International Journal of Plasticity 78 (2016) 242–265

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Unraveling the temperature dependence of the yield strength in single-crystal tungsten using atomistically-informed crystal plasticity calculations

David Cereceda [a, b, c], Martin Diehl [d], Franz Roters [d], Dierk Raabe [d], J.Manuel Perlado [c], Jaime Marian [a, *]

[a] Department of Materials Science and Engineering, University of California Los Angeles, Los Angeles, CA 90095, USA
[b] Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, CA, USA
[c] Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, E-28006 Madrid, Spain
[d] Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

ARTICLE INFO

Article history:
Received 8 June 2015
Received in revised form 19 August 2015
Available online 14 September 2015

Keywords:
Bcc crystal plasticity
Yield stress
Non-Schmid effects
Screw dislocations
Single crystal tungsten

ABSTRACT

We use a physically-based crystal plasticity model to predict the yield strength of body-centered cubic (bcc) tungsten single crystals subjected to uniaxial loading. Our model captures the thermally-activated character of screw dislocation motion and full non-Schmid effects, both of which are known to play critical roles in bcc plasticity. The model uses atomistic calculations as the sole source of constitutive information, with no parameter fitting of any kind to experimental data. Our results are in excellent agreement with experimental measurements of the yield stress as a function of temperature for a number of loading orientations. The validated methodology is employed to calculate the temperature and strain-rate dependence of the yield strength for 231 crystallographic orientations within the standard stereographic triangle. We extract the strain-rate sensitivity of W crystals at different temperatures, and finish with the calculation of yield surfaces under biaxial loading conditions that can be used to define effective yield criteria for engineering design models.

1. Background and motivation

The plastic behavior of body-centered cubic (bcc) single crystals at low to medium homologous temperatures is governed by the motion of ½⟨111⟩ screw dislocations on close-packed crystallographic planes. There are two particularities that make bcc metals unique in relation to their deformation characteristics. The first one is the thermally-activated nature of screw dislocation glide, a consequence of the compact (non-planar) structure of the dislocation core at the atomistic level (Vitek, 2004; Wurster et al., 2010; Li et al., 2012; Samolyuk et al., 2013). This feature is also responsible for the high intrinsic friction stresses reported in the literature for bcc metals and their alloys (Romaner et al., 2010; Samolyuk et al., 2013). The second is the breakdown of the standard geometric projection rule of the resolved shear stress (RSS) from the total stress tensor known as *Schmid law* (Schmid and Boas, 1935). This is owed to both specific crystallographic properties of the bcc lattice structure as well as to the coupling between the dislocation core and non-glide components of the stress tensor, which —to

* Corresponding author.
E-mail address: jmarian@ucla.edu (J. Marian).

http://dx.doi.org/10.1016/j.ijplas.2015.09.002
0749-6419/

the best of our understanding– is unique to bcc crystals (Bulatov et al., 1999; Brinckmann et al., 2008; Woodward and Rao, 2001; Chaussidon et al., 2006; Gröger and Vitek, 2005). These anomalies have been the subject of much research and discussion going back to the 1960's (Takeuchi et al., 1967; Hull et al., 1967; Duesbery, 1969; Duesbery and Foxall, 1969), both experimentally and –more recently– using computational atomistic models.

In regards to the first point above, at low stresses slip proceeds via the thermally activated nucleation of steps on the dislocation line, known as *kink pairs*, and their subsequent sideward relaxation. For a constant strain rate, this gives rise to the characteristic temperature dependence of the flow stress in bcc single crystals, which has been observed for all refractory metals and is considered to be a principal signature of their plastic response (Seeger, 1981; Ackermann et al., 1983; Taylor, 1992; Gordon et al., 2010; Chaussidon et al., 2006; Yang et al., 2001). The flow stress is considered to be composed of thermal and athermal contributions, with the latter depending on temperature only as the elastic moduli. Dislocation glide is thought to occur on {110}, {112}, and even {123} planes, depending on temperature and stress, over a periodic energy landscape known as the *Peierls* potential U_P. The connection between the experimentally measured flow stress and this periodic energy potential is via the critical stress for which U_P vanishes at zero temperature, known as the Peierls stress σ_P. Theoretically then, the flow stress at very low temperatures ($\lesssim$25 K) is thought to represent the macroscopic equivalent of σ_P as the temperature approaches 0 K. σ_P can thus be unequivocally defined and has been the object of considerable numerical work since the first atomistic models were devised by Vitek and co-workers starting in the 1970s (Vitek and Yamaguchi, 1973).

