocations), and a dislocation substructure interaction stress, τ_{sub}^s (dependent on the organized distribution of dislocations at the later stages of deformation):

$$\tau_c^s(\dot{\epsilon}, T) = \tau_{o,f}^s(\dot{\epsilon}, T) + \tau_{o,HP}^s + \tau_{for}^s(\dot{\epsilon}, T) + \tau_{sub}^s(\dot{\epsilon}, T). \quad (2)$$

Non-Schmid effects are incorporated in the calculation of τ^s in Eq. (1) and of the friction stress $\tau_{o,f}^s$, which contributes to the total slip resistance τ_c^s in Eq (2). The first method is an extension of the conventional Schmid law (Schmid and Boas, 1950), where yielding in a system occurs when the resolved shear stress, τ^s (the stress resolved in the Burgers direction, $\mathbf{b}^s$, on the glide plane, $\mathbf{n}^s$), reaches the slip resistance, τ_c^s . The resolved shear stress, τ^s , is given by $\mathbf{P}_s^s : \boldsymbol{\sigma}'$, where $\mathbf{P}_s^s$ is the Schmid tensor, defined as:

$$\mathbf{P}_s^s = c_o \cdot 0.5 (\mathbf{b}^s \otimes \mathbf{n}^s + \mathbf{n}^s \otimes \mathbf{b}^s). \quad (3)$$

With non-Schmid effects included, the resolved shear stress is given by

$$\tau^s = \mathbf{P}_s^s : \boldsymbol{\sigma}' + \mathbf{P}_{ns}^s : \boldsymbol{\sigma}', \quad (4)$$

where $\mathbf{P}_{ns}^s$ is the non-Schmid tensor, which provides a weighted projection of the stress tensor along the remaining components as :

$$\mathbf{P}_{ns}^s = c_1(\mathbf{t}^s \otimes \mathbf{b}^s) + c_2(\mathbf{t}^s \otimes \mathbf{n}^s) + c_3(\mathbf{n}^s \otimes \mathbf{n}^s) + c_4(\mathbf{t}^s \otimes \mathbf{t}^s) - (c_3 + c_4)(\mathbf{b}^s \otimes \mathbf{b}^s). \quad (5)$$

and where $\boldsymbol{\sigma}'$ is the deviatoric stress and $\mathbf{t}^s$ is the slip system direction perpendicular to the Burgers vector and normal directions, $\mathbf{t}^s = \mathbf{n}^s \times \mathbf{b}^s$. In Lim et al. (2013), the non-Schmid coefficients, c_i , were characterized using single crystal Ta deformation data from (Byron, 1968). We adopt these in the present study ($c_1 = 0.15$, $c_2 = -0.13$, $c_3 = -0.07$, and $c_4 = 0.04$). Both, Schmid and non-Schmid effects are applied to the $\{110\}$ and $\{112\}$ slip modes. We utilize the generalized yield criterion of (Dao and Asaro, 1993; Lim et al., 2013) since it allows each component of stress acting on the slip system to be incorporated independently. While the above non-Schmid parameters were established for the $\{110\}$ slip systems, we assumed the same non-Schmid effects same for the $\{112\}$ slip systems due to lack of an exact data in current literature for the $\{112\}$ slip systems. Additionally, the non-Schmid parameters are reported to be a function of temperature (Lim et al., 2013). However, in order to keep the number of fitting parameters in the present model to a minimum we only incorporate temperature effects via the thermally activated dislocation density hardening law.

A second non-Schmid effect incorporated here is the dependence of slip resistance of $\{112\}$ dislocations on the stress resolved normal to the Burgers vector and in the glide plane, i.e. $\tau_m^s = (\mathbf{t}^s \otimes \mathbf{n}^s) : \boldsymbol{\sigma}'$ (Ito and Vitek, 2001; Wang and Beyerlein, 2011). We use an empirical function for the Peirels stress taken from (Wang and Beyerlein, 2011), which was characterized directly from molecular dynamics simulation results of (Ito and Vitek, 2001). The dependence on τ_m^s has been adopted for the friction stress, $\tau_{o,f}^\alpha$ (dependent on the Peierls stress, precipitates and the initial content of dislocation debris) as follows:

