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Mechanisms of deformation and ductility in tungsten – A review

Brady G. Butler^{a,b,*}, James D. Paramore^{a,c}, Jonathan P. Ligda^a, Chai Ren^c, Z. Zak Fang^c, Scott C. Middlemas^d, Kevin J. Hemker^{b,e}

^a Lightweight and Specialty Metals Branch, U.S. Army Research Lab, Aberdeen, Proving Ground, MD 21005, USA

^b Department of Materials Science and Engineering, Johns Hopkins University, 3400 North Charles Street, Baltimore, MD 21218, USA

^c Department of Metallurgical Engineering, University of Utah, 135 S. 1460 E., Room 412, Salt Lake City, UT 84112, USA

^d Post Irradiation Examination Department, Idaho National Laboratory, P.O. Box 1625, MS 6184, Idaho Falls, ID 83415, USA

e Department of Mechanical Engineering, Johns Hopkins University, 3400 North Charles Street, Baltimore, MD 21218, USA

ABSTRACT

The physical, chemical, and mechanical properties of tungsten are at the far limits of all engineering materials. These unique properties, particularly ultra-high strength, density, and melting point, create enticing prospects for using tungsten in extreme engineering environments for nuclear, military and space applications. However, these environments also require materials that resist fracture, which presents a significant challenge for tungsten, particularly at low temperatures. This review discusses several significant factors that affect the ductile to brittle transition and low temperature ductility of tungsten. The effects of crystal structure, dislocation structure, and microstructure to describe competing factors in the plasticity and fracture of tungsten at low temperatures are assessed. In particular, the dislocation structure and the mechanisms of dislocation mobility are shown to be critical to understanding plasticity at low temperatures.

1. Introduction

Although metallic tungsten was first isolated in 1783 [1], its widespread use as an engineering material did not occur until the early 1900s, when special processing procedures were employed to enhance the formability, and more generally, the ductility of tungsten. Driven by the desire for ultra-high-temperature materials for the lighting industry, William D. Coolidge, a research scientist at the General Electric Research Laboratory, became intimately accustomed to the refractory nature of tungsten. In a paper to the American Institute of Electrical Engineers [2], Coolidge stated "When work was first started on the problem of producing a ductile form of tungsten, the metal looked very uncompromising. It was so hard that it could not be filed without detriment to the file, and was, at ordinary temperatures, very brittle." Through careful control of impurities and additives, and by extensive cold working at temperatures below the recrystallization temperature, Coolidge was able to demonstrate ductile behavior at room temperature. Despite this early progress, significant research efforts around the world are still devoted to understanding and optimizing the low temperature plasticity of tungsten over a century later.

Tungsten is generally considered to be brittle at room temperature with only a few notable exceptions; single crystals [3-6], heavily cold worked materials (e.g. drawn wire [7-9] and rolled foils [10-12]), and

tungsten-rhenium alloys [13–16] have each demonstrated ductile behavior at room temperature. The deformation of crystalline materials is best described by the defects that accommodate plasticity at stresses far below the theoretical strength of the crystal. In the case of tungsten, the plastic behavior is effectively mediated by dislocations over a range of temperatures, compositions, and strain rates. There are a few notable cases where twinning accommodates deformation in tungsten, particularly at low temperatures, high strain rates, and in impure materials. However, these are special cases that are generally beyond the scope of this review. A thorough understanding of dislocation behavior in tungsten can help to describe general features of ductility, strain rate sensitivity, thermal softening, fracture toughness, and the ductile to brittle transition temperature (DBTT) of tungsten.

The plastic behavior of tungsten is often counterintuitive, defying some of the most basic principles of deformation in metals. For instance, (1) most metals and alloys show lower strain to failure with excessive plastic deformation, but tungsten demonstrates improved ductility after cold working [2,10], (2) most pure metals are strengthened by solid solution alloying, but certain alloy additions actually soften and ductilize tungsten at low temperatures [17–19], and (3) tungsten exhibits several clear violations of Schmid's law [20,21]. These peculiarities in plastic behavior make it difficult to understand and manipulate this highly refractory material. However, this detailed

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^{*} Corresponding author at: Lightweight and Specialty Metals Branch, U.S. Army Research Lab, Aberdeen, Proving Ground, MD 21005, USA. *E-mail address:* brady.g.butler.civ@mail.mil (B.G. Butler).

review of the crystal structure, dislocation structure, and the nuances of dislocation mobility has been undertaken to help illuminate the mechanisms of plasticity and design better materials for extreme engineering environments.