For their part, non-Schmid effects were detected in tests done in the 1930's by Taylor in the wake of his seminal works on plastic flow and strain hardening (Taylor, 1928, 1934a, 1934b). Subsequent observations and measurements (Šesták and Zárubová, 1965; Sherwood et al., 1967; Zwiesele and Diehl, 1979; Christian, 1983; Pichl, 2002; Escaig, 1968, 1974), and a rigorous theoretical formulation of the problem (Duesbery and Vitek, 1998; Ito and Vitek, 2001; Woodward and Rao, 2001; Gröger and Vitek, 2005; Chaussidon et al., 2006; Gröger et al., 2008a,b; Soare, 2014) have established non-Schmid behavior as a principal tenet of bcc plasticity that must be accounted for in order to understand bcc plastic flow. In terms of phenomenology, the two essential aspects to bear in mind are (i) that the resolved shear stress is not independent of the sign of the stress in glide planes of the ⟨111⟩ zone (the so-called *twinning/anti-twinning* asymmetry), and (ii) that non-glide components of the stress tensor –*i.e.* those which are perpendicular to the Burgers vector– play a role on the magnitude and sign of the RSS on the glide plane of interest.

Areas where we do not have a complete understanding of bcc plastic picture include the value of the flow stress at near zero absolute temperatures, the meaning of the so-called *knee* temperature, and the onset of athermal flow. In the last two decades, computer simulation has unquestionably emerged as discipline capable of shedding light on these processes on a similar footing with experiments, providing physically-substantiated explanations across a range of temporal and spatial scales. These include the use and application of density-functional theory methods (Ventelon and Willaime, 2007; Ventelon et al., 2013; Weinberger et al., 2013; Dezerald et al., 2014, 2015), semi empirical atomistic calculations and molecular dynamics calculations (Gilbert et al., 2011; Queyreau et al., 2011; Chang et al., 2001; Komanduri et al., 2001), kinetic Monte Carlo (Lin and Chrzan, 1999; Cai et al., 2002; Deo and Srolovitz, 2002; Scarle et al., 2004; Stukowski et al., 2015), and crystal plasticity (CP) (Qin and Bassani, 1992; Dao and Asaro, 1993; Brünig, 1997), to name but a few. In general, while there is no doubt that the intricacies associated with ½⟨111⟩ screw dislocation glide –including its thermally activated nature and deviations from Schmid law– cannot but be resolved using methods capable of atomistic resolution, one must recognize that, at the same time, flow is a phenomenon potentially involving statistically-significant amounts of dislocations and –as such– cannot be captured resorting to atomistic calculations only.

Modeling thermally-activated flow and non-Schmid effects in bcc systems has been the subject of much work, starting in the 1980s and, particularly, in recent times. Different authors have considered different subsets of the {110}, {112}, and {123} families of glide planes, without (Raphanel and Van Houtte, 1985; Hölscher et al., 1991, 1994; Raabe et al., 1994; Raabe, 1995a,b; Peeters et al., 2000; Stainier et al., 2002; Erieau and Rey, 2004; Ma et al., 2007; Hamelin et al., 2011; Kitayama et al., 2013) and with non-Schmid effects (Lee et al., 1999; Kuchnicki et al., 2008; Koester et al., 2012; Weinberger et al., 2012; Alankar et al., 2014; Lim et al., 2013; Narayanan et al., 2014; Patra et al., 2014; Knezevic et al., 2014; Lim et al., 2015a,b). Of particular interest are some recent simulations where the flow rule is directly formulated on the basis of screw dislocation properties in Fe (Yalcinkaya et al., 2008; Koester et al., 2012; Alankar et al., 2014; Narayanan et al., 2014; Patra et al., 2014; Lim et al., 2015b), Ta (Kuchnicki et al., 2008; Lim et al., 2013; Knezevic et al., 2014; Lim et al., 2015a), Mo (Yalcinkaya et al., 2008; Weinberger et al., 2012; Lim et al., 2013, 2015a), W (Lee et al., 1999; Weinberger et al., 2012; Lim et al., 2013; Knezevic et al., 2014; Lim et al., 2015a), and Nb (Yalcinkaya et al., 2008; Lim et al., 2015a). These works also include non-Schmid effects following the model proposed by Vitek and Bassani (Duesbery and Vitek, 1998; Qin and Bassani, 1992; Gröger et al., 2008a,b). However, albeit very useful for certain applications, all these works resort to (i) a partial consideration of non-Schmid effects, and/or (ii) some kind or another of parameter fitting with experimental data, which prevents their use in regions of the parameter space outside the range of fitting and does not link the effective (*macroscopic*) response to exclusively fundamental material properties and features.

In this work, we provide a unified computational methodology consisting of rate-dependent crystal plasticity calculations parameterized entirely and exclusively to atomistic calculations. We show that a full description of non-Schmid effects, together with the state of the art in terms of our understanding of thermally-activated screw dislocation motion, suffices to capture the experimentally measured temperature dependence of the flow stress in tungsten. This is achieved in a fully classical framework, without the need for quantum effects recently invoked to explain the long standing discrepancy observed between