$$\frac{\tau_{o,f}^s}{\tau_{oo,f}^s} = \begin{cases} \infty & \text{if } \tau_m^s / \tau_{oo,f}^s < -0.055 \\ 1.12 \exp\left(\frac{0.0567}{\tau_m^s / \tau_{oo,f}^s - 0.5}\right) & \text{if } -0.055 \leq \tau_m^s / \tau_{oo,f}^s \leq 0.36 \\ 0.75 & \text{if } \tau_m^s / \tau_{oo,f}^s > 0.36 \end{cases} \quad (6)$$

where $\tau_{oo,f}^s$ is the initial slip resistance. When τ_m^s is negative, $\tau_{o,f}^s$ is made infinitely high rendering the (112) dislocation immobile. When τ_m^s is positive, $\tau_{o,f}^s$ decreases as τ_m^s increases

according to the exponential function in Eqn. 6. When τ_m^s becomes large, $\tau_{o,f}^s$ saturates to a small value, such that $\{112\}$ glide becomes easy. For $\{110\}$ glide, $\tau_{o,f}^s = \tau_{oo,f}^s$.

The initial slip resistances per slip system, $\tau_{oo,f}^s(\dot{\epsilon}, T)$, is taken to be the same for all slip systems belonging to mode α , decays exponentially with temperature and increases logarithmically with strain rate as:

$$\tau_{oo,f}^\alpha(\dot{\epsilon}, T) = A^\alpha (1 + B^\alpha \ln(\dot{\epsilon})) \exp\left(-\frac{T}{C^\alpha}\right) \quad (7)$$

where A^α , B^α , and C^α are constants, whereas T and $\dot{\epsilon}$ are the current temperature and strain rate, respectively. Such expression was used for several other metals in earlier studies (Knezevic et al., 2014a; Knezevic et al., 2013d). The grain size effect, $\tau_{o,HP}^\alpha$, is accounted for through a Hall-Petch-like equation:

$$\tau_{o,HP}^\alpha = \mu H^\alpha \sqrt{\frac{b^\alpha}{d_g}}, \quad (8)$$

where b^α is the magnitude of the Burgers vector, d_g is the initial grain size, μ is the effective shear modulus, and H^α is the Hall-Petch-like constant. $\tau_{oo,f}^\alpha$ and $\tau_{o,HP}^\alpha$ are contributions to the slip resistance that do not evolve with plastic strain.

The forest term, $\tau_{for}^\alpha(\dot{\epsilon}, T)$, contribution is based on the evolution of the forest dislocation densities per plane, $\rho_{for}^\alpha(\dot{\epsilon}, T)$ through the Taylor relationship (Mecking and Kocks, 1981):

$$\tau_{for}^\alpha(\dot{\epsilon}, T) = \chi^\alpha(\dot{\epsilon}) b^\alpha \mu \sqrt{\rho_{for}^\alpha(\dot{\epsilon}, T)}, \quad (9)$$

where χ^α is a dislocation interaction parameter. The values of the χ^α parameter were reported to be in the range 0.05-2.6 and dependent on crystal structure, temperature, strain rate and alloying (Lavrentev, 1980). Consistent with earlier evidence (Hirsch and Lally, 1965; Lawley and Gaigher, 1964), we assume that χ^α decreases with strain rate following the logarithmic form:

$$\chi^\alpha = \chi_o^\alpha - \ln \frac{|\dot{\epsilon}|}{E^\alpha}, \quad (10)$$

where χ_o^α is the initial value and E^α is a constant. A rationale for such behavior is that the interactions are stronger at lower rates because the crossing dislocations have more chances to interact and form locks.

Based on (Mecking and Kocks, 1981), the evolution of the stored forest density per slip mode, $\rho_{for}^\alpha(\dot{\epsilon}, T)$, is a competition between the rate of storage and the rate of dynamic recovery:

$$\frac{\partial \rho_{for}^\alpha}{\partial \gamma^\alpha} = \frac{\partial \rho_{gen,for}^\alpha}{\partial \gamma^\alpha} - \frac{\partial \rho_{rem,for}^\alpha}{\partial \gamma^\alpha} = k_1^\alpha \sqrt{\rho_{for}^\alpha} - k_2^\alpha(\dot{\epsilon}, T) \rho_{for}^\alpha, \quad \Delta \rho_{for}^\alpha = \frac{\partial \rho_{for}^\alpha}{\partial \gamma^\alpha} \Delta \gamma^\alpha, \quad \Delta \gamma^\alpha = \sum_{s=1}^{N_s} |\Delta \gamma^s|, \quad (11)$$

where N_s is the total number of slip systems per slip mode, α , k_1^α is a rate-insensitive coefficient for dislocation storage by statistical trapping of mobile dislocations and k_2^α is a rate-sensitive coefficient that accounts for dynamic recovery by thermally activated mechanisms. The latter coefficient, k_2^α , is given by (Beyerlein and Tomé, 2008)

$$\frac{k_2^\alpha}{k_1^\alpha} = \frac{\chi^\alpha b^\alpha}{g^\alpha} \left(1 - \frac{kT}{D^\alpha b^3} \ln \left(\frac{\dot{\epsilon}}{\dot{\epsilon}_o} \right) \right). \quad (12)$$