2. Crystal structure effects on plasticity

Some of the most peculiar aspects of plasticity in tungsten are the result of the body-centered-cubic (BCC) crystal structure and the crystallographic defects that are characteristic of this structure. These unusual features include the demonstration of "anomalous slip" (i.e. slip on planes that do not exhibit the maximum resolved shear stress (MRSS)), asymmetric stress response to the direction of slip referred to as a "twinning anti-twinning asymmetry" [4,21-23], and a glide dependence on stresses normal to the slip plane [24]. Each of these examples violate Schmid's law. Furthermore, tungsten exhibits a very strong dependence of flow stress as a function of temperature [20,25] and strain rate [26]. All of these features may be accounted for by the theory of dislocations in BCC metals, which is discussed in-depth in several books and review articles [27-31]. However, the refractory properties of tungsten, specifically its ultra-high modulus and melting point, exacerbate many features associated with plasticity in BCC metals.

The establishment of the primary slip systems in BCC metals is critical to understanding and modeling the deformation behavior of these materials. The BCC structure is close packed along <111> directions in the lattice and the smallest Burgers vector for slip is $\frac{1}{2}$ < 111 > . There are no close packed planes in the BCC lattice, but the planes of highest density are types {110} and {112}, as shown in Fig. 1 [32]. Historically, slip planes have been identified by slip traces on deformed single crystals; however, this treatment determines the "effective" slip plane without defining the elementary mechanisms of dislocation propagation [33]. For tungsten (and BCC metals in general), there are some discrepancies regarding the primary slip plane reported using this technique and slip traces are often wavy and ill-defined [33-35]. Although there is no clear consensus, it has been proposed that primary slip occurs on the closest packed {110} type planes, with the possibility of activating slip on higher order planes at higher temperatures [36]. It has been suggested for decades [37,38] that these higher order slip planes could be accommodated by coordinated cross slip of screw dislocations on different {110} planes. In recent studies, Marichal et al. [39,40] utilized micropillar testing in conjunction with in situ Laue micro-diffraction from a synchrotron source to quantitatively demonstrate that coordinated slip on {110} type planes do form {112} and higher order slip traces. This has also been recently

demonstrated using atomistic [23] and discrete dislocation dynamics simulations [41].

Establishing the elementary slip planes in tungsten is important for understanding the fundamental barriers to dislocation motion. According to the von Mises principal, plastic deformation of a polycrystalline material requires a minimum of five independent slip systems in order to accommodate an arbitrary strain field [42-46], as such a condition is essential to maintaining continuity between grains during deformation of a polycrystal. Even if slip is restricted to {110} type planes, there would be a total of 12 unique {110} 111 slip systems. This provides 384 combinations of five independent systems to accommodate an arbitrary strain field [46,47]. By this assessment, there is no fundamental crystallographic reason that tungsten should exhibit poor ductility, so long as these elementary slip systems are fully active. The transition from ductile to brittle behavior as a function of strain rate and temperature may be understood based on the mobility of dislocations, which is rooted in the dislocation character, the structure of the dislocation core, and the thermally activated mechanisms for propagation.

3. Character and structure of dislocations

The dislocation character (i.e. the orientation between the Burgers vector and the dislocation line) plays an important role in the structure and mobility of $\frac{1}{2} < 111 >$ dislocations in a BCC lattice. The geometry of a screw dislocation, with Burgers vector parallel to the dislocation line, results in a compact and inherently non-planar dislocation core structure as shown in Fig. 2. This screw dislocations shows reduced mobility in comparison to edge and mixed dislocations at low temperatures [48,49]. Deformation behavior is fundamentally linked to the rate limiting step in transmitting strain through the lattice [50,51]. In essence, screw dislocations mediate plasticity at low temperatures, and the reduced mobility of these dislocations may be understood based on the structure of the screw dislocation core.

The Peierls stress (σ_p , Eq. (1)) describes the amount of external stress required to move a dislocation from one local minimum in potential energy to the adjacent minimum, without any consideration of thermal activation (i.e. at absolute zero temperature) [30,31,37,52].

$$\sigma_{\rm p} = \frac{2\mu}{1-\nu} \exp\left(\frac{-2\pi w}{b}\right) \tag{1}$$

where μ is the shear modulus, ν is Poisson's ratio, w is the effective width of the dislocation in the slip plane, and b is the magnitude of the Burger's vector associated with the dislocation. While this one dimensional description has significant limitations [53], it does provide basic



Fig. 1. The atomic structure of planes critical to fracture and plasticity in BCC metals, (a) 100} predominant fracture plane, despite the lower surface energy of the more closely packed {110} type planes, and an example of a sessile dislocation with Burgers vector, $\vec{b} = a[010]$, where *a* is the lattice parameter of tungsten, (b) {110} primary slip plane and Burgers vector, $\vec{b} = \frac{a}{2}[10]$, associated with mobile dislocations, and (c) {112} twinning plane, and contested slip plane for higher temperature deformation. Figures were prepared using VESTA [32].

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