Here, k , $\dot{\epsilon}_o$, g^α , and D^α are, respectively, the Boltzmann constant, a reference strain rate, an effective activation enthalpy and a drag stress.

The development of substructure within grains, such as cells, cell blocks, and dislocation sheets (e.g. Kuhlmann-Wilsdorf, 1989), is believed to cause Stage IV hardening. Stage IV hardening in Ta polycrystals has been observed by (Mitchell and Spitzig, 1965; Sargent et al., 1962). In this model, a separate substructure density is introduced to capture Stage IV hardening. Dislocations belonging to all active slip modes can contribute to the evolution of substructure. Accordingly, the rate of substructure development is given as:

$$\Delta \rho_{sub} = \sum_{\alpha} q^\alpha b^\alpha \frac{\partial \rho_{rem,for}^\alpha}{\partial \gamma^\alpha} |\Delta \gamma^\alpha| \quad (13)$$

where q^α is a dislocation recovery rate coefficient defining the fraction of α -type dislocations that do not annihilate but become substructure. The substructure density resists slip for all slip modes. Justification for the above equation arises from the basic processes involving climb and cross slip known to be responsible for pattern formation (Jackson, 1985; Kocks and Mecking, 2003; Peeters et al., 2001; Wang et al., 2007). Dislocation dipoles, jogs, and locks are examples of patterns generated due to dislocation interactions and it is believe that they can self-organize

into lower energy patterns, such as cells, cell blocks, and dislocation sheets (e.g. Kuhlmann-Wilsdorf, 1989). While the hardening model considers a large fraction of these processes to contribute recovery of forest dislocations, it also assumes that a smaller fraction adds to substructure development. We should note that this model neglects the length scales and pattern type associated with substructure. These aspects can lead to directional hardening and strongly affect flow stress and work hardening during strain path changes (Beyerlein and Tomé, 2007; Mahesh et al., 2004; Peeters et al., 2001). As our present interests lie in modeling non-Schmid effects, advancing the substructure model and applications to strain path changes are left for future work.

4.0 Results and discussion

Using the model described above, we simulate simple compression and tension tests on polycrystalline Ta-10W over a wide range of temperatures and strain rates. Loading in either the axial (AX) or transverse (TR) directions of the bar was simulated by imposing 0.001 strain increments along the loading direction, while enforcing zero average stress along the other two sample directions. We represent the initial textures of Fig. 2 using 10,000 orientations and we assign an initially spherical shape to the representative grain ellipsoids according to the EBSD maps in Fig. 2. As deformation proceeds, the grain shapes are permitted to evolve.

4.1 Calibration of parameters

First, we compared simulated and measured stress-strain curves to determine the following material parameters for the $\{110\}$ and $\{112\}$ slip modes: $\tau_{o,f}^\alpha$, trapping rate coefficient, k_1^α , activation barrier for de-pinning, g^α , and drag stress, D^α . Advantageously, each parameter largely affects a different portion of the stress-strain curve. For example, $\tau_{o,f}^\alpha$ is mainly responsible for the yield stress, k_1^α mainly governs the initial slope of the stress-plastic strain curve, and k_2^α the onset and character of Stage III hardening. Consequently, it is possible to obtain a reasonable estimate of these parameters even from one stress-strain curve.

We used half of the stress-strain data for parameter characterization. Specifically: axial compression in region 1 (AXC1) and axial tension in region 1 (AXT1) at 298 K under 10^{-3} s^{-1} and 1 s^{-1} , AXC1 at 473 K under 0.001 s^{-1} and 2400 s^{-1} , and AXC1 at 673 K under 2400 s^{-1} . The comparison of the model (dash) and experimental curves (solid) is given in Fig. 3. The

corresponding set of hardening parameters is given in Table I. This single set was used in all subsequent calculations discussed below. The remaining experimental stress-strain curves and all measured textures were used to test the model's predictive capabilities with this set.

4.2 Predictions of mechanical response

Axial compression and tension tests were performed on samples cut either from Region 1 or Region 2 of the bar to determine the effects of microstructural variation from processing. We found that the mechanical responses in Region 1 and Region 2 are similar. Figure 3a shows this result at two strain rates, 0.001/s and 1/s suggesting that the mechanical response was not sensitive to the differences in grain structure and texture between regions 1 and 2.

To explore plastic anisotropy, compression tests were performed in the transverse direction. Figures 3a and 3b reveal small plastic anisotropy between axial and transverse directions. We attribute this plastic anisotropy to the difference in texture, which exhibits a stronger component of the relatively harder [111] orientation along the TR direction.

To evaluate tension-compression asymmetry, compression and tension tests were performed in the axial and transverse directions. Figure 3b and 3c show little plastic asymmetry along the AX direction and more plastic asymmetry along the TR direction. For both the axial and transverse tests, the compression flow stresses were higher than those in tension.

Based on the above results, we elected to further study rate effects on mechanical response using compression samples cut from Region 1. Compression tests were carried out over a wide range of temperatures from 298 K to 673 K and for strain rates 10^{-3} to 2400 s^{-1} . Results are shown in the Figs. 3d and 3e. We observe that the flow stresses and hardening rates of Ta-10W strongly depend on strain rate and temperature. Dislocation slip is known to be more difficult to activate if strain rate increases or if temperature decreases. Therefore, the flow stress decreases as strain rate decreases and temperature increases. The stress-strain curves recorded under quasi-static deformation conditions exhibit a classical decreasing hardening rate throughout. This decrease of the hardening rate is more pronounced with increasing temperature due to the thermal activation of dislocation slip (Chen and Gray, 1996; Lau et al., 1967). It is seen that the work hardening rate at high strain rate is rather constant.

A key achievement of this work is that the model is shown to provide excellent agreement for all stress-strain responses using a single set of parameters. Specifically, the small plastic anisotropy, the slight tension-compression asymmetry, and the strong rate sensitivity are

simultaneously captured. As many of these features in flow stress and rate sensitivity of Ta-W are similar to those in other BCC metals, the present modeling framework is expected to be useful for a wider set of materials in addition to Ta alloys. While the model successfully captures stress-strain response and texture evolution, a more rigorous test for the model would be predicting mechanical response and texture evolution during deformation strain-path changes.

4.3 Predictions of texture evolution

The EBSD maps of the microstructure deformed at room temperature to a strain of 0.2 under 0.001 s^{-1} and to a strain of 0.15 under 2000 s^{-1} are shown in Fig. 4a and b, respectively. The maps show that microstructure and intra-grain heterogeneities develop similarly at quasi-static and high-rate deformation conditions. Texture development was also measured and a few measurements are presented in the form of pole figures in Fig. 5 and 45° orientation distribution function (ODF) sections (Kalidindi et al., 2009) in Fig. 6. The corresponding model predictions are provided alongside the measured textures, and we find that the agreement is qualitatively good. Note that the calculated textures are predicted and not used for model calibration. Figure 6 compares the locations of fibers and texture components in a $\varphi_2 = 45^\circ$ section of Euler space and our measured and predicted results in the same ODF section. Consistency in texture predictions is not sufficient proof of the validity of the model. However, since texture is a consequence of system activity, which in itself depends on the relative CRSS between, it provides indirect support for the model. Interestingly, the texture evolution is not a function of strain rate or temperature, indicating that the basic deformation mechanisms are active at about the same ratios for all temperature and rate conditions tested. Similar independence was recently reported for a cobalt based superalloy (Knezevic et al., 2014a).

4.4 Predictions of slip activity

Achieving good agreement over a broad suite of stress-strain response data and texture evolution is a good indication that the model is capturing well the underlying slip activity. To indicate slip activity, we use as a measure the relative contribution to shear per mode α to the total contribution of all slip systems, given by:

$$Activity^\alpha = \frac{\sum_{s=1}^{N_s} \dot{\gamma}^s}{\sum_{\alpha=1}^{N_\alpha} \sum_{s=1}^{N_s} \dot{\gamma}^s} \quad (14)$$

where $N\alpha$ and Ns are the total number of slip modes and the total number of slip systems per slip mode, respectively. As an example, the predictions for slip activity in the room-temperature, quasi-static conditions are given in Fig. 7. We find that for a given test the slip activity is achieved in the initial stages of deformation and remains steady with respect to straining. Both $\{110\}$ and $\{112\}$ slip modes are found to contribute substantially to deformation, with the $\{110\}$ slip mode contributing more in every case.

Table I Slip system hardening parameters (the same values apply to both $\{110\}$ and $\{112\}$ planes)

b^α [nm]	k_1^α [m ⁻¹]	$\dot{\epsilon}_o$ [s ⁻¹]	g^α	D^α [MPa]	H^α [MPa]	q^α	μ [MPa]
0.28579	1.15e+08	10 ⁷	0.35	220	50	10	69000

A^α	B^α	C^α	E^α	χ_o^α
505	0.053	630	19	0.52

Figure 3 Measured and simulated stress-strain response on samples of Ta-10W in compression (C) and tension (T) along the axial (AX) and transverse (TR) directions and at the temperatures and strain-rates indicated in the plots. Also 1 and 2 indicate regions where the samples were machined from the extruded Ta-10W bar. The solid lines are the experimental curves and the dashed lines are the model calculations.

Figure 4 Orientation maps of the deformed microstructure for axial 1 compression at room temperature under strain rates of (a) 0.001 s^{-1} and (b) 2000 s^{-1} . The compression axis in the orientation maps is vertical and the colors indicate the orientation of the compression axis with respect to the crystal reference frame.

Figure 5 Pole figures showing comparisons of measured (on the left) and predicted (on the right) texture evolution at a strain of 0.2 under quasi-static deformation conditions at room temperature in: (a) axial compression in region 1 (AXC1), (b) axial compression in region 2 (AXC2), (c) axial tension in region 1 (AXT1), (d) transverse compression in region 1 (TRC1), and (e) transverse compression in region 2 (TRC2). (f) shows the comparison of texture for high strain-rate axial compression at a strain of 0.15 at a strain-rate of 2000 s^{-1} in region 1 (AXC1). The center of all pole figures is the rod central axial. The transverse direction is to the right.

Figure 6 Section of $\phi_2 = 45^\circ$ in Euler space with indicated locations of the important fibers and texture components (Lee and Han, 2013). $\phi_2 = 45^\circ$ ODF sections showing the measured and predicted texture corresponding to the Fig. 5.

Figure 7 Predicted relative activities of slip modes for the deformation conditions indicated in the plots.

5.0 Conclusions

The deformation behavior of Ta-10W is examined using quasi-static and high strain-rate testing, EBSD characterization and crystal plasticity modeling. The microstructure characterization reveals gradients in grain structure and crystallographic texture along the radial direction of the bar. In particular, texture transitions from $\{110\}$ fiber in the center to $\{001\}$ fiber in the periphery of the bar. Texture was found to play the dominant role in plastic anisotropy between axial and transverse direction. The flow stress and hardening rates were sensitive to strain-rate and temperature. We use the measured data to calibrate and validate a polycrystal model. The model couples a non-Schmid yield criterion with a dislocation density hardening law within the VPSC crystal plasticity model and is capable of predicting well the mechanical response and texture evolution of Ta-10W over a wide range of temperatures and strain rates. Based on the good predictions, we find that both $\{110\}$ and $\{112\}$ slip modes contribute substantially to the plasticity of Ta-10W. As many of the features in the microstructure and the flow stress response of Ta-10W are similar to those in other BCC metals, the present multiscale model is expected to work well for a wider set of materials in addition to Ta alloys.

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Figure 1 EBSD orientation maps showing axial and transverse sections of the initial microstructure in the Ta-10W bar from the center to the surface of the bar. The colors in the maps are based on the unit IPF triangle and indicate the crystal direction normal to the section plane. Note a gradient in grain structure and crystal orientations from Region 1 over the transition region to Region 2. The IPF triangle has the crystal reference frame defined as [001] in the center, [101] to the right, and [111] upward.

Figure 2 Initial texture in Region 1 (left) and Region 2 (right) of the Ta-10W bar. Centerline of the bar is in the center of the pole figures. The transverse direction is to the right.

Figure 3 Measured and simulated stress-strain response on samples of Ta-10W in compression (C) and tension (T) along the axial (AX) and transverse (TR) directions and at the temperatures and strain-rates indicated in the plots. Also 1 and 2 indicate regions where the samples were machined from the extruded Ta-10W bar. The solid lines are the experimental curves and the dashed lines are the model calculations.